

## Current Situation & Goals

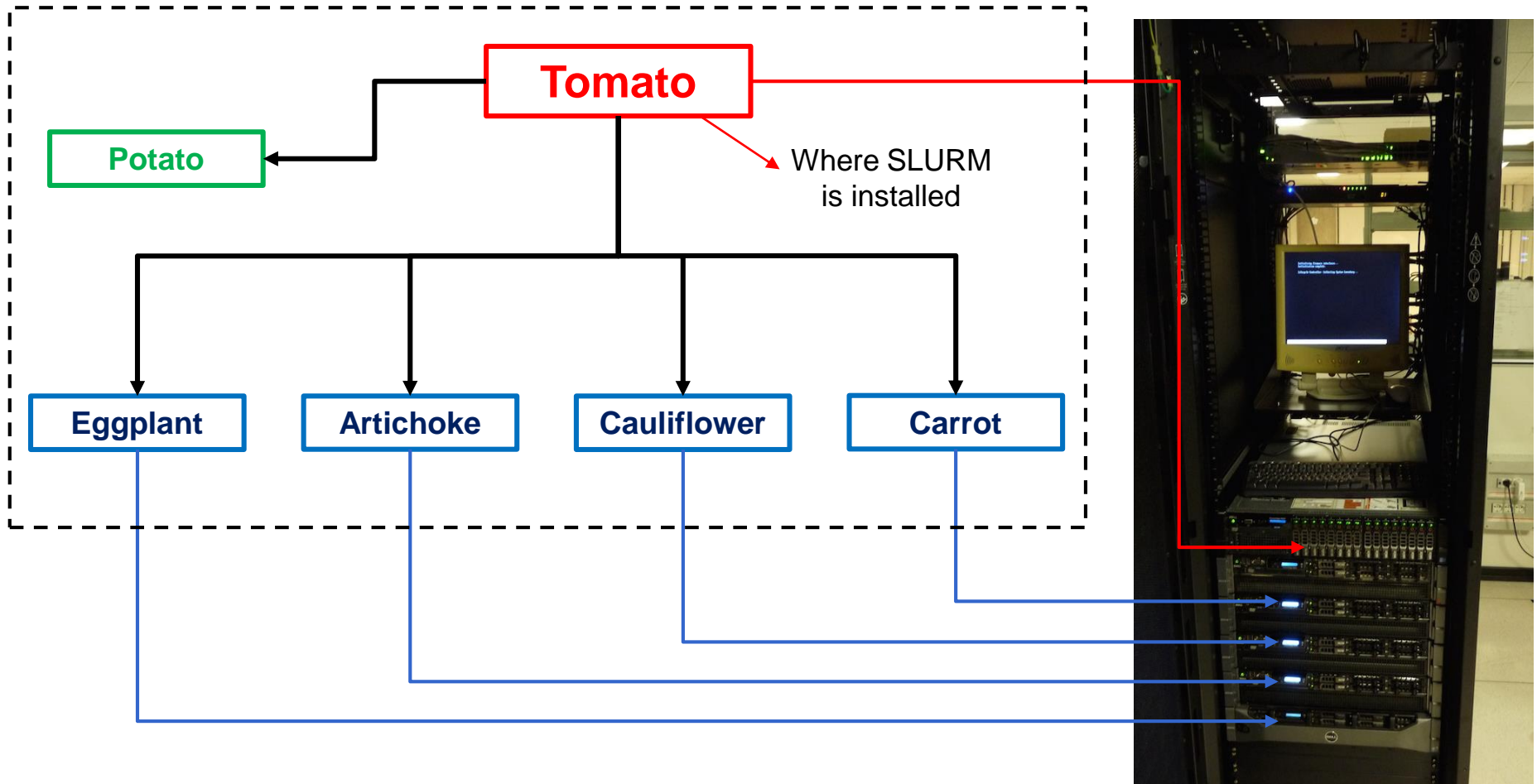
- People run simulations on Tomato «wildly»
- Computation nodes are under-used
- Data are stored randomly on the disks



So...

- Optimize** computational nodes with SLURM
- Teaching** how to use SLURM
- Give a set of **good practice rules**
- Add **new features** into the server

