PRACE Course: Intermediate MPI
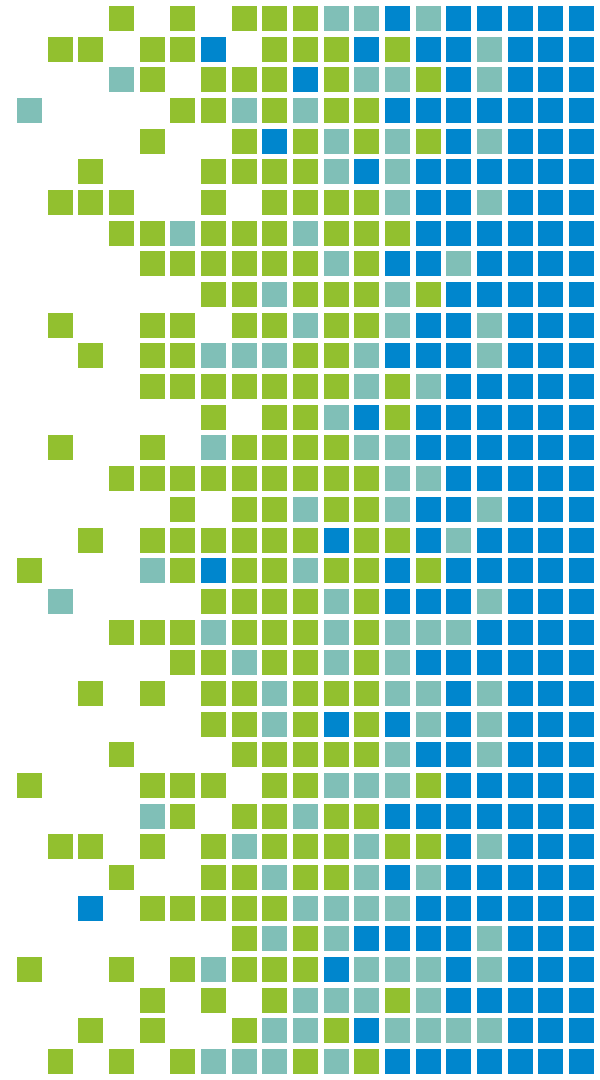
9-11 November 2022

