



# Introduction to HPC

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# Roadmap today



# Roadmap today



Connection

Accounts

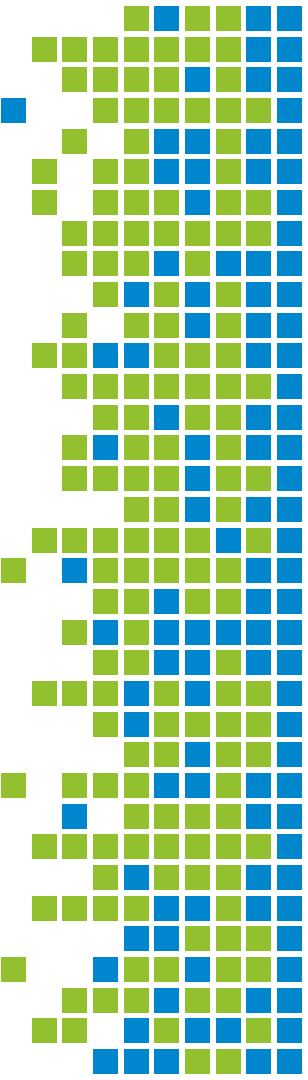
Transfer

Modules

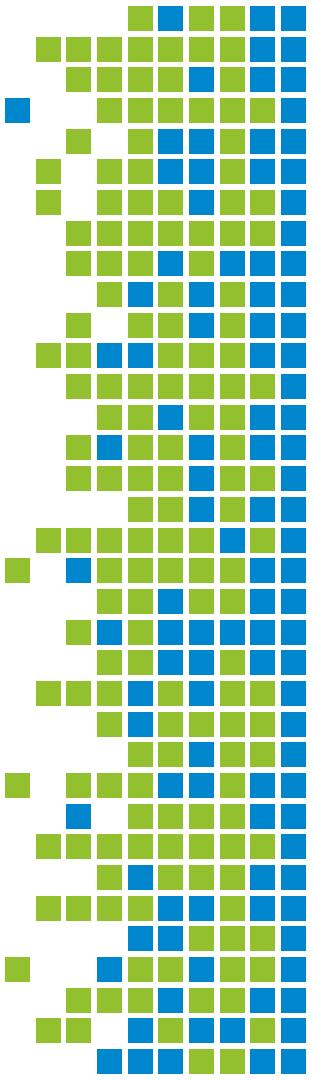
Submission



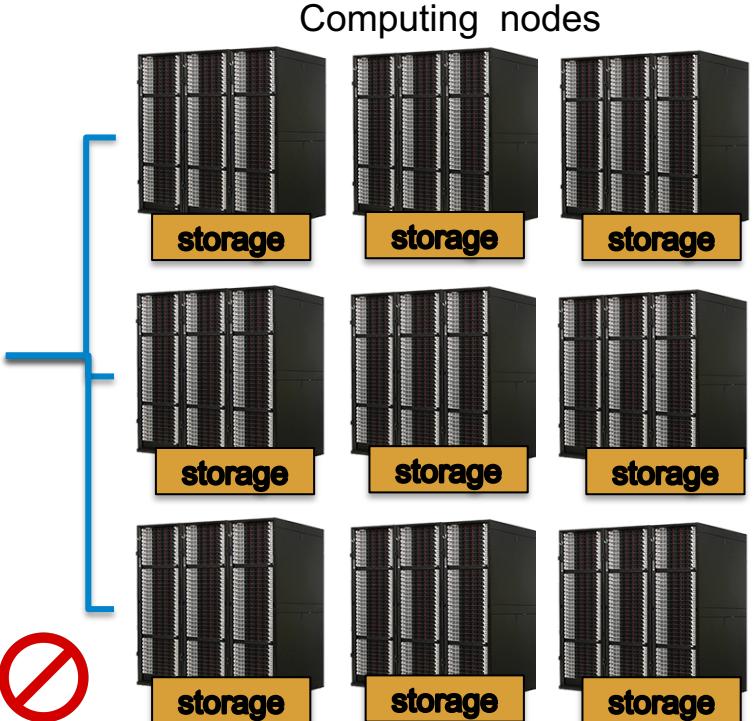
- How to ssh
- SSH-Keys
- Login & Compute nodes



