Introduction to High Performance Computing

Forschung und Wissenschaftliche Informationsversorgung
IT.SERVICES

RUHR UNIVERSITÄT BOCHUM RUB

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What is High Performance Computing?

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RUB

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High end personal computer:

AMD 6900HX	3.7 TFlops
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High end supercomputers:

El Capitan	1742.00 PFlops
Frontier	1206.00 PFlops
Aurora	1012.00 PFlops

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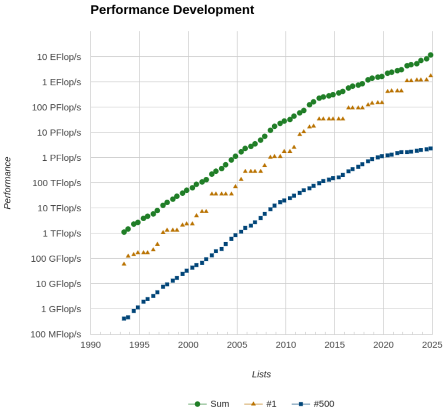
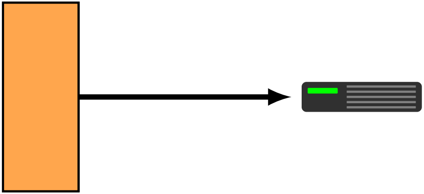
The Fastest Computes



- The performance of the fastest computers grows exponentially.[1]

[1] https://www.top500.org/

How Can an HPC System be so Fast?



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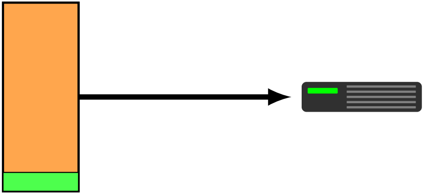

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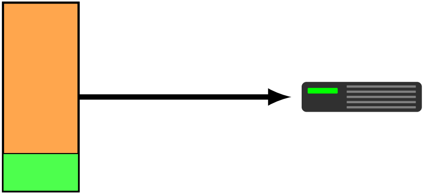

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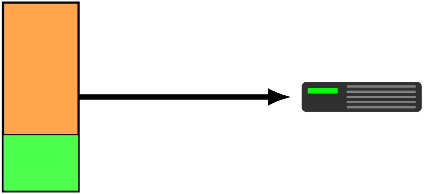