## Server Architecture Scheme



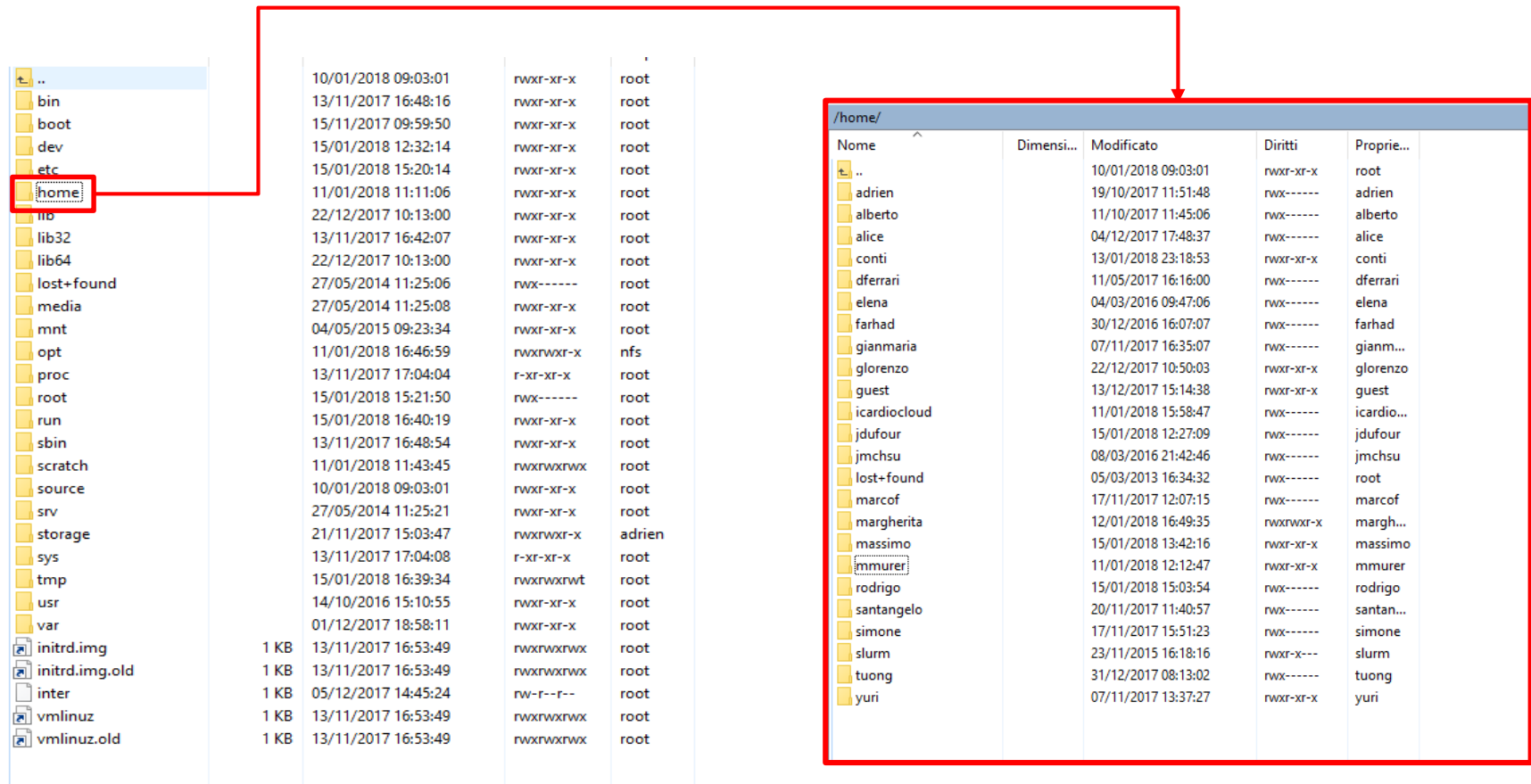
## Shared Folders

- /home: it's your working directory and it is shared by all the nodes. (96 GB out of 824 GB available)
- /opt: where software and libraries are installed (programs and libraries source)
- /scratch: it's the working directory where temporary files are generated
- /storage: where you results and data files have to be saved (all that is in /scratch will be deleted at the next simulation). Contains files you have used or will use for next simulations (3.1 TB out of 8.2 TB available)

..	10/01/2018 09:03:01	rwxf-xf-x	root
bin	13/11/2017 16:48:16	rwxf-xf-x	root
boot	15/11/2017 09:59:50	rwxf-xf-x	root
dev	15/01/2018 12:32:14	rwxf-xf-x	root
etc	15/01/2018 15:20:14	rwxf-xf-x	root
home	11/01/2018 11:11:06	rwxf-xf-x	root
lib	22/12/2017 10:13:00	rwxf-xf-x	root
lib32	13/11/2017 16:42:07	rwxf-xf-x	root
lib64	22/12/2017 10:13:00	rwxf-xf-x	root
lost+found	27/05/2014 11:25:06	rw-x-----	root
media	27/05/2014 11:25:08	rwxf-xf-x	root
mnt	04/05/2015 09:23:34	rwxf-xf-x	root
opt	11/01/2018 16:46:59	rwxf-rwxf-x	nfs
proc	13/11/2017 17:04:04	r-xf-xf-x	root
root	15/01/2018 15:21:50	rw-x-----	root
run	15/01/2018 16:40:19	rwxf-xf-x	root
sbin	13/11/2017 16:48:54	rwxf-xf-x	root
scratch	11/01/2018 11:43:45	rwxf-rwxf-rwx	root
source	10/01/2018 09:03:01	rwxf-xf-x	root
srv	27/05/2014 11:25:21	rwxf-xf-x	root
storage	21/11/2017 15:03:47	rwxf-rwxf-x	adrien
sys	13/11/2017 17:04:08	r-xf-xf-x	root
tmp	15/01/2018 16:39:34	rwxf-rwxf-rwt	root
usr	14/10/2016 15:10:55	rwxf-xf-x	root
var	01/12/2017 18:58:11	rwxf-xf-x	root
initrd.img	1 KB 13/11/2017 16:53:49	rwxf-rwxf-rwx	root
initrd.img.old	1 KB 13/11/2017 16:53:49	rwxf-rwxf-rwx	root
inter	1 KB 05/12/2017 14:45:24	rw-r--r--	root
vmlinuz	1 KB 13/11/2017 16:53:49	rwxf-rwxf-rwx	root
vmlinuz.old	1 KB 13/11/2017 16:53:49	rwxf-rwxf-rwx	root

## Shared Folders

- `/home`: it's your working directory and it is shared by all the nodes.



