Introduction to
IJC computational infrastructure

Angelika Merkel (Head of Bioinformatics)
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IT Team

Franciso Contreras

(Network administration/
 Windows support)

Marc Jubany

(Head of IT)

José Alcántara

(HPC administration/
 Linux support)

Office: 0.00.04 (ground floor)

Email: helpdesk@carrerasresearch.org
https://tickets.carrerasresearch.org/

IJC Bioinformatics

Angelika Merkel

(Head of Unit)

Izar de Villasante

(Bioinformatician)

(Software engineer)

Office: 1.31.01 (1st floor); phone: 4300

https://carrerasresearch.sharepoint.com/sites/BIT

https://www.carrerasresearch.org/en/bioinformatics-unit

Data analysis
- Processing
- Analysis
- Visualization
- Report

Consulting
- Experimental design
- Statistical advice
- Recommend analysis workflow and tools

Data services
- File transfers (collaborators)
- Data upload to public repositories (GEO, SRA)
- Data download from public repositories and databases

Training
- Internships (master)
- Seminars
- Workshops

Tool development
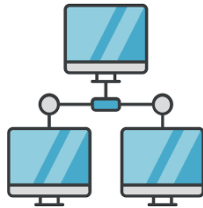- Custom (bio)informatic solutions

Overview:

Resources

Shared resources

Filesharing

Data management

IJC network & working remotely

Network

Connecting from the outside

Cybersecurity

High performance computing (HPC) c

Architecture

Scheduling

Shared network resources (IJC only)

INVESTIGACIO

- Shared folder for research group or core facility. By default contains a private folder for the group leader and a shared folder accessible by anyone in the group

- **For Office documents and results only!** No RAW DATA or big images.

- **Back-up**

SHARED FOLDER

- Folders shared with specific groups or people. They are created by the IT department upon request.

- Some default folders shared with all groups: TRAVEL_UNIT, LABORATORIES, UNITAT_MICROSCOPIA

- **For Office documents and results only!** No RAW DATA or big images.

- **Back-up**

NAS SYNOLOGY BIODATA (OLD!)

- Network attached storage (100TB) for data storage,

- Shared folder for each group \BDgroupleadername, (IP: 10.110.20.7) set up by IT

- Predates the current HPC and will become obsolete in the future

- **NO back-up!**

HPC

- High-performance computing

- ISILON file storage system (**RAW DATA, large files**)

- **Back-up**

Shared network resources (IJC only)

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NAS... ...TA (OLD!)

- Network at... ...storage,
- Shared f... ...ame, (IP: 10.110.20.7)
- Pre... ...e current HPC and will become... ...e in the future
- **NO back-up!**

HPC

- High-performance computing
- ISILON file storage system (**RAW DATA, large files**)
- **Back-up**

File sharing (via web browser)

Access your files from everywhere through a browser and share them easily via link or email

ONE DRIVE/ SHAREPOINT (MICROSOFT)

- https://carrerasresearch-my.sharepoint.com/

- Pros: Desktop compatible, integrated with office 365
- Cons: Data is located on MS servers off site

NEXTCLOUD

1. Core facilities:
   - https://nextcloud_micro.carrerasresearch.org/
   - Share data files or results with collaborators
2. Personal:
   - https://nextcloud_ijc.carrerasresearch.org/
   - Access to > INVESTIGACIO, > SHARED_FOLDER, > BD$GROUP
   - In the future only accessible through VPN portal
3. On request
   - Request a custom link from IT to share files

- Pros: Highly customizable access (time, groups, etc.)
- Cons: limited file viewing properties for office documents

File sharing via FTP

Move files from inside the IJC network to the internet and vice versa

Secure FTP

- transfer large data files
- 5TB temporary storage <u>shared</u> amongst users
- Host: ftpbios.carrerasresearch.org Port 4242
- Access over the internet **only with credentials**