Introduction to ICHEC Cluster

Roadmap

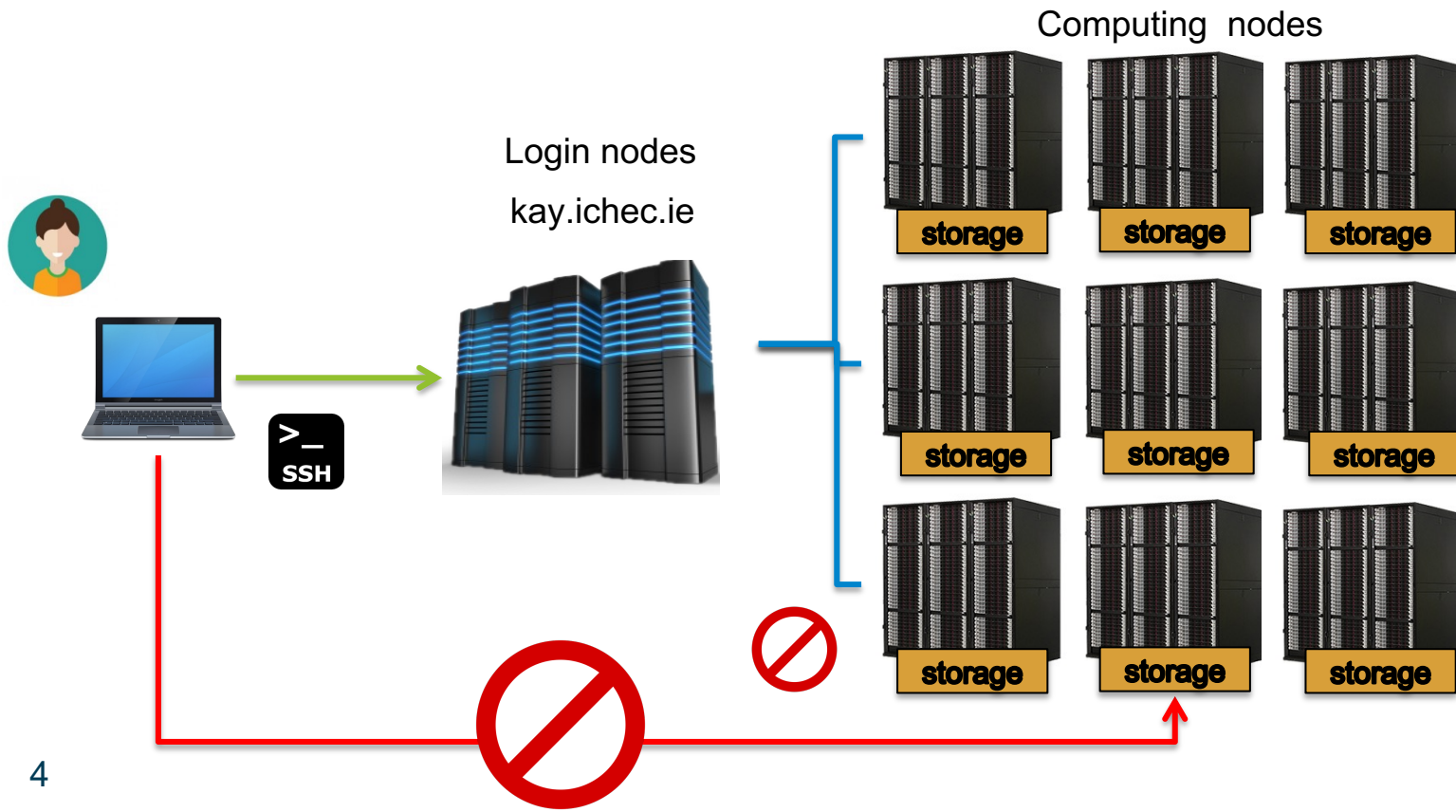Connection Accounts Transfer Modules Submission

Roadmap

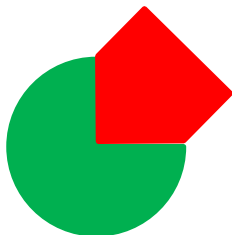Connection · Accounts · Transfer · Modules · Submission

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

Login & Compute Nodes

Computing nodes

Login nodes

kay.ichec.ie

SSH

storage

storage

storage

storage

storage

storage

storage

storage

storage

Ssh-keys

Generate the ssh-key

Private: id_ed25519

Public: id_ed25519.pub

$USER_PROFILE/.ssh/id_ed25519

$HOME/.ssh/authorized_keys

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

Ssh-keys
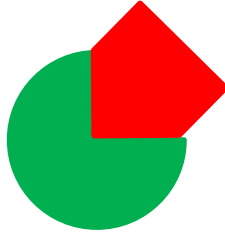
Match

wrong private   *wrong public*

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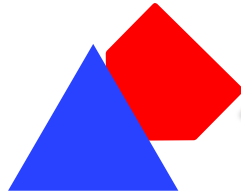
Roadmap

Connection Accounts Transfer Modules Submission

- Ground rules
- Home folders
- Useful commands

User and project account

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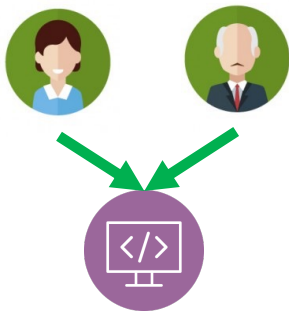- **/ichec/home/users/courseXX**
- Storage: 25GB

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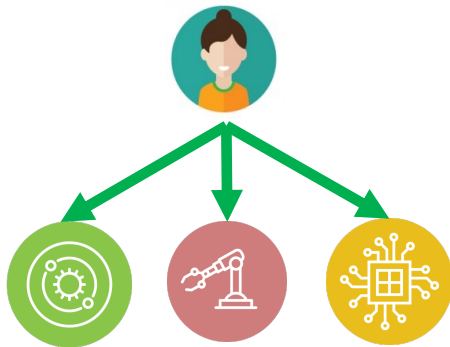- Required to access kay