Nome	Dimensi...	Modificato	Diritti	Proprie...
..		10/01/2018 09:03:01	rw-r--r--	root
adrien		19/10/2017 11:51:48	rw-r--r--	adrien
alberto		11/10/2017 11:45:06	rw-r--r--	alberto
alice		04/12/2017 17:48:37	rw-r--r--	alice
conti		13/01/2018 23:18:53	rw-r--r--	conti
dferrari		11/05/2017 16:16:00	rw-r--r--	dferrari
elena		04/03/2016 09:47:06	rw-r--r--	elena
farhad		30/12/2016 16:07:07	rw-r--r--	farhad
gianmaria		07/11/2017 16:35:07	rw-r--r--	gianm...
glorenzo		22/12/2017 10:50:03	rw-r--r--	glorenzo
guest		13/12/2017 15:14:38	rw-r--r--	guest
icardiocloud		11/01/2018 15:58:47	rw-r--r--	icardi...
jdufour		15/01/2018 12:27:09	rw-r--r--	jdufour
jmchsu		08/03/2016 21:42:46	rw-r--r--	jmchsu
lost+found		05/03/2013 16:34:32	rw-r--r--	root
marcof		17/11/2017 12:07:15	rw-r--r--	marcof
margherita		12/01/2018 16:49:35	rw-r--r--	margh...
massimo		15/01/2018 13:42:16	rw-r--r--	massimo
mmurer		11/01/2018 12:12:47	rw-r--r--	mmurer
rodrigo		15/01/2018 15:03:54	rw-r--r--	rodrigo
santangelo		20/11/2017 11:40:57	rw-r--r--	santan...
simone		17/11/2017 15:51:23	rw-r--r--	simone
slurm		23/11/2015 16:18:16	rw-r--r--	slurm
tuong		31/12/2017 08:13:02	rw-r--r--	tuong
yuri		07/11/2017 13:37:27	rw-r--r--	yuri



# CompMech Server Architecture



## Shared Folders

- /opt: where software and libraries are installed (programs and libraries source).

The image shows a file manager interface with a sidebar on the left and a main pane on the right. The sidebar lists various system directories, with /opt highlighted. The main pane displays the contents of /opt as a table with columns for Name, Dimensions, Modified, Permissions, and Properties.

Nome	Dimensi...	Modificato	Diritti	Proprie...
.		10/01/2018 09:03:01	rw-r--r--	root
abacus		05/07/2017 12:10:30	rw-rw-r--	2003
acml		30/04/2015 10:46:29	rw-rw-r--	adrien
adhocpp		11/01/2018 18:06:08	rw-r--r--	massimo
adrien		10/01/2018 09:48:00	rw-rw-r--	adrien
amd64		02/02/2017 11:12:16	rw-rw-r--	santan...
gotoblas		20/05/2014 10:26:52	rw-rw-r--	adrien
intel		10/01/2018 10:09:43	rw-rw-r--	adrien
intel_parallel_xe_clust...		10/01/2018 10:09:49	rw-r--r--	root
lapack		20/05/2014 10:34:34	rw-rw-r--	adrien
lifev-env		17/03/2017 17:44:49	rw-rw-r--	adrien
MATLAB		13/12/2017 11:52:12	rw-rw-r--	adrien
modules		30/11/2017 15:58:02	rw-rw-r--	adrien
mpich-3.1		22/08/2017 14:32:50	rw-rw-r--	2003
openblas		20/05/2014 10:35:22	rw-rw-r--	adrien
openmpi-1.6.5		26/06/2014 16:25:34	rw-rw-r--	santan...
openmpi-3.0.0		08/01/2018 10:06:58	rw-r--r--	root
test-michele		30/06/2015 10:57:37	rw-rw-r--	2003
vmgtk		30/11/2017 16:01:04	rw-rw-r--	adrien
slurmctld.log	54.371 KB	15/01/2018 16:45:04	rw-r--r--	slurm
slurmd.log	435.141 KB	27/11/2017 15:36:40	rw-r--r--	nobody

## Shared Folders

- `/scratch`: it's the working directory where temporary files are generated.

..	10/01/2018 09:03:01	rw-r--r--	root
bin	13/11/2017 16:48:06	rw-r--r--	root
boot	15/11/2017 09:59:30	rw-r--r--	root
dev	15/01/2018 12:32:04	rw-r--r--	root
etc	15/01/2018 15:20:04	rw-r--r--	root
home	11/01/2018 11:11:06	rw-r--r--	root
lib	22/12/2017 10:13:00	rw-r--r--	root
lib32	13/11/2017 16:42:07	rw-r--r--	root
lib64	22/12/2017 10:13:00	rw-r--r--	root
lost+found	27/05/2014 11:25:06	rw-r--r--	root
media	27/05/2014 11:25:08	rw-r--r--	root
mnt	04/05/2015 09:23:34	rw-r--r--	root
opt	11/01/2018 16:46:39	rw-r--r--	nfs
proc	13/11/2017 17:04:04	r-xr-xr-x	root
root	15/01/2018 15:21:00	rw-r--r--	root
run	15/01/2018 16:40:09	rw-r--r--	root
sbin	13/11/2017 16:48:04	rw-r--r--	root
<b>scratch</b>	11/01/2018 11:43:45	rw-rw-rw-	root
source	10/01/2018 09:03:01	rw-r--r--	root
srv	27/05/2014 11:25:21	rw-r--r--	root
storage	21/11/2017 15:03:47	rw-rw-rw-	adrien
sys	13/11/2017 17:04:08	r-xr-xr-x	root
tmp	15/01/2018 16:39:34	rw-rw-rwt	root
usr	14/10/2016 15:10:55	rw-r--r--	root
var	01/12/2017 18:58:11	rw-r--r--	root
initrd.img	1 KB 13/11/2017 16:53:49	rw-rw-rw-	root
initrd.img.old	1 KB 13/11/2017 16:53:49	rw-rw-rw-	root
inter	1 KB 05/12/2017 14:45:24	rw-r--r--	root
vmlinuz	1 KB 13/11/2017 16:53:49	rw-rw-rw-	root
vmlinuz.old	1 KB 13/11/2017 16:53:49	rw-rw-rw-	root