Public FTP

- e.g. for software requiring public URLs to upload data (genome browser)
- account needs to be configured by IT
- Host: bios.carrerasresearch.org Port 22
- https://username.carrerasresearch.org
- Allows access over the internet **without credentials**

Transfer files with:

1) ftp client like Filezilla or

2) via Terminal

```
sftp –P 4242 username@ftpbios.carrerasresearch.org (secure)          sftp bios.carrerasresearch.org  (public)
    > mput myfile
    > get myfile
```

External filesharing tools

| Interface	Tool	Access	Recommended for	File location
Web browser	OneDrive	https://carrerasresearch-my.sharepoint.com/	Documents	Windows servers (off-site)
Web browser	NextCloud	https://nextcloud_ijc.carrerasresearch.org	Documents, data <1GB	IJC servers (on-site)
Software	Filezilla	Available for MacOS, Windows, Linux	Data > 1GB	IJC sftp server (on-site)
Terminal	Sftp (public)	https://username.carrerasresearch.org sftp username@bios.carrerasresearch.org > mput my_file; > mget my_file	Public data < 5GB	IJC sftp server (on-site)
Terminal	Sftp (secure)	sftp – P 4242 username@ftpbios.carrerasresearch.org > mput my_file; > mget my_file	Data > 1GB	IJC sftp server (on-site)

Data management best practices:

- Important documents and data should be stored on IJC servers, with centralized management and frequent backups. (Intellectual property concerns, IJC servers are managed by IT).

- Local workstations serve to interact with IJC file servers, for development and temporary storage. There is no back-up (Workstations supervised by IT but are still managed by the user).

- **No back-up** on external hard drives.

- Repositories of databases and software should be centralized (when possible) and associated with a user/user group. The repository should be revised when the associated user or user group changes or leaves.

- User data and accounts are terminated after the employee leaves. Before leaving the institute the user shall remove irrelevant data, assure important data is kept accordingly and is well documented. (@Bioinformaticians: Use RELATIVE PATHS in your scripts avoid ABSOLUTE PATHS!)

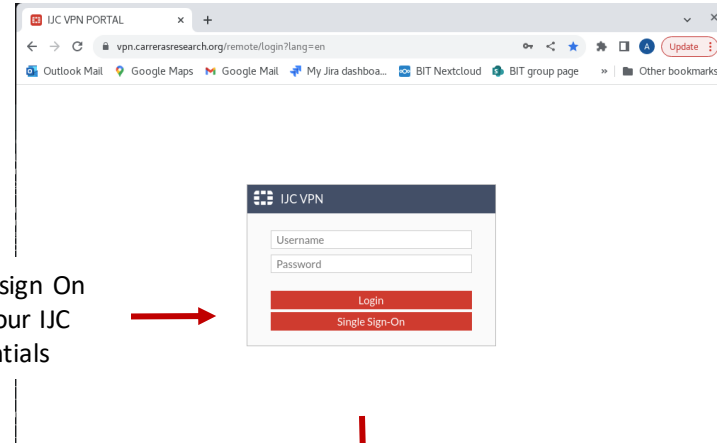**Avoid multiple copies of data!**
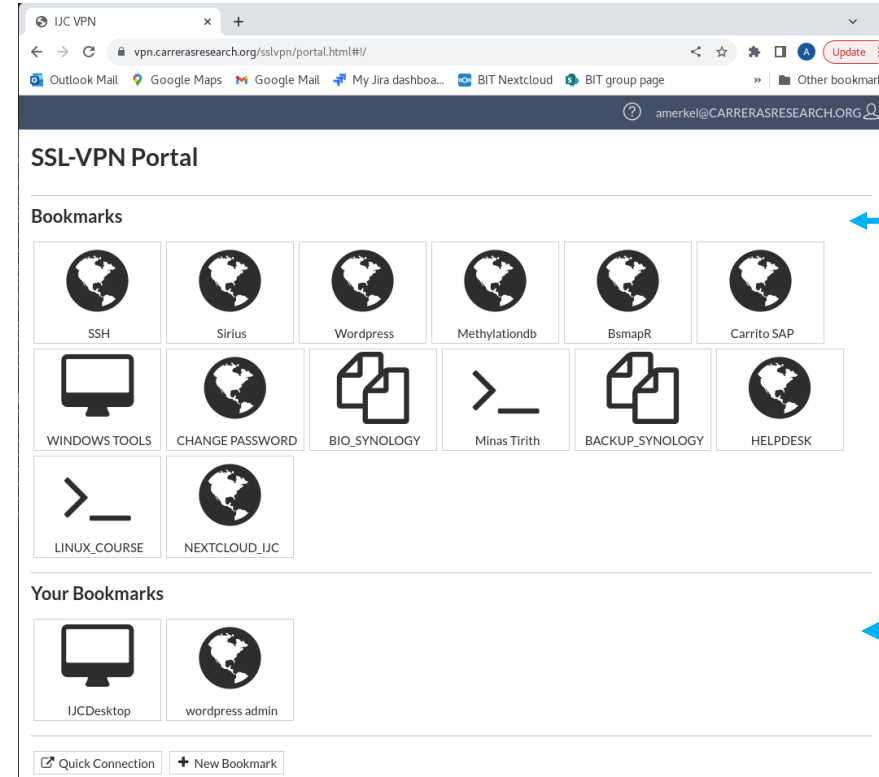
The IJC network & remote connections

The network

The IJC VPN portal

https://vpn.carrerasresearch.org/
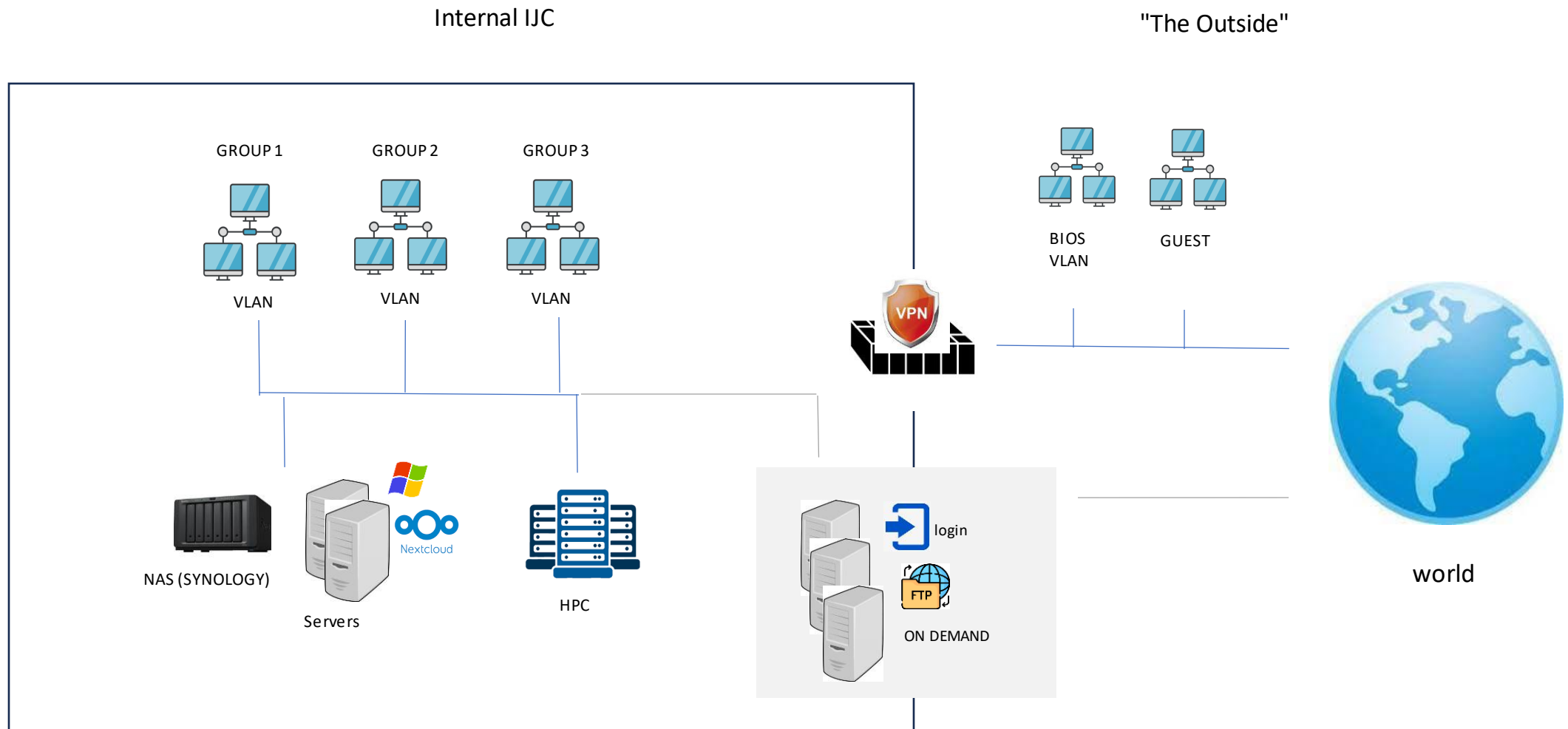
Single-sign On with your IJC credentials

2 – Factor- Authentication

Shared bookmarks (by IT)

Personal bookmarks (by you, only bios profile)

The login node

If you are connecting from outside the IJC (or you are using a computer that is not administrated by IT) you can connect through the 'login node'.

You need:

1. an SSH client (bash for Linux/zsh for Mac, or putty for windows)
2. an active domain user
3. your smartphone with a 2 Factor Authentication app (and configured by IT!).

You can access the machine with the following command:

```
ssh -P 4242 username@loginnode.carrerasresearch.org
Password: (your windows/mail password)
Verification code: (your 2FA app code)

Now you can ssh to minastitrith or you r workstation
```

IT administrated & non-IT administrated computers

IT

- Software installation and maintenance by IT
- No 'sudo' rights

Pros:

- IJC network 600Mb/s internet
- ISILON filesystem is permanently mounted (-> allows file access with GUI applications)
- Connection from the outside directly to the IJC network with vpnclient (Linux/Mac via biosvpn with IT certicate)
- As-you-go printing (all IJC printer)

Cons:

- (-> limited control, IT dependent)

Non-IT

- Software installation and maintenance by user
- 'sudo' rights

Pros:

- full control

Cons:

- Separate network (bios) without backup, 100Mb/s internet
- ISILON access only via ssh client through minastirith, no mount (-> no file access for GUI applications)
- Connection from the outside to the IJC network only via VPN portal or login node
- Printing only on guest printers (next auditorium, 2nd floor)

Cybersecurity best practices

- Do not open email with suspicious attachments or from unknown senders (if in doubt verify with IT)

- Do not plugin external hard disks with unverified content

- Do create/ maintain unsanctioned network connections between the IJC network and the outside world

- Do not share your IJC credentials (IT or your PI never will/ should ask for your credentials)

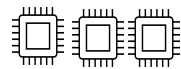- Do not approve 2FA if you are not accessing your account at the time

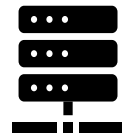# High performance computing (HPC)

HPC cluster

User

Master Node (Minastirith)
12 cores 128Gb Ram

Computational nodes
c01 128 cores 1Tb Ram
c02 128 cores 1Tb Ram
c03 128 cores 1Tb Ram GPU

Fast temporary storage
100Tb
/mnt/beegfs/$USERNAME
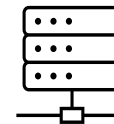
slurm workload manager

ISILON storage 1Ptb

/ijc/LABS/$GROUP/RAW = 45TB
                /DATA = 5TB
                /LTS
/ijc/USERS/$USER   = 500GB
/ijc/PROJECTS/$PROJECT = on request

Connecting to the cluster

You can connect to the cluster (masternode = minastirith) in several ways:

1. From anywhere with a browser via VPN Portal: https://vpn.carrerasresearch.org (bookmark 'Minastirith')

2. From your machine (Linux/Mac) with a terminal:

    $ ssh username@minastirith

3. From your machine using a ssh client (e.g. PUTTy for windows) connect directly to the host:

    minastirith

To connect from outside the IJC network you need to connect to the SSHlogin node first.

Using the software

Available as modules

Description	Command
see all available modules	`module avail`
load/unload a module	`module load/unload`
see all loaded modules	`module list`
unload all modules	`module purge`

Executing a job

All tasks (jobs) executed on the cluster computational nodes are managed by SLURM (the scheduler)

https://docs-research-it.berkeley.edu/services/high-performance-computing/user-guide/
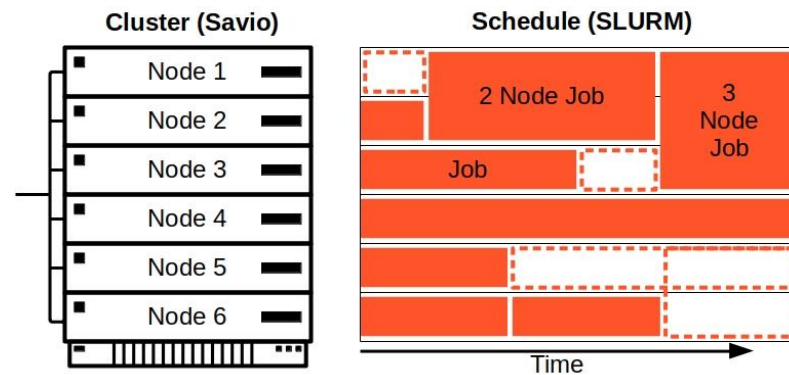
SLURM schedules each job based on available resources (CPU, memory, nodes, execution time, etc)

SLURM partitions (queues)

There are multiple partitions on the cluster depending to which jobs can be submitted depending on the required resources

#SBATCH --partition

Partition	Max time	Default time	Max CPU*	Max mem/CPU*	Max memory*	Priority
default	72:00:00	01:00:00	80	-	500	20
highMem	24:00:00	01:00:00	4	-	800	30
highCPU	72:00:00	01:00:00	200	4	-	30

*NOTE: If the resource requirement is not specified, default value = max value

(implementation in progress)

SLURM script

./my_clusterjob.sh   # basic serial job

```bash
#!/bin/bash


# SLURM arguments
#SBATCH --job-name=job_serial      # Job name
#SBATCH --cpus-per-task=1          # Run on a single CPU
#SBATCH --mem=1gb                  # Job memory request
#SBATCH --time=00:10:00            # Time limit hrs:min:sec
#SBATCH --output=job_%j.log        # Standard output and error log


# load software

module load R


# message something

echo "Running R script on a single CPU core"

# run
Rscript myscript.r
```

%j = jobid

Slurm Commands

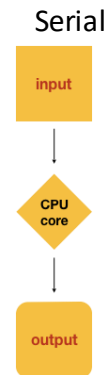| Command	Description
sbatch my_clusterjob.sh	Submit job for execution
squeue	Show the actual job queue
scancel jobid	Cancel a job
sacct –j jobid	Job accounting infos
seff -j jobid	Report on the efficiency of a job's cpu and memory utilization (after the job has finished)
salloc	Allocate resource for an interactive shell

Do's & Don't's

DO

- only request resources that you need

- check if the resources you requested were efficiently used (use seff -j jobid or similar)

- check if your job should be submitted to a special queue

- submit resource intensive jobs at low peak times (over night or the weekend)

- break large jobs down into smaller ones
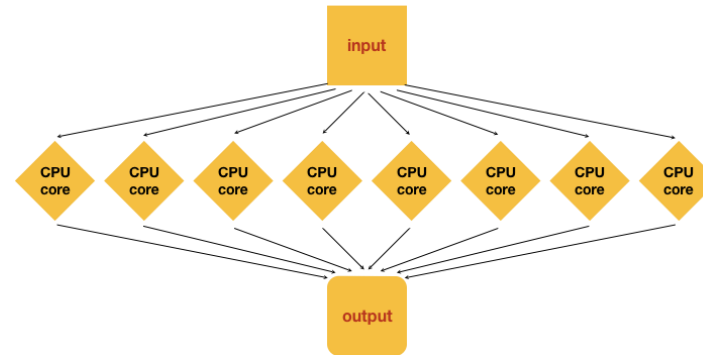
- optimize your code

DON'T

- ask for unnecessary resources (+ 10/15% time or memory are usually sufficient)

- execute any resource intensive task on the master node, use an interactive shell instead

- forget to close your interactive session

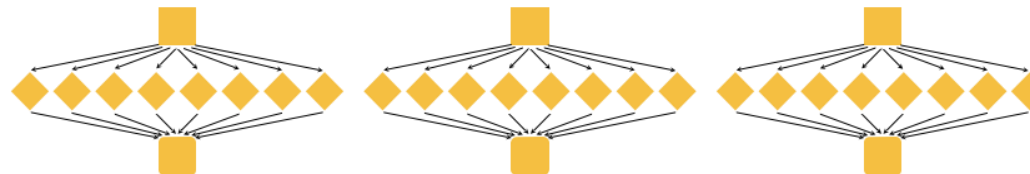# Parallelization increases speed

Serial

input

1. Single input + single task

CPU core

output

Multithreaded

input

CPU core | CPU core | CPU core | CPU core | CPU core | CPU core | CPU core | CPU core

output

2. Single input + multiple threads

Multithreaded and Parallel

3. Multiple inputs + multiple threads

Multi-processing vs multi-threading

In **multi-processing** multiple processes are executed on multiple CPUs:

- #SBATCH —-ntask=number_of_processes

In **multi-threading** a single process is executed with multiple threads (e.g. multiple code segments):

1. Shared-memory multi-threading application (threaded, OpenMP, PTHREADS) can use multiple cpus but only on a single node:
   - #SBATCH ---nodes=1
   - #SBATCH —-ntask=1
   - #SBATCH —-cpus-per-task=number_of_threads
2. OpenMPI applications allow to share threads across nodes:
   - #SBATCH —-ntask=1
   - #SBATCH –cpus-per-task=number_of_threads

Job arrays

Execute the same job over multiple inputs (samples/data sets/parameter sets)

```
#!/bin/bash


# SLURM arguments
#SBATCH --job-name=array_job          # Job name
#SBATCH --ntasks=1                     # Run a single task
#SBATCH --mem=1gb                      # Job Memory
#SBATCH --time=00:05:00                # Time limit hrs:min:sec
#SBATCH --output=array_%A-%a.log       # Standard output and error log
#SBATCH --array=1-5                    # Array range



# load module
module load python

# message something
echo This is task $SLURM_ARRAY_TASK_ID

# run
infile=$(ls *.txt | sed -n ${SLURM_ARRAY_TASK_ID}p)      # multiple input files (*.txt)

myscript.py $infile
```

How to get help

- contact IT for help with resource requirements, software and permissions
- contact BIT for help with coding and workflows
- check the documentation @:
    https://wordpress.carrerasresearch.org/
    https://vpn.carrerasresearch.org/ > wordpress
- check the BIT pages @:
    https://carrerasresearch.sharepoint.com/sites/BIT

- Teams: ijcbioinfo
- Bioinfo coffee club: Tuesdays 10.30am cafeteria

Questions?