# Kay: Login & Compute Nodes

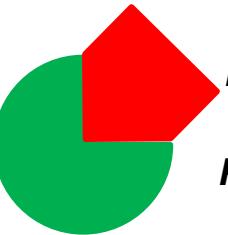


>  
\_  
SSH



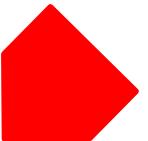
# ssh-keys

Generate the ssh-key



*Private: id\_ed25519*

*Public: id\_ed25519.pub*

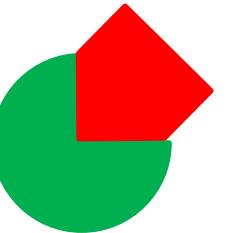


**\$USER\_PROFILE/.ssh/id\_ed25519**

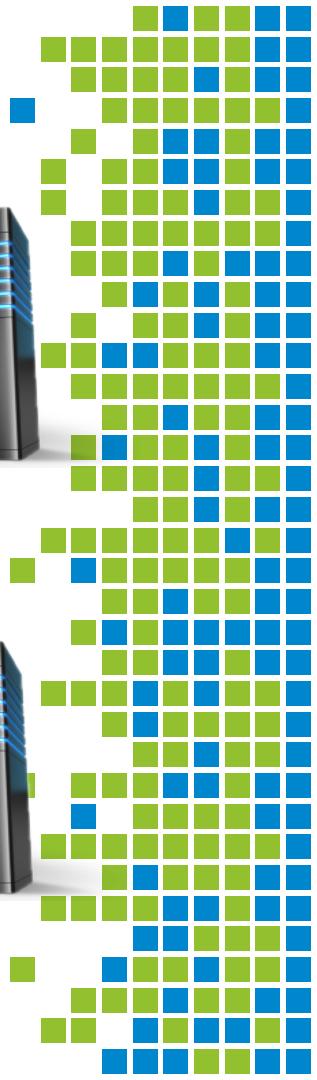


**\$HOME/.ssh/authorized\_keys**

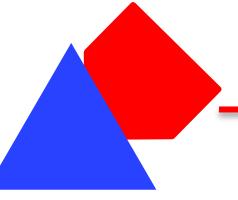
# ssh-keys



*Match*



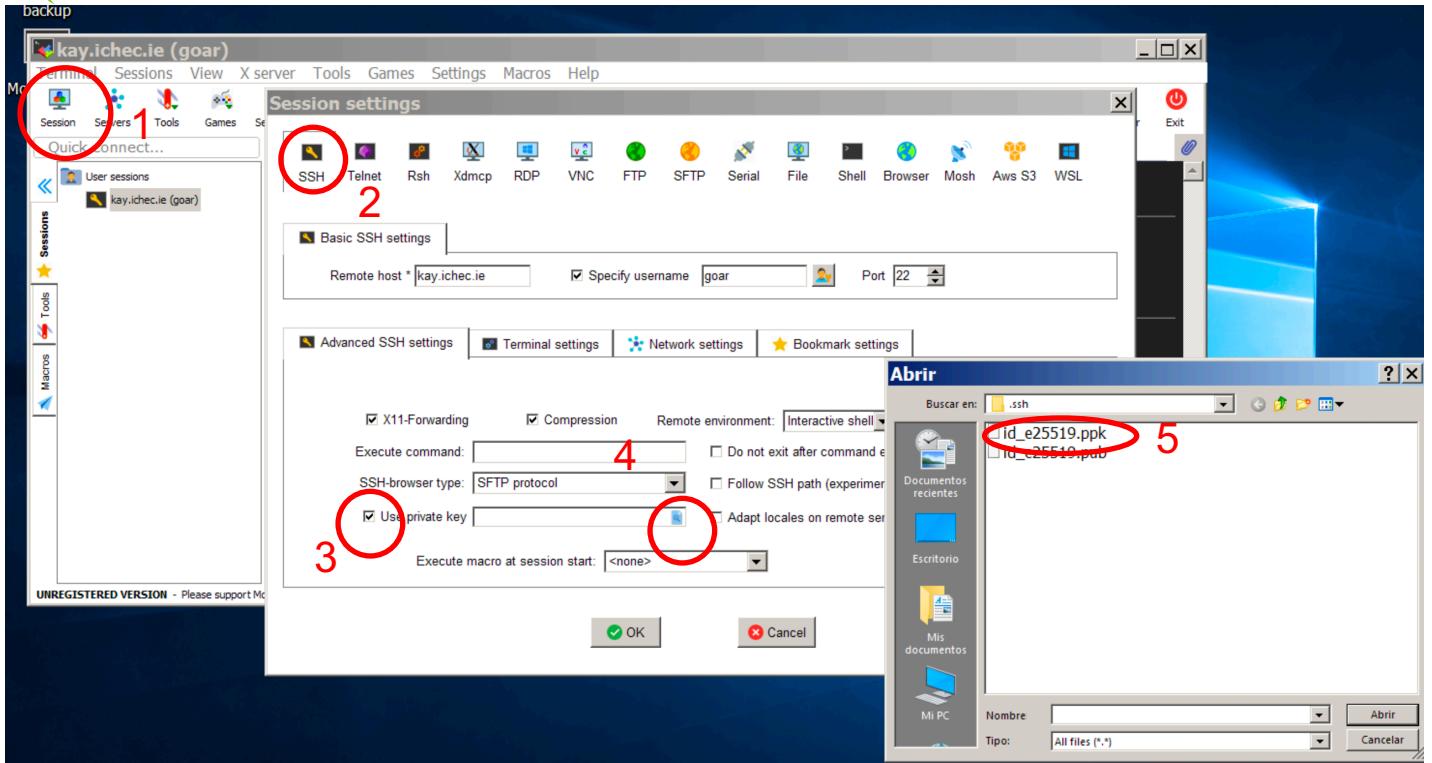
*wrong  
private*



*wrong  
public*



# Mobaxterm Connection



<https://www.ichec.ie/academic/national-hpc/documentation/tutorials/setting-ssh-keys>

## Roadmap today



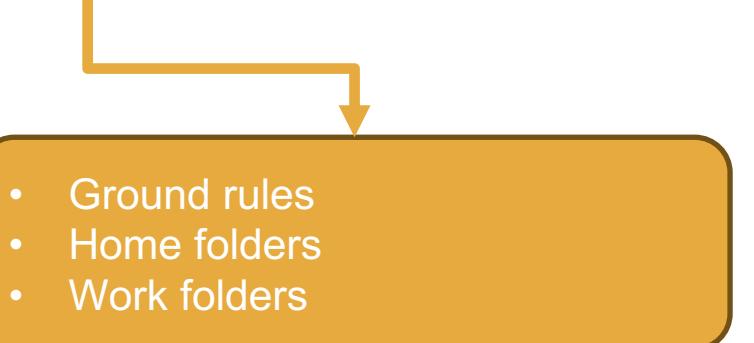
Connection

Accounts

Transfer

Submission

Gaussian

- 
- Ground rules
  - Home folders
  - Work folders

# User and project account



## User Account

- Unique: username
- Same across all ICHEC services
- Required to access kay
- `/ichec/home/users/courseXX`
- Storage: 25GB

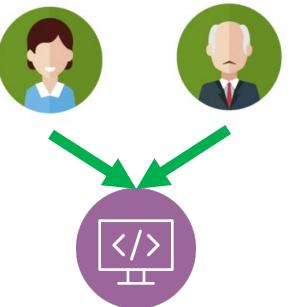


## Project Account

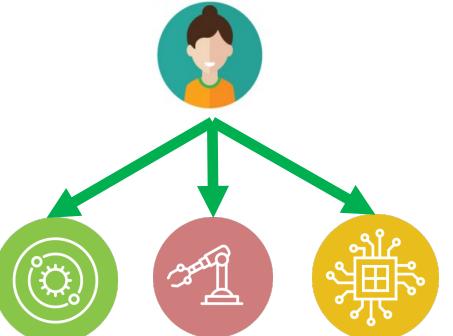
- ID name **course**
- PI manage the account
- Required to access kay

**You need an user account + project to connect to kay**

Multiple users can share a **project** account



Multiple **projects** can be assigned to a user account



**Sharing users accounts is strictly forbidden**



# User and project account



## Useful commands

- quota

```
[course00@login1 ~]$ quota
Disk quotas for user course00 (/ichec/home/users/course00):
      Used: 0.00 GB    Soft: 25.00 GB  Hard: 27.50 GB
[course00@login1 ~]$
```

- mybalance

```
[course00@login3 ~]$ mybalance
=====
Core Hours Allocation Information for account : course
=====
Allocated Core Hours      :      833333.33
Project Consumed Core Hours :      160791.67
Percentage of Project Consumed :      19.30
=====
[course00@login3 ~]$
```

## Roadmap today



Connection

Accounts

Transfer

Modules

Submission



- Transfer files
- Ssh
- MobaXterm

# Transferring files

## Transferring files:

- Putting files from your laptop to Kay

```
scp SOURCE username@kay.ichec.ie:DESTINATION
```



```
goar@815-goar:~$ scp myfiles goar@kay.ichec.ie:/ichec/staff/goar
```