`/scratch/`

Nome	Dimensi...	Modificato	Diritti	Proprie...
massimo		17/01/2018 18:36:12	rw-r--r--	root

`/scratch/massimo/`

Nome	Dimensi...	Modificato	Diritti	Proprie...
adhocpp_release		19/01/2018 09:58:38	rw-r--r--	massimo
CMakeFiles		11/01/2018 14:59:31	rw-r--r--	massimo
gcc-5.5.0		09/01/2018 10:58:04	rw-r--r--	massimo
lib		09/01/2018 11:06:37	rw-r--r--	massimo
lib64		09/01/2018 11:06:46	rw-r--r--	massimo
libexec		09/01/2018 11:06:04	rw-r--r--	massimo
cmake_install.cmake	5 KB	11/01/2018 14:11:53	rw-r--r--	massimo
CMakeCache.txt	2 KB	11/01/2018 14:59:31	rw-r--r--	massimo
CPackConfig.cmake	4 KB	11/01/2018 14:02:46	rw-r--r--	massimo
CPackSourceConfig.c...	4 KB	11/01/2018 14:02:46	rw-r--r--	massimo
gcc-5.5.0.tar.gz	120.915 KB	10/10/2017 14:42:32	rw-r--r--	massimo
test.m	1 KB	16/01/2018 09:30:58	rw-r--r--	massimo

## Shared Folders

- **/storage:** where you results and data files have to be saved (all that is in /scratch will be deleted at the next simulation). Contains files you have used or will use for next simulations.

..				
bin				
boot				
dev				
etc				
home				
lib				
lib32				
lib64				
lost+found				
media				
mnt				
opt				
proc				
root				
run				
sbin				
scratch				
source				
srv				
<b>storage</b>				
sys				
tmp				
usr				
var				
initrd.img	1 KB	13/11/2017 16:53:49	root	
initrd.img.old	1 KB	13/11/2017 16:53:49	root	
inter	1 KB	05/12/2017 14:45:24	root	
vmlinux	1 KB	13/11/2017 16:53:49	root	
vmlinux.old	1 KB	13/11/2017 16:53:49	root	

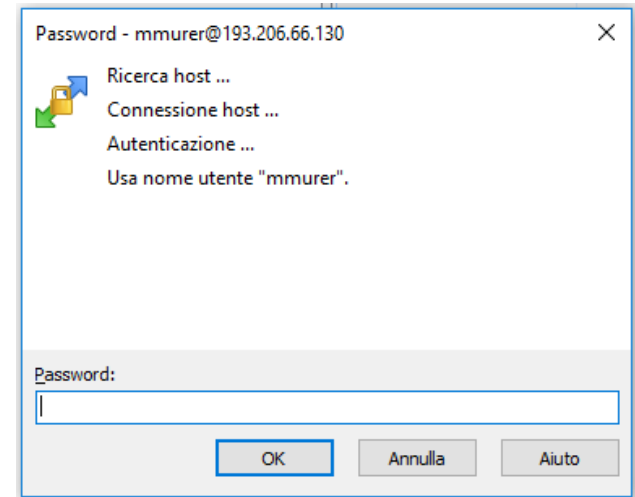
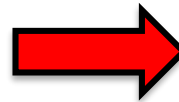
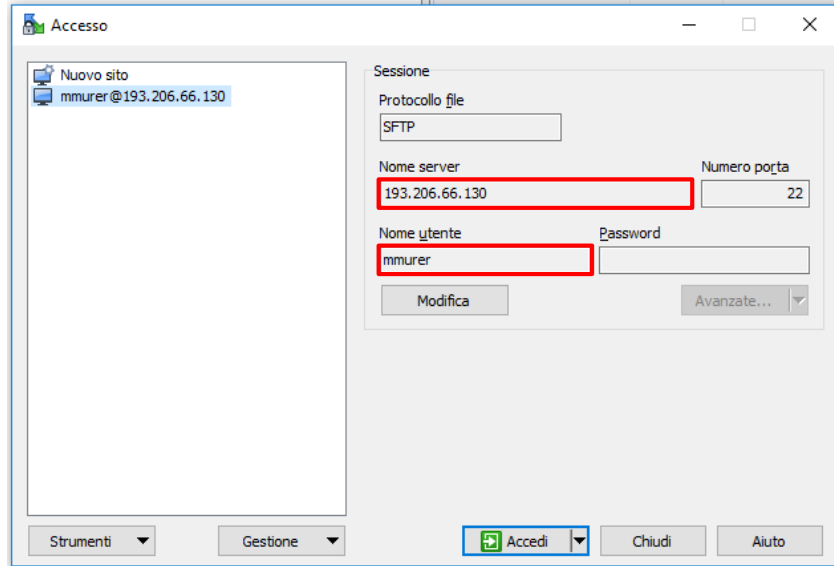
10/01/2018 09:03:01	root		
13/11/2017 16:48:16	root		
15/11/2017 09:59:50	root		
15/01/2018 12:32:14	root		
15/01/2018 15:20:14	root		
11/01/2018 11:11:06	root		
22/12/2017 10:13:00	root		
13/11/2017 16:42:07	root		
22/12/2017 10:13:00	root		
27/05/2014 11:25:06	root		
27/05/2014 11:25:08	root		
04/05/2015 09:23:34	root		
11/01/2018 16:46:59	nfs		
13/11/2017 17:04:04	root		
15/01/2018 15:21:50	root		
15/01/2018 16:40:19	root		
13/11/2017 16:48:54	root		
11/01/2018 11:43:45	root		
10/01/2018 09:03:01	root		
27/05/2014 11:25:21	root		
21/11/2017 15:03:47	adrien		
13/11/2017 17:04:08	root		
15/01/2018 16:39:34	root		
14/10/2016 15:10:55	root		
01/12/2017 18:58:11	root		
13/11/2017 16:53:49	root		
13/11/2017 16:53:49	root		
05/12/2017 14:45:24	root		
13/11/2017 16:53:49	root		
13/11/2017 16:53:49	root		

