

# Introduction to IJC computational infrastructure

Angelika Merkel (Head of Bioinformatics)  
21/11/2023



Angelika Merkel  
(Head of Unit)



Izar de Villasante  
(Bioinformatician)



Emilio Lario  
(Software engineer)



Marta Meroño  
(Master student)

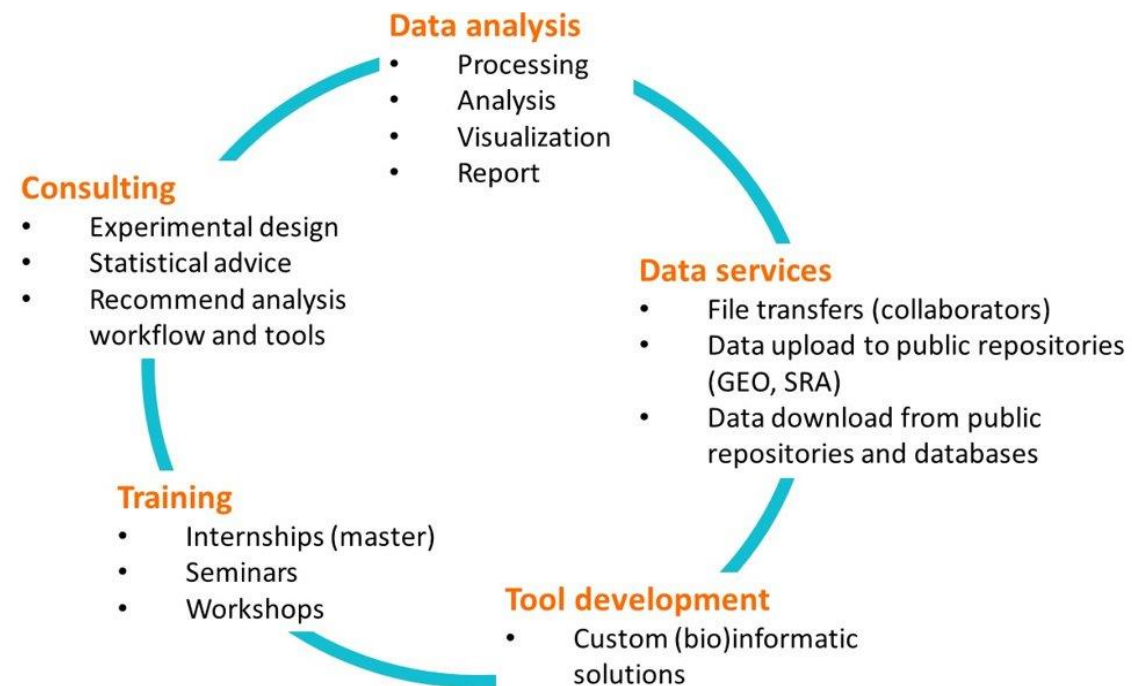
Office: Sala Prof. Albert Grañena (1st floor)(1st floor); phone: 4300

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

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



Tues: 10.30-11am, Cafeteria



# 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)

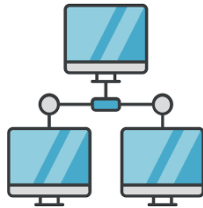
Email: [helpdesk@carrerasresearch.org](mailto:helpdesk@carrerasresearch.org)  
<https://tickets.carrerasresearch.org/>

# Overview:



## Resources

Shared resources  
Filesharing  
Data management



## IJC network & working remotely

Network  
Connecting from the outside  
Cybersecurity



## High performance computing (HPC)

Architecture  
Scheduling

## 1. Resources & file sharing

# Shared network resources (IJC only)

## INVESTIGACIO



- Shared folder for research 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)

## 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 STORAGE (OLD!)

- Network attached storage,
- Shared folder name, (IP: 10.110.20.7)
- Predecessor of 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**

# 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/](https://nextcloud_micro.carrerasresearch.org/)
    - Share data files or results with collaborators
  2. Personal:
    - [https://nextcloud\\_ijc.carrerasresearch.org/](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 shared 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)
> mput myfile
> get myfile
```