# Transferring files

## Transferring files:

- Bringing files from Kay to your laptop

```
scp goar@kay.ichec.ie:SOURCE DESTINATION
```



```
goar@815-goar:~$ scp goar@kay.ichec.ie:/ichec/staff/goar/myfiles .
```

# SCP/SFTP Clients



## Windows

- **Mobaxterm**
- Filezilla
- Bitvise
- WinSCP
- Cyberduck

<https://mobaxterm.mobatek.net/>



## Mac OS

- **Cyberduck**

<https://cyberduck.io/download/>



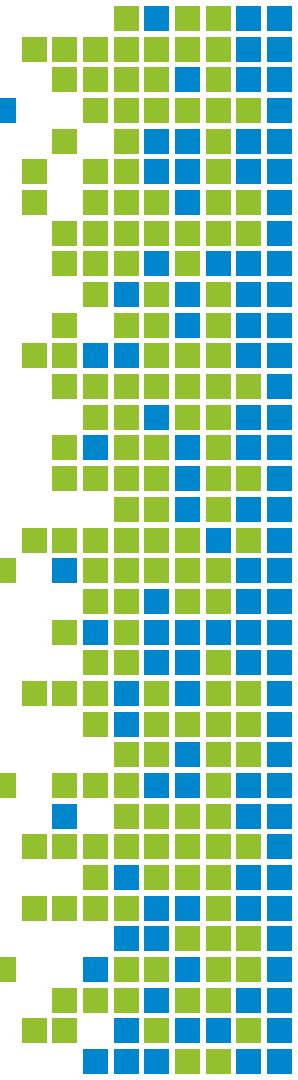
## Linux

- **Filezilla**

<https://filezilla-project.org/>



# Transferring Files



## OPTIONS

- *-r : recursive, to transfer folders*
- *~ : home directory*
  
- ***Transfer files from your laptop into fionn***
  - Create a text file
  - Transfer it to Kay
  
- ***Transfer files from Kay into your laptop***
  - Modify the text file
  - Transfer the new file into your laptop
  
- ***Transfer folders (recursive)***
  - Create a folder
  - Create n-files into that folder
  - Transfer that folder

## Roadmap today



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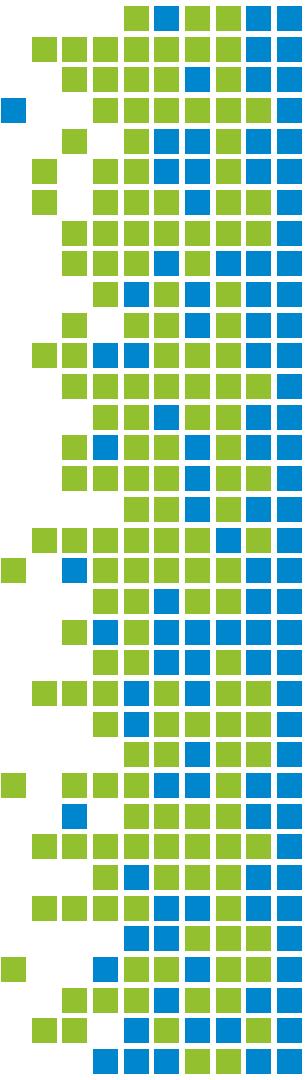
Modules

Submission

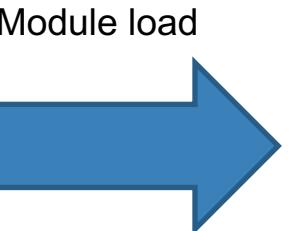


- Modules
- Load, list, delete

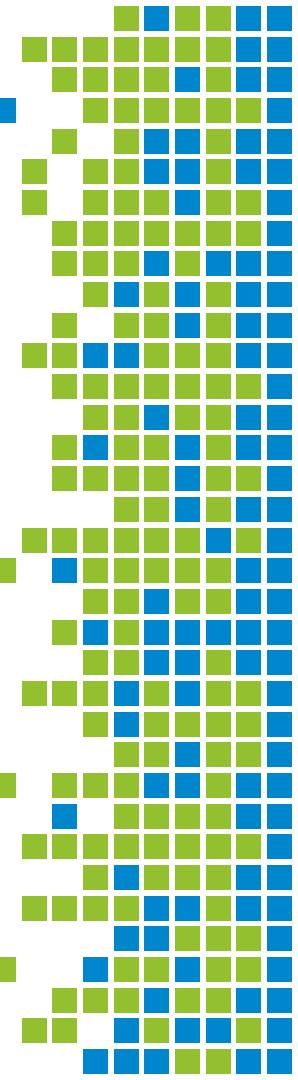
# Modules



- Modules allow access to certain software, compilers, etc. in Kay
- Prevent mismatch or interference with other libraries
- Allow using different versions of a program/compiler/etc.
- Access to python and conda environments