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

Register an account: https://register.ichec.ie

Condominium Access

Projects

    Class C (1 year) : **small** resources:100k CPUh/250GB

    Class B (1.5 year) : **medium** resources:1M CPUh/1TB

    Class A (2 years) : **large** resources:10M CPUh/5TB

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

Connection　Accounts　Transfer　Modules　Submission

- Transfer files
- Scp clients

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
- Git bash

Mac OS
- **Cyberduck**

Linux
- **Filezilla**

https://mobaxterm.mobatek.net/

https://cyberduck.io/download/

https://filezilla-project.org/

Roadmap

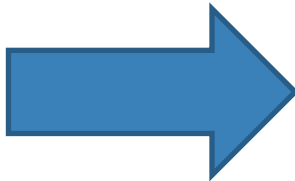Connection → Accounts → Transfer → Modules → Submission

- 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

module load

Modules

Syntax: module [command] *arguments*

 module: shows all options

 mo**dule 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
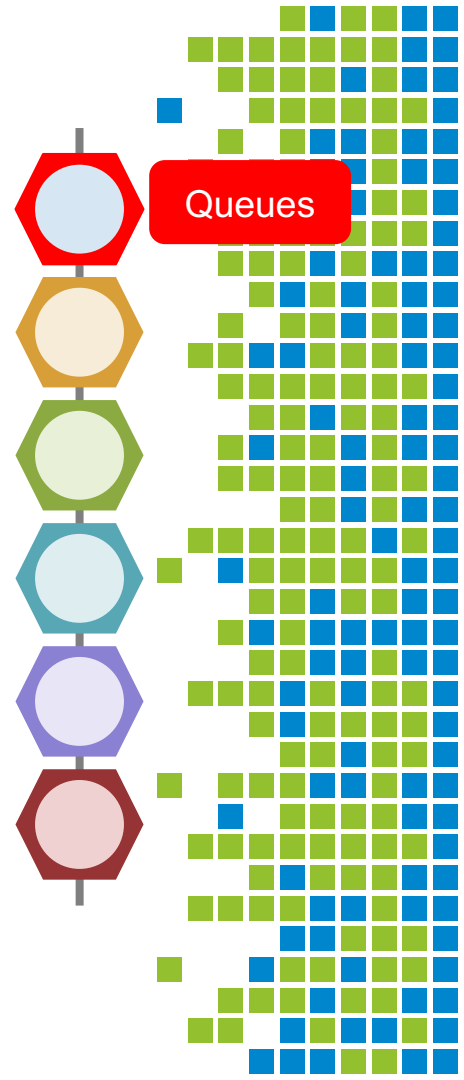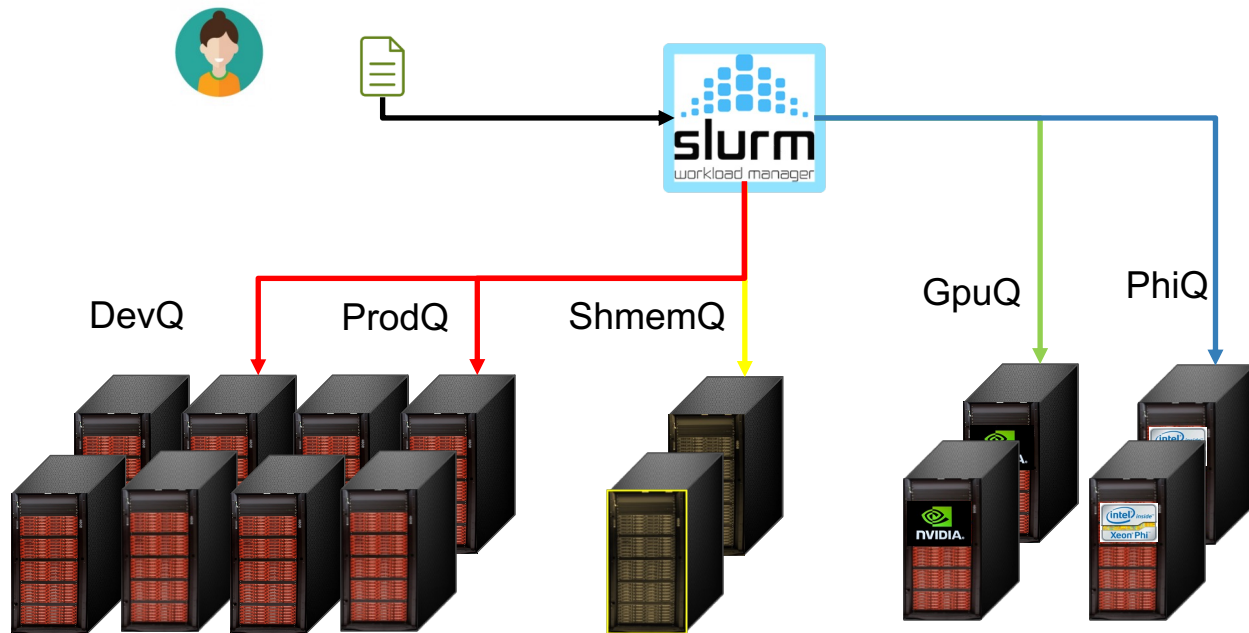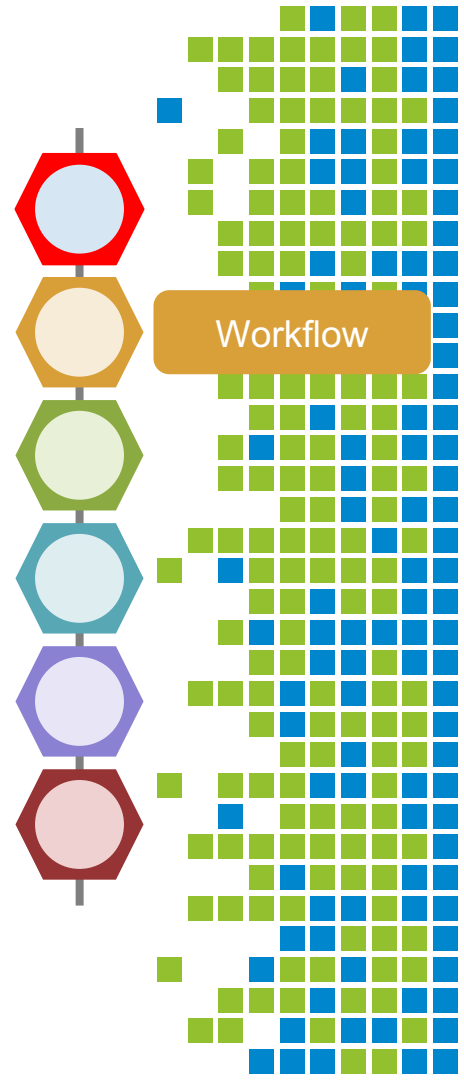
Roadmap today