Nome	Dimensi...	Modificato	Diritti	Proprie...
adrien		10/01/2018 09:03:01	root	
alberto		02/06/2016 15:57:11	adrien	
alice		19/07/2017 17:38:40	alberto	
alice		01/03/2017 16:29:03	alice	
conti		29/12/2017 19:26:31	conti	
dferrari		10/05/2017 20:30:34	dferrari	
elena		03/03/2016 14:44:19	elena	
farhad		30/11/2016 12:53:36	farhad	
gianmaria		09/06/2017 18:21:33	gianmaria	
guest		29/05/2017 01:20:37	guest	
icardiocloud		17/03/2015 11:20:26	icardiocloud	
jdfour		12/01/2016 11:11:58	jdfour	
jmchsu		04/03/2016 15:10:11	jmchsu	
lifer		19/01/2017 09:44:07	rodrigo	
luigi		09/11/2017 15:19:21	santan...	
marcof		23/09/2017 16:00:31	marcof	
margherita		14/10/2017 19:14:30	margherita	
massimo		09/01/2018 16:57:01	massimo	
matlab		11/07/2015 10:48:52	adrien	
matlab_install		11/07/2015 10:50:23	adrien	
motif		09/02/2016 23:44:41	adrien	
rescue		13/10/2014 16:51:36	adrien	
rodrigo		13/12/2017 09:53:14	rodrigo	
save		30/10/2017 09:33:06	adrien	
simulations		28/07/2014 19:54:10	adrien	
sync		03/07/2014 10:17:22	adrien	
tuong		22/02/2016 13:39:31	tuong	
yuri		18/10/2015 00:47:41	yuri	

## Windows Users - WinSPC

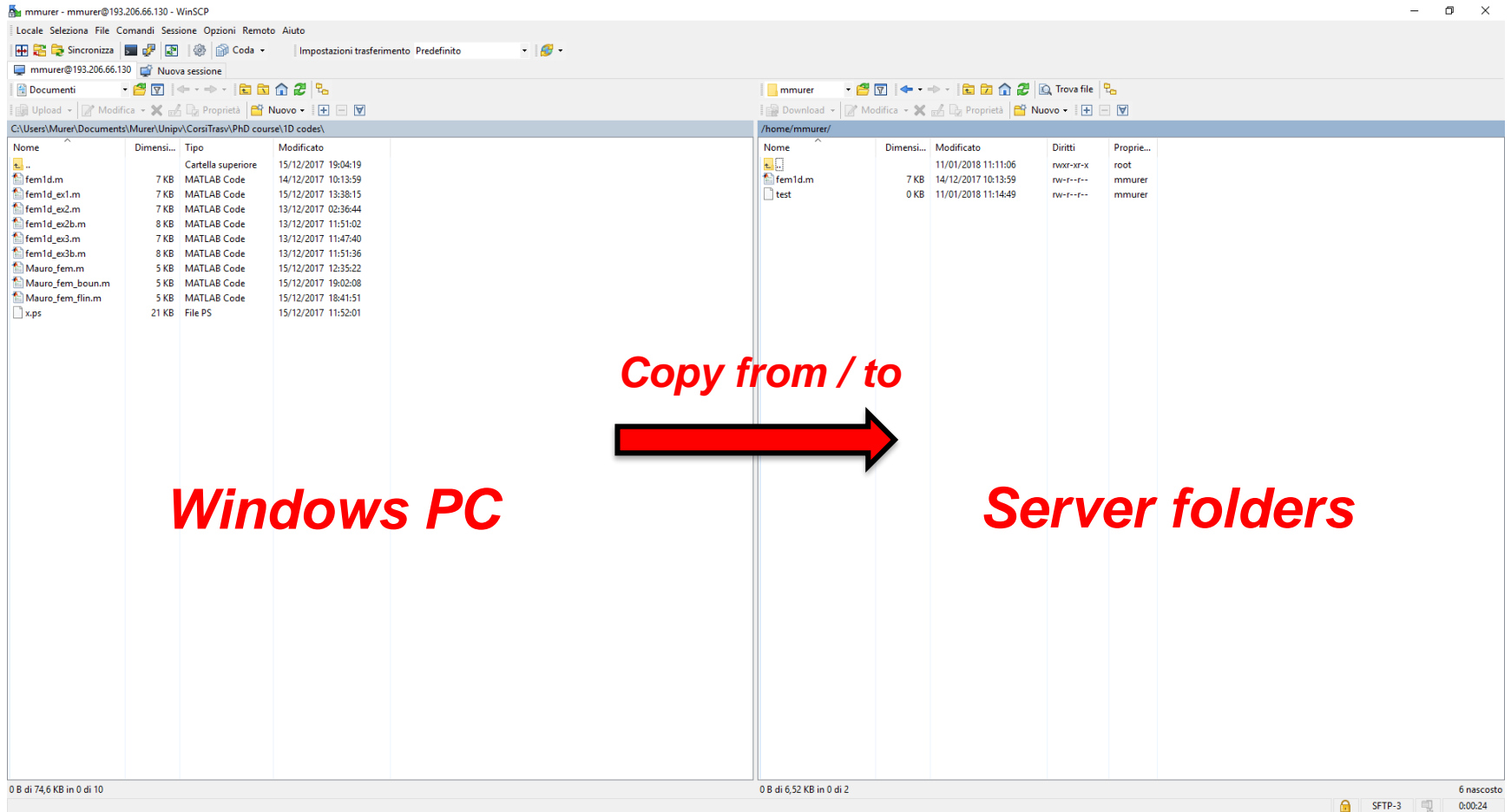
**WinSPC:** allow you to transfer/copy files from your PC to server folders  
Download from: <https://winscp.net/eng/download.php>