# Modules

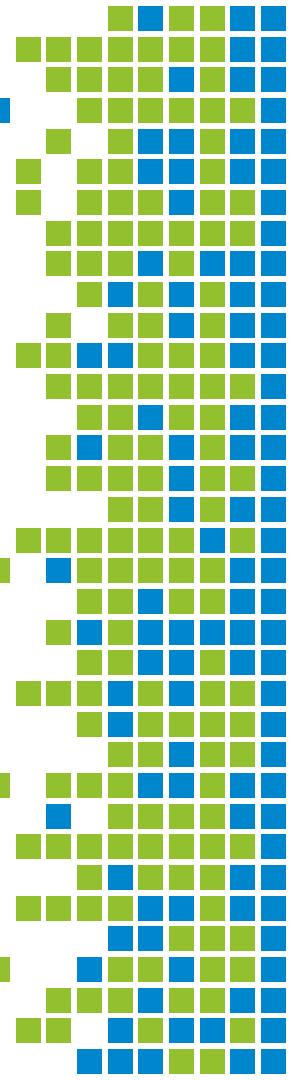


Syntax: `module [command] arguments`

- **module**: shows all options
- **module av/avail**: shows modules available in the system
- **module load *name***: loads *name*
- **module unload *name*** : unloads *name*
- **module list**: lists all modules currently loaded
- **module purge**: unload all modules

Let's do it live...

# Transferring Files



- ***Load modules***
  - Load any module
  - Load an intel module
  - Load another intel module. What happens?
  - List all modules loaded
- ***Unload modules***
  - Load any module
  - Unload the same module
  - Load several modules and unload them one by one
  - Load several modules and purge them
- ***Additional exercise***
  - Load a compiler
  - Compile a hello\_world program (choose your preferred language)

## Roadmap today



Connection

Accounts

Transfer

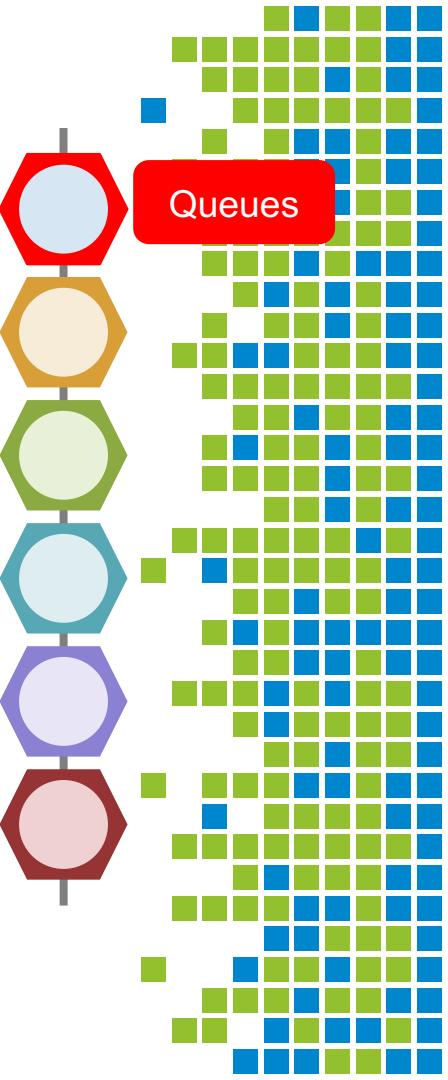
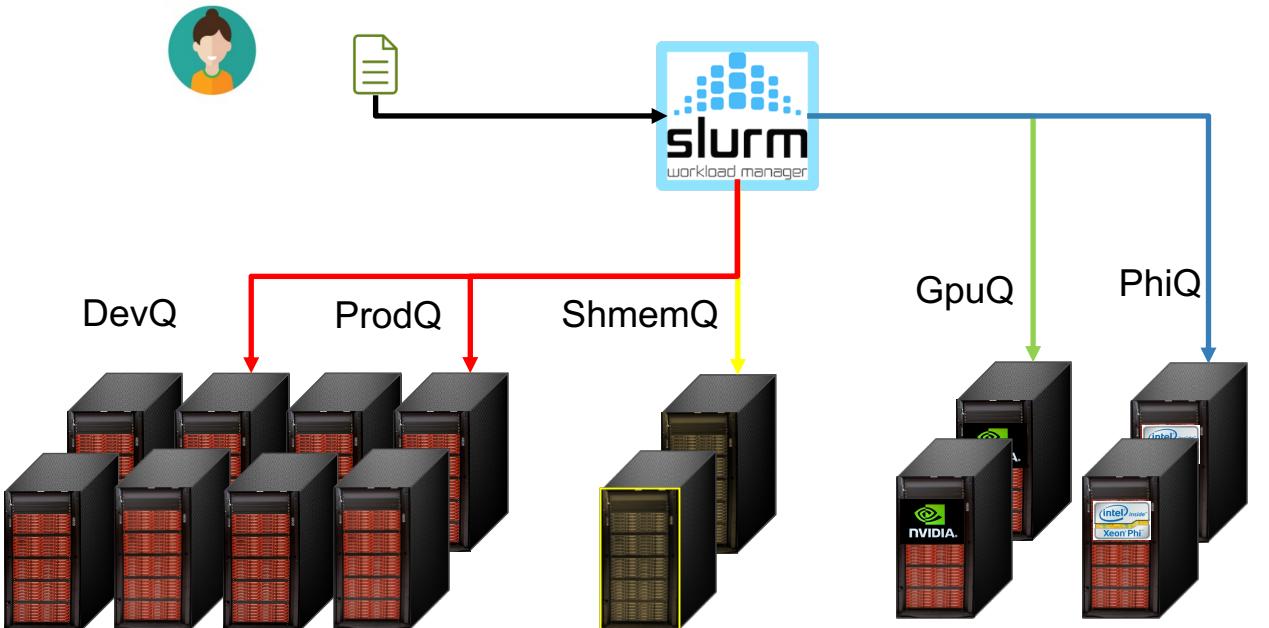
Modules