Connection   Accounts   Transfer   Modules   Submission

- Queues
- Submission Script
- Jobs control

Slurm Manager

DevQ ProdQ ShmemQ GpuQ PhiQ

Queues
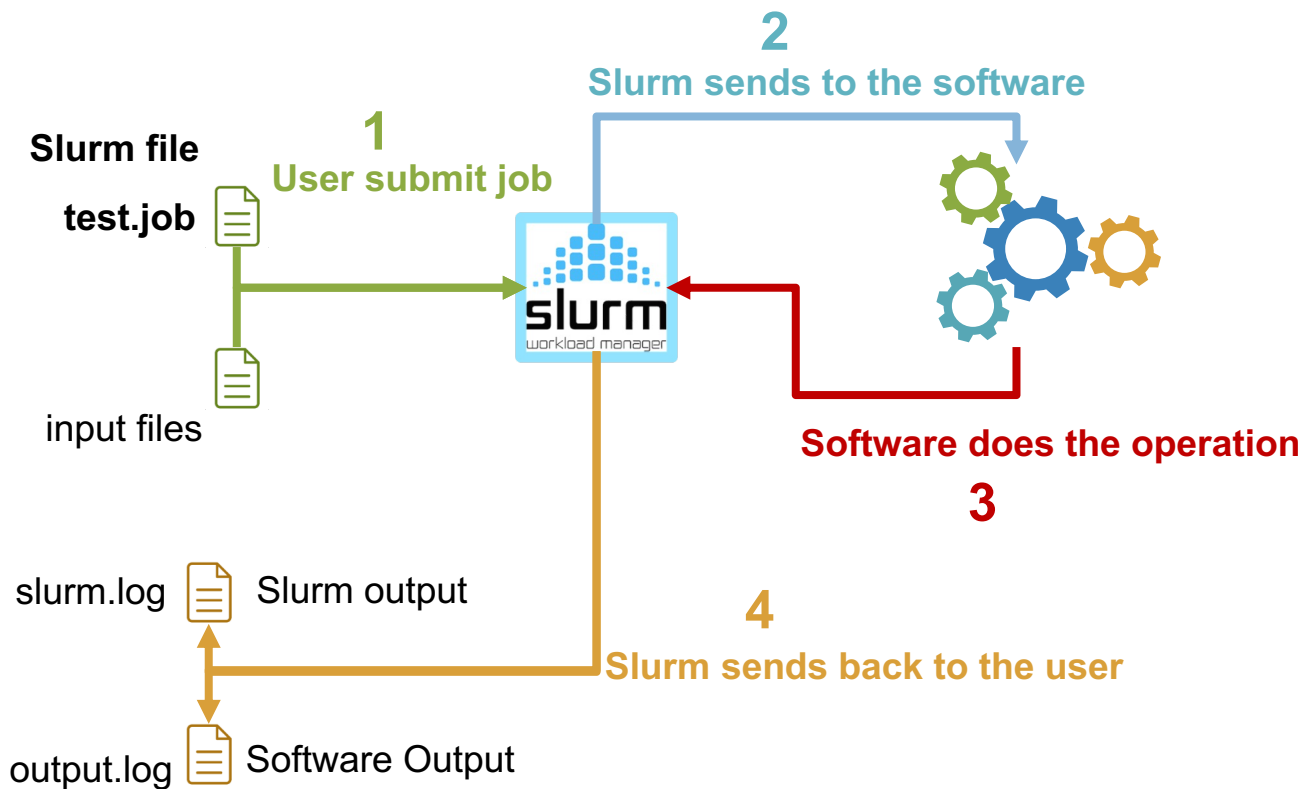
Workflow

Slurm file
test.job

input files

1
User submit job

2
Slurm sends to the software

Software does the operation
3

4
Slurm sends back to the user

slurm.log — Slurm output

output.log — Software Output

Workflow

20

Workflow

Slurm submission file
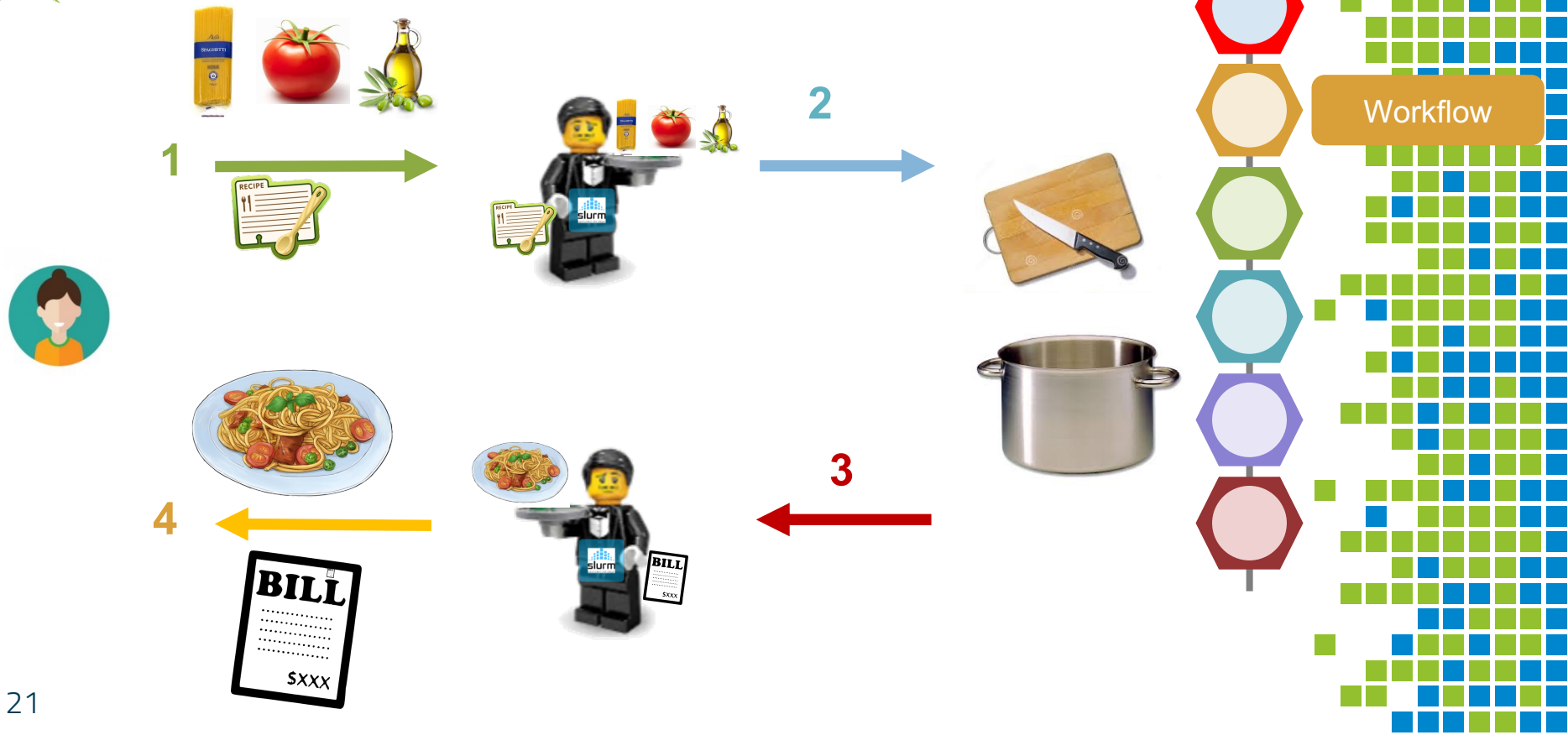
Slurm file

test.job

Slurm file

```bash
#!/bin/bash

#Slurm flags