- How it works





## Windows Users - WinSPC



**Copy from / to**

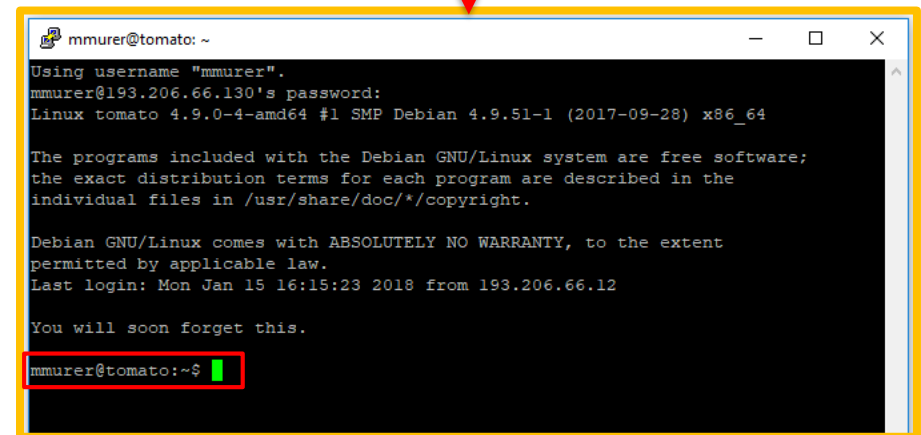
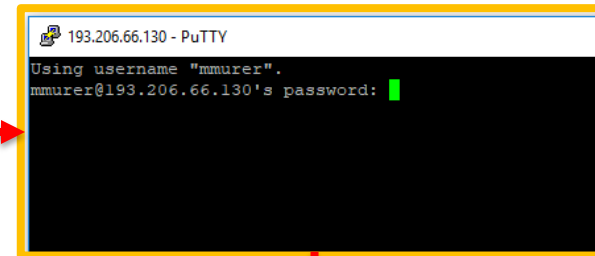
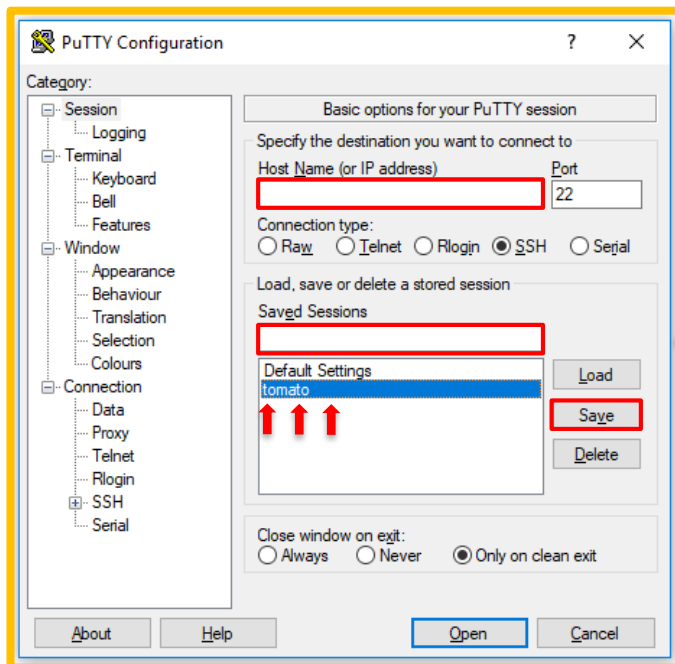
**Windows PC** → **Server folders**

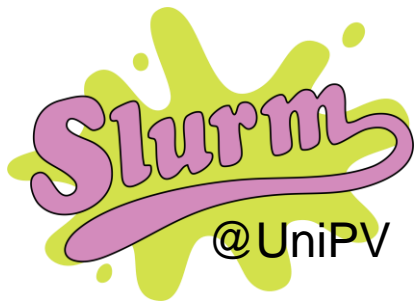
Nome	Dimensi...	Tipo	Modificato	Diritti	Proprie...
..		Cartella superiore	15/12/2017 19:04:19		
fem1d.m	7 KB	MATLAB Code	14/12/2017 10:13:59	rw-r--r--	root
fem1d_ex1.m	7 KB	MATLAB Code	15/12/2017 13:38:15	rw-r--r--	mmurer
fem1d_ex2.m	7 KB	MATLAB Code	13/12/2017 02:36:44	rw-r--r--	mmurer
fem1d_ex2b.m	8 KB	MATLAB Code	13/12/2017 11:51:02		
fem1d_ex3.m	7 KB	MATLAB Code	13/12/2017 11:47:40		
fem1d_ex3b.m	8 KB	MATLAB Code	13/12/2017 11:51:36		
Mauro_fem.m	5 KB	MATLAB Code	15/12/2017 12:35:22		
Mauro_fem_boun.m	5 KB	MATLAB Code	15/12/2017 19:02:08		
Mauro_fem_flin.m	5 KB	MATLAB Code	15/12/2017 18:41:51		
x.ps	21 KB	File PS	15/12/2017 11:52:01		

## Windows Users - Putty

**Putty:** allows you to enter the server. Download from: <http://www.putty.org/>

- How it works





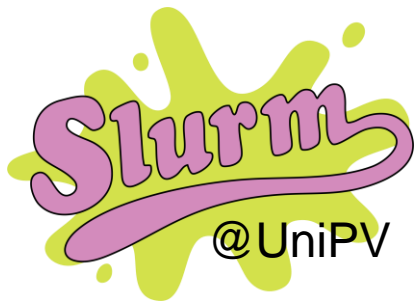
## What is SLURM

Slurm is an open source, fault-tolerant, and highly scalable cluster management and job scheduling system for large and small Linux clusters

1. It allocates exclusive and/or non-exclusive access to resources (compute nodes) to users for some duration of time so they can perform work
2. It provides a framework for starting, executing, and monitoring work (normally a parallel job) on the set of allocated nodes.
3. It arbitrates contention for resources by managing a queue of pending work.

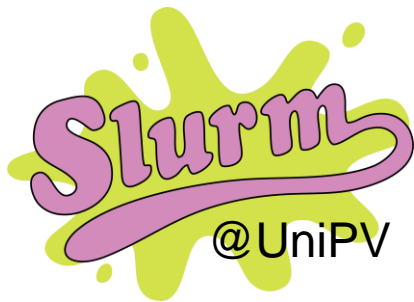


**SLURM allows tomato to run simulations on the other nodes (Carrot, Artichoke, ecc..) for you.**



## SLURM Commands

- ❖ **/srun**: run simulations through SLURM
- ❖ **/sbatch**: run simulation in background through a batch file
- ❖ **/squeue**: shows the "jobs" in progress on the server
- ❖ **/scancel**: cancel the specified job ID
- ❖ **/scontrol**: allows you to control/manage the processes that SLURM is running at that time



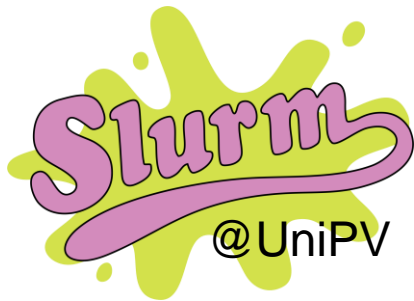
## Summary

### Good Practice Rules

- **ALWAYS** run computations through SLURM
- **ALWAYS** store your data in /storage
- **ALWAYS** work locally

### Sys Admins Contact (Just in case of emergency !!!!!!!)

- John-Eric «Giorgione» Dufour
- Massimo Carraturo
- Mauro Murer ☺



## Summary

### When contact Sys Admins

- I need the library xxxx...
- Update/Upgrade softwares
- If software says: «contact server administrator»

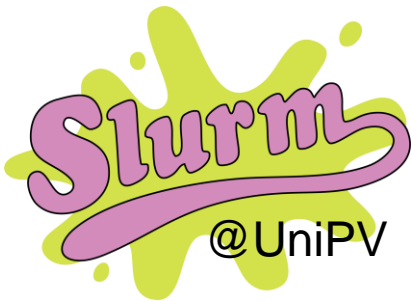
### When **NOT** contact Sys Admins

- Set up your (any software) input file
- Where are my data?
- My job is in queue but I really need the results...



## Upcoming features

- CompMech@GitLab
- New softwares (Ansys, etc...)
- Wiki page
- VPN connection
- Suggestions from the users! :)



## Run file

/home/massimo/tutorial.sh - mmurer@193.206.66.130 - Editor - WinSCP

```
#!/bin/bash -l

### Specify max memory the job can use.
#SBATCH --mem=1000mb
### Do not export the environment into the job
#SBATCH --export=NONE
### The number of CPUs per task
#SBATCH --cpus-per-task=4
### The name of the partition we want (debug=tomato, general=artichoke,carrot,cauliflower,eggplant)
#SBATCH --partition=general
### The name of the job
#SBATCH --job-name=tutorial
### working directory (scratch/USERNAME/PATH_TO_WORKSPACE)
#SBATCH -D /scratch/massimo/
### If you don't care about that output, leave 'none'
#SBATCH --output=sbatch.%j.out
#SBATCH --error=sbatch.%j.err

cd $PWD
echo $PWD

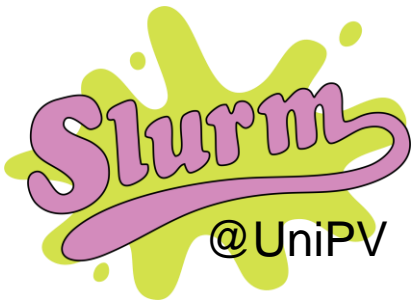
echo "Hello World"

### move the working directory containing the file in the scratch/USERNAME" on the node
cp -r workspace/ /scratch/massimo/
cd /opt/MATLAB/bin

### run MATLAB -sd folder (to start matlab in the working directory) -r MATLABCommand (to run a matlab command)
./matlab -sd '/scratch/massimo/workspace/' -noFigureWindows -r "try; run('test.m'); catch; end; quit"
```

Options





## Run file

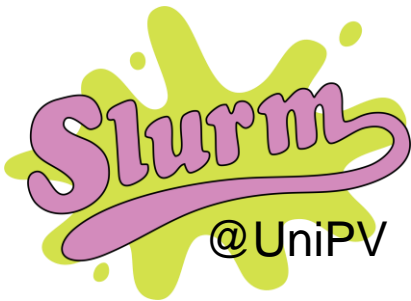
```
/home/massimo/tutorial.sh - mmurer@193.206.66.130 - Editor - WinSCP
# /bin/bash -l
### Specify max memory the job can use.
#SBATCH --mem=1000mb
### Do not export the environment into the job
#SBATCH --export=NONE
### The number of CPUs per task
#SBATCH --cpus-per-task=4
### The name of the partition we want (debug=tomato, general=artichoke,carrot,cauliflower,eggplant)
#SBATCH --partition=general
### The name of the job
#SBATCH --job-name=tutorial
### working directory (scratch/USERNAME/PATH_TO_WORKSPACE)
#SBATCH -D /scratch/massimo/
### If you don't care about that output, leave 'none'
#SBATCH --output=sbatch.%j.out
#SBATCH --error=sbatch.%j.err

cd $PWD
echo $PWD
echo "Hello World"

### move the working directory containing the file in the scratch/USERNAME" on the node
cp -r workspace/ /scratch/massimo/
cd /opt/MATLAB/bin

### run MATLAB -sd folder (to start matlab in the working directory) -r MATLABCommand (to run a matlab command)
./matlab -sd '/scratch/massimo/workspace/' -noFigureWindows -r "try; run('test.m'); catch; end; quit"
```

Print the working directory and fancy sentences to check if the simulation starts



## Run file

```
/home/massimo/tutorial.sh - mmurer@193.206.66.130 - Editor - WinSCP
# /bin/bash -l
### Specify max memory the job can use.
#SBATCH --mem=1000mb
### Do not export the environment into the job
#SBATCH --export=NONE
### The number of CPUs per task
#SBATCH --cpus-per-task=4
### The name of the partition we want (debug=tomato, general=artichoke,carrot,cauliflower,eggplant)
#SBATCH --partition=general
### The name of the job
#SBATCH --job-name=tutorial
### working directory (scratch/USERNAME/PATH_TO_WORKSPACE)
#SBATCH -D /scratch/massimo/
### If you don't care about that output, leave 'none'
#SBATCH --output=sbatch.%j.out
#SBATCH --error=sbatch.%j.err

cd $PWD
echo $PWD

echo "Hello World"

### move the working directory containing the file in the scratch/USERNAME" on the node
cp -r workspace/ /scratch/massimo/
cd /opt/MATLAB/bin

### run MATLAB -sd folder (to start matlab in the working directory) -r MATLABCommand (to run a matlab command)
./matlab -sd '/scratch/massimo/workspace/' -noFigureWindows -r "try; run('test.m'); catch; end; quit"
```

Copy working files in the working directory (/scratch)



## Run file

```
/home/massimo/tutorial.sh - mmurer@193.206.66.130 - Editor - WinSCP
# /bin/bash -l
### Specify max memory the job can use.
#SBATCH --mem=1000mb
### Do not export the environment into the job
#SBATCH --export=NONE
### The number of CPUs per task
#SBATCH --cpus-per-task=4
### The name of the partition we want (debug=tomato, general=artichoke,carrot,cauliflower,eggplant)
#SBATCH --partition=general
### The name of the job
#SBATCH --job-name=tutorial
### working directory (scratch/USERNAME/PATH_TO_WORKSPACE)
#SBATCH -D /scratch/massimo/
### If you don't care about that output, leave 'none'
#SBATCH --output=sbatch.%j.out
#SBATCH --error=sbatch.%j.err

cd $PWD
echo $PWD

echo "Hello World"

### move the working directory containing the file in the scratch/USERNAME" on the node
cp -r workspace/ /scratch/massimo/
cd /opt/MATLAB/bin

### run MATLAB -sd folder (to start matlab in the working directory) -r MATLABCommand (to run a matlab command)
./matlab -sd '/scratch/massimo/workspace/' -noFigureWindows -r "try; run('test.m'); catch; end; quit"
```

→ Run Matlab