Submission

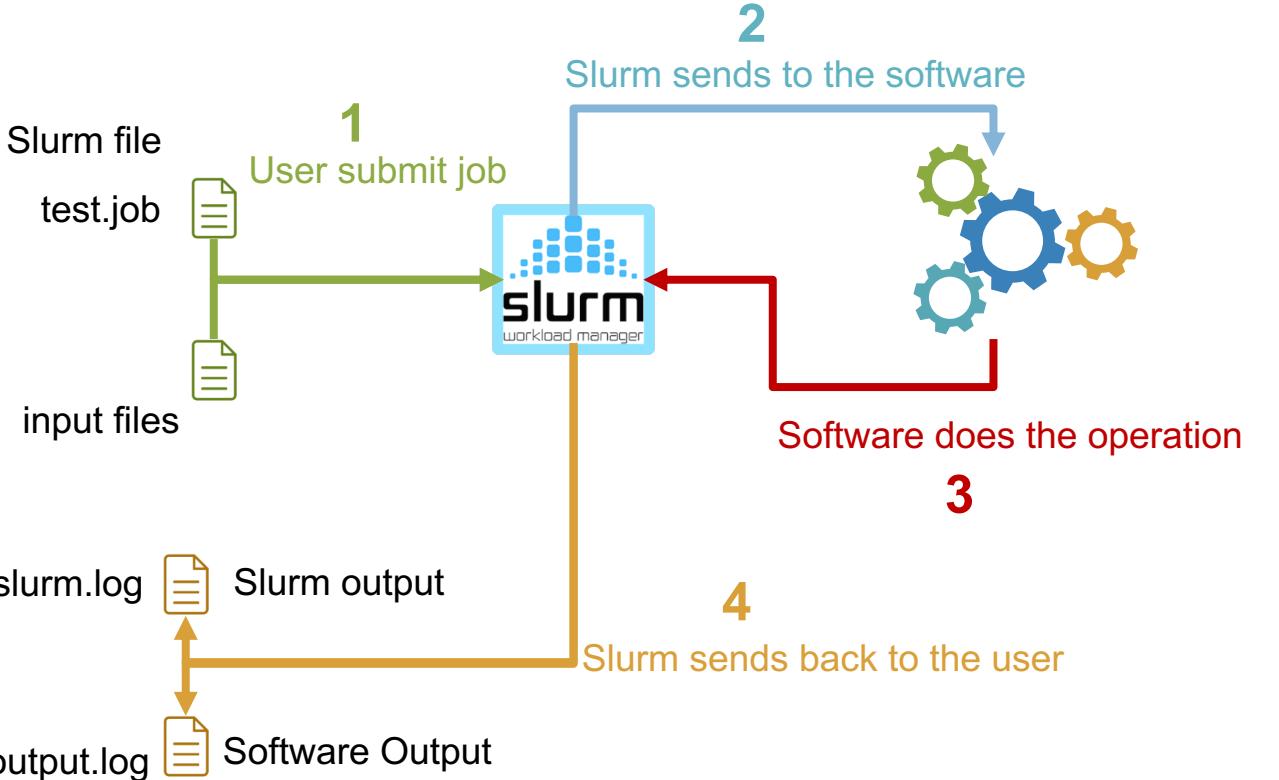


- Queues
- Submission Script
- Jobs control

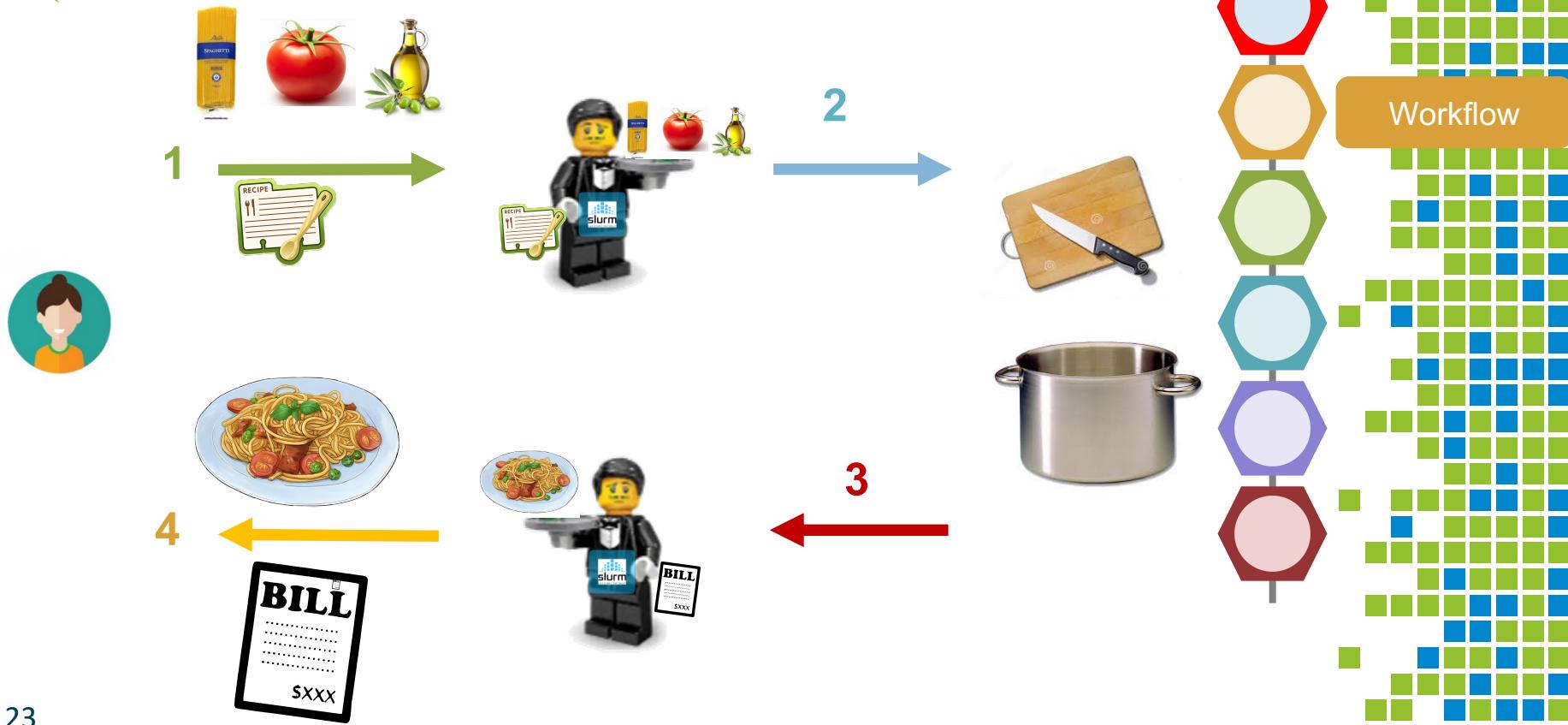
# Slurm Manager



# Workflow



# Workflow



# Slurm Submission file

Slurm file



test.job

```
#!/bin/bash

#Slurm flags
#SBATCH --partition=CourseDevQ
#SBATCH --nodes=1
#SBATCH --time=00:30:00
#SBATCH --job-name=test
#SBATCH --account=course
#SBATCH --output=slurm.log
#SBATCH --mail-user=myemailaddress@universityname.ie
#SBATCH --mail-type=BEGIN,END

cd $SLURM_SUBMIT_DIR

#Load module

module load XXXXX

#do something
```