#SBATCH --partition=CourseDevQ
#SBATCH --reservation=CourseMar2
#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 --reservation=CourseMar2
#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/8.2.0

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

Slurm file

Submit a job

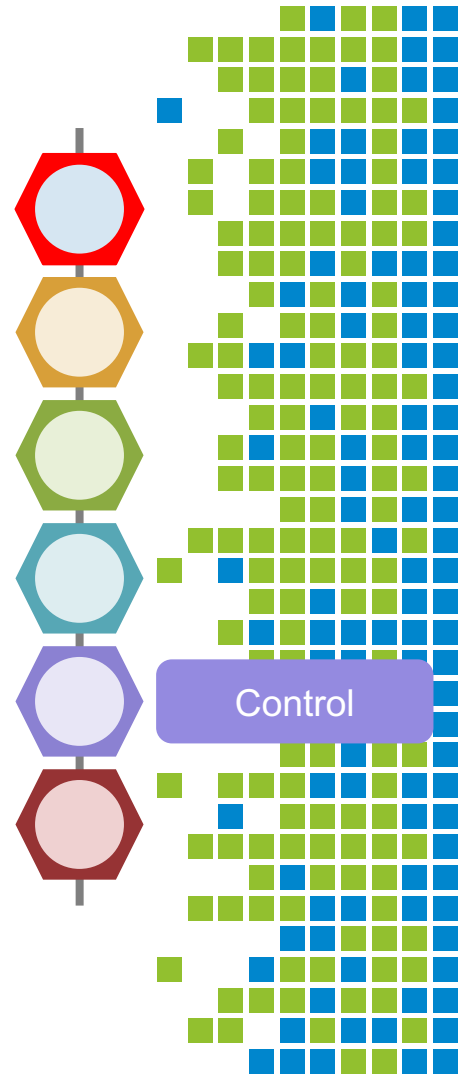Slurm file

 test.job

```
goar@login1:~$ sbatch test.job
```

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

Submission

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**

Control

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