```
sftp bios.carrerasresearch.org (public)
```

# External filesharing tools

Interface	Tool	Access	Recommended for	File location
Web browser	OneDrive	<a href="https://carrerasresearch-my.sharepoint.com/">https://carrerasresearch-my.sharepoint.com/</a>	Documents	Windows servers (off-site)
Web browser	NextCloud	<a href="https://nextcloud_ijc.carrerasresearch.org">https://nextcloud_ijc.carrerasresearch.org</a>	Documents, data <1GB	IJC servers (on-site)
Software	Filezilla	Available for MacOS, Windows, Linux	Data > 1GB	IJC sftp server (on-site)
Terminal	Sftp (public)	<a href="https://username.carrerasresearch.org">https://username.carrerasresearch.org</a> 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)

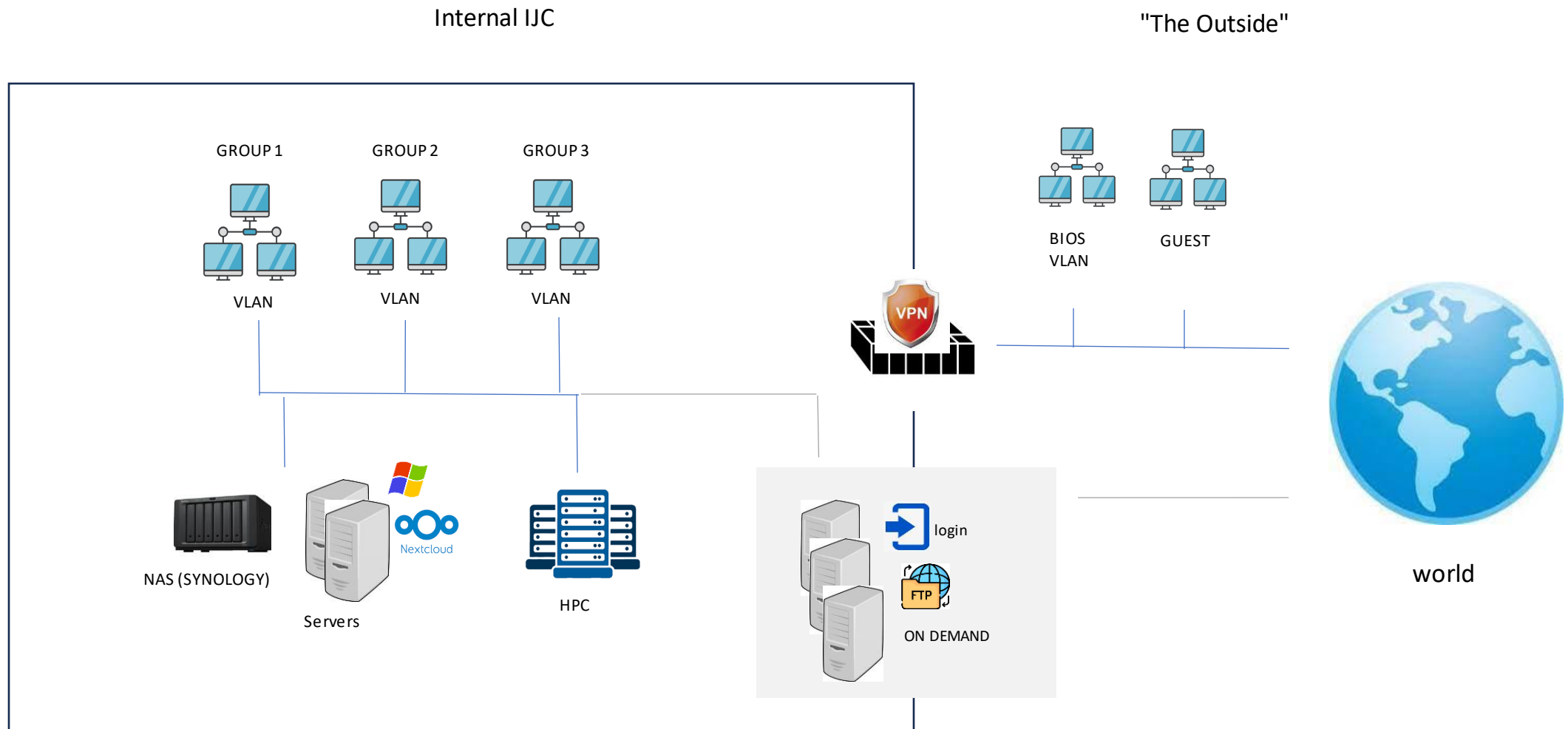
# Data management best practices:

- 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!**

## 2. The IJC network & remote connections

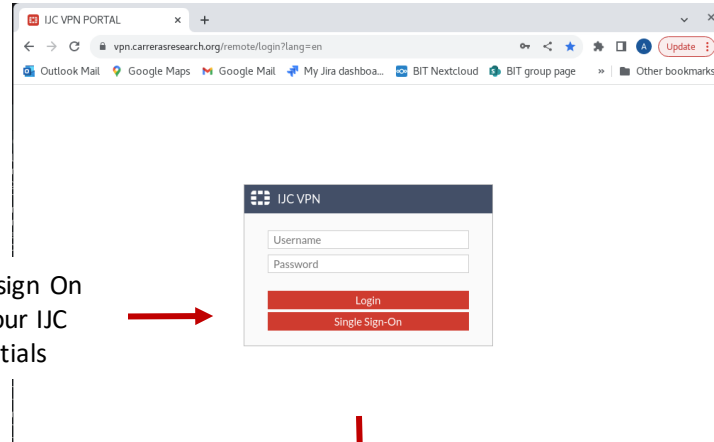
# The network



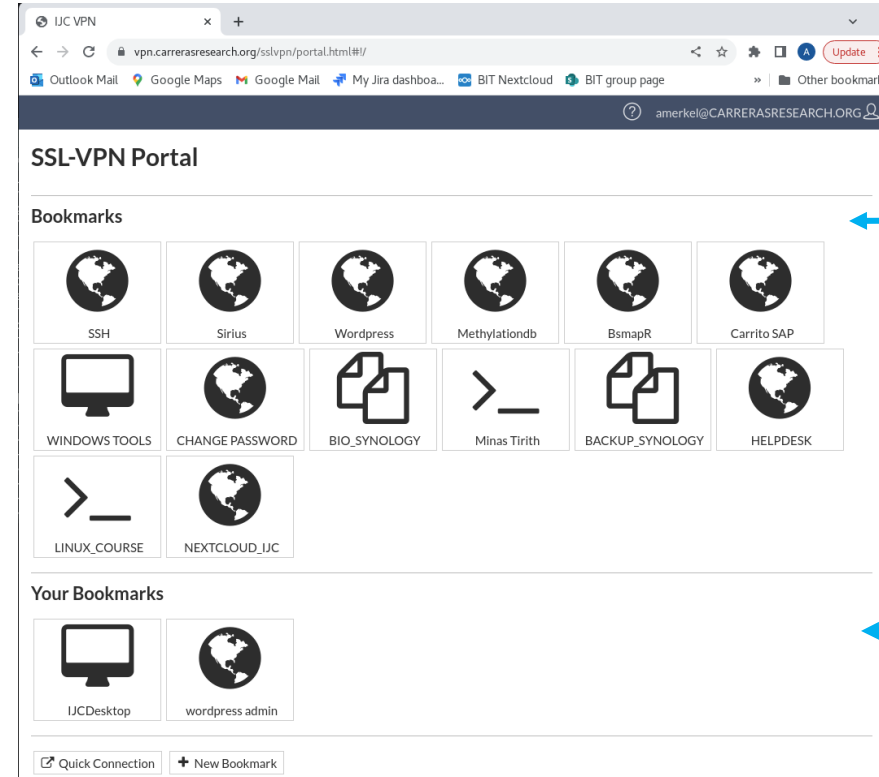
# The IJC VPN portal

<https://vpn.carrerasresearch.org/>

Single-sign On  
with your IJC  
credentials



2 – Factor- Authentication



Shared bookmarks  
(by IT)

Personal bookmarks (only  
bioinformatics 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 minastitrit or your 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 certificate)
- 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:

- Isolated bios network (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)

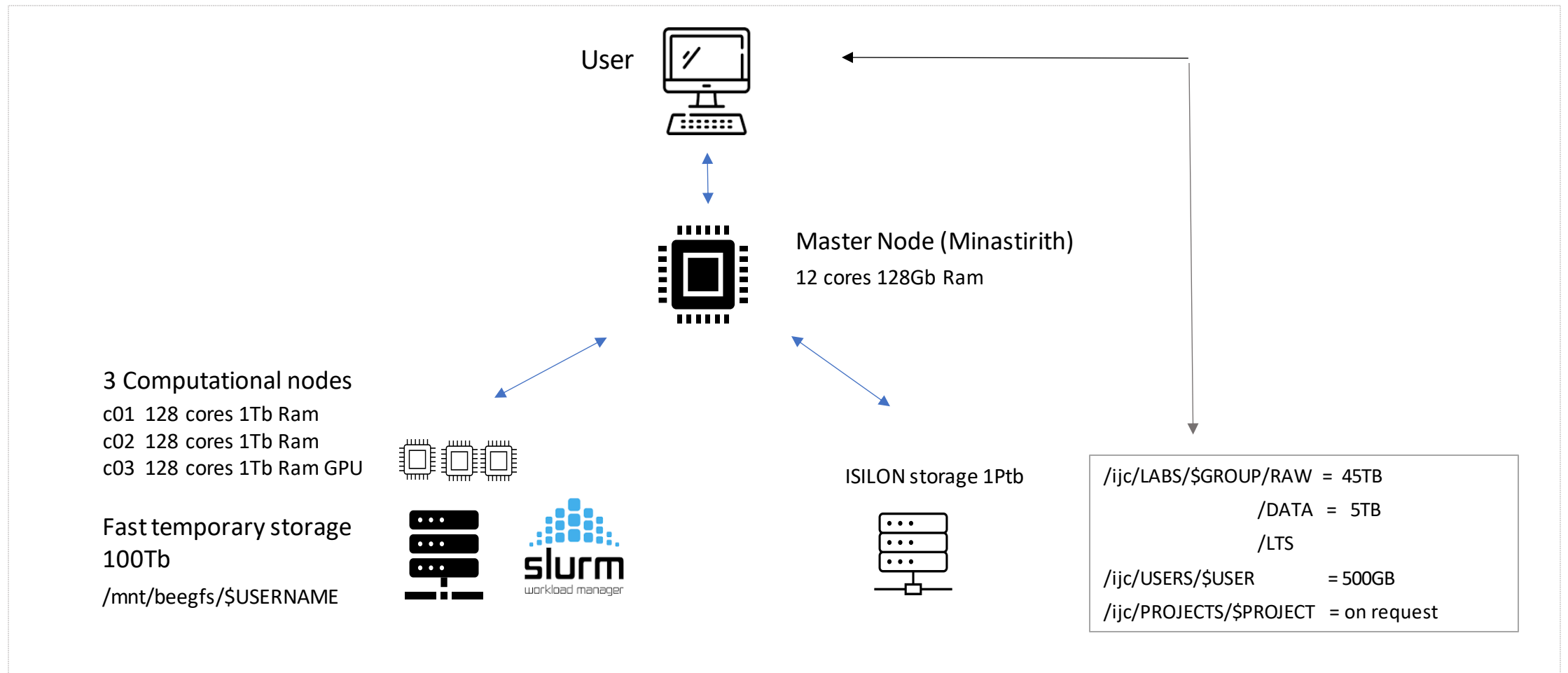


# Cybersecurity best practices

- 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 not 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

### 3. High Performance Computing (HPC)

# HPC cluster

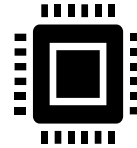


# HPC cluster



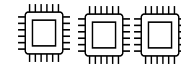
- Master Node (Minastirith)

= connects user, computational nodes (+ flash storage), isilon  
-> Shared resource, do not run your jobs here!



- Computational nodes

= computing (job execution via SLURM)  
-> Shared resource, use wisely!



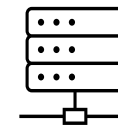
- Flash storage '/ijc/beegfs/'

= attached storage to computational nodes for fast read/write access  
-> Shared resource, for temporary data storage only!



- Isilon

= centralized, backed-up storage  
/ijc/LABS/\$GROUP/RAW = 45TB (raw data, static)  
/DATA = 5TB (analysis data, dynamic)  
/LTS (long term storage, archive data for tape back-up)  
/ijc/USERS/\$USER = 500GB (user directory)  
/ijc/PROJECTS/\$PROJECT = on request (project directory with special permissions created by IT upon request)



# Connecting to the cluster

You can connect to the cluster (master node = 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.

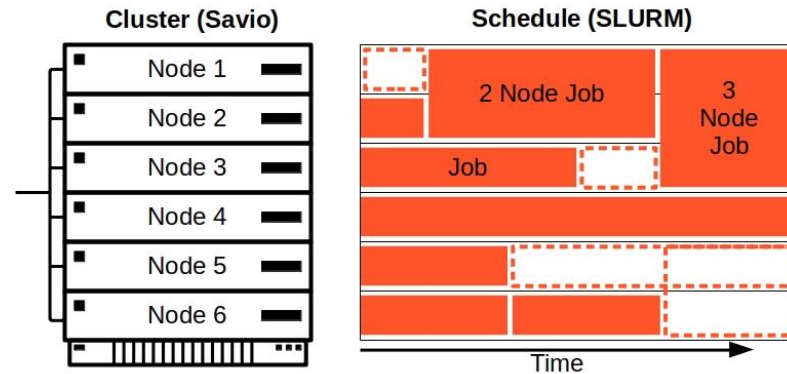
# Using the software

## Available as modules

Description	Command
see all available modules	<code>module avail</code>
load/unload a module	<code>module load/unload</code>
see all loaded modules	<code>module list</code>
unload all modules	<code>module purge</code>

# 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 Name	Max Time	Default Time	Max CPU x Node	Max Mem x CPU	Def Mem x CPU	Max Mem x Node
fast	2 hours	1h	64	4000M	2000M	256000M
highMem	1 Day	1h	8	-	-	800000M
hpc	3 Days	4h	86	200000M	4000M	-

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



# SLURM script

`./my_clusterjob.sh # basic serial job`

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

# Do's & Don't's

## DO

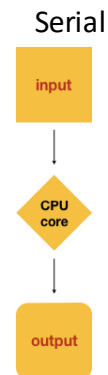
- only request resources that you need
- check if the resources you requested were efficiently used (use `seff -j jobid` or similar)
- check if your job should be submitted to a special queue
- submit resource intensive jobs at low peak times (over night or the weekend)
- break large jobs down into smaller ones
- optimize your code

## DON'T

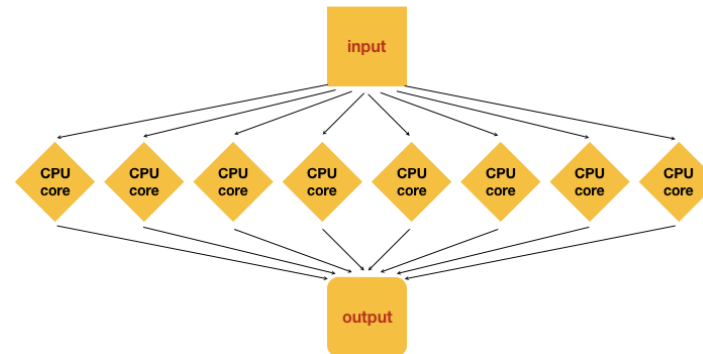
- ask for unnecessary resources (+ 10/15% time or memory are usually sufficient)
- execute any resource intensive task on the master node, use an interactive shell instead
- forget to close your interactive session

# Parallelization increases speed

- 1 Single input +  
· single task

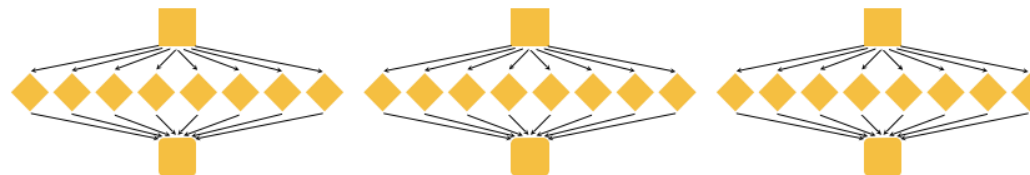


Multithreaded



- 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 workshop pages @:  
[https://ijcbit.github.io/Workshops/Trainings/HPC/Intro to IJC HPC.html](https://ijcbit.github.io/Workshops/Trainings/HPC/Intro%20to%20IJC%20HPC.html)
- Teams: ijcbioinfo
- Bioinfo coffee club: Tuesdays 10.30am cafeteria

Questions?