# Slurm Submission file

Slurm file



test.job

```
#!/bin/bash

#Slurm flags
#SBATCH --partition=CourseDevQ
#SBATCH --nodes=1
#SBATCH --time=00:30:00
#SBATCH --job-name=myjob
#SBATCH --account=course
#SBATCH --output=slurm.log
#SBATCH --mail-user=goar.sanchez@ichec.ie
#SBATCH --mail-type=BEGIN,END

cd $SLURM_SUBMIT_DIR

#Load compiler's module

module load gcc/8.3.1

#compile the program
g++ -o helloworld.o hello_world.cpp
```



Slurm file

Slurm file



type: sbatch test.job



#### Hints:

- You need 1 slurm file per job
- You need all the necessary input files

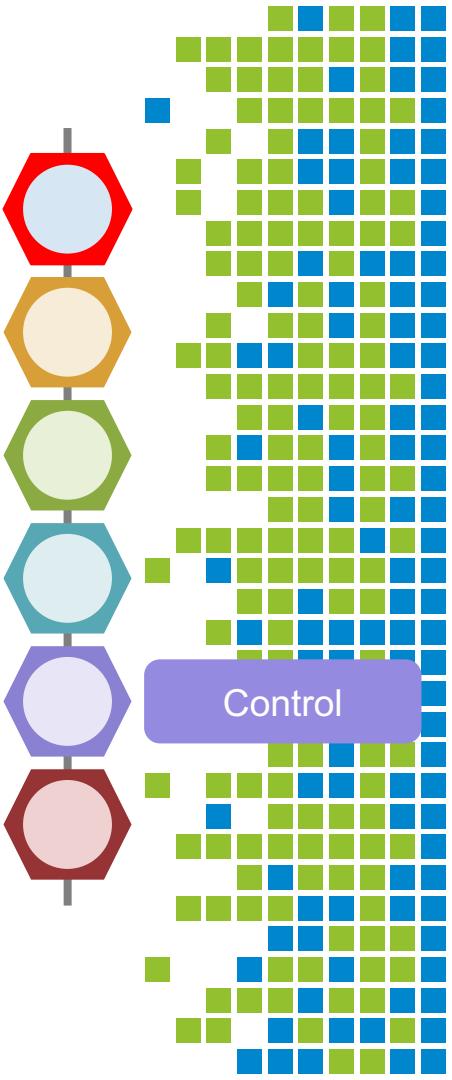
# Submit a job



# Slurm Manager

Slurm file

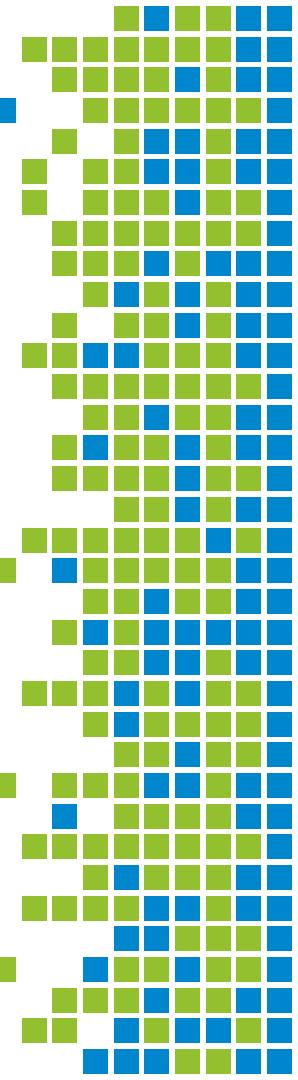
Description	Command
Queue Status	sinfo
Submit Job	sbatch job.sh
Check Job Status	squeue -u \$USER
Cancel Job	scancel 123213
Check Project Account Balance	mybalance



# Exercises

1. **Copy** files from `/ichec/home/users/course00/slurm/example` to your folder
2. **Copy** files from `/ichec/home/users/course00/slurm/exercises` to your folder

# Getting Help



## Frequently Asked Questions

<https://www.ichec.ie/academic/national-hpc/FAQ>

## Documentation

<https://www.ichec.ie/academic/national-hpc/documentation>

## Helpdesk

<https://www.ichec.ie/academic/national-hpc/user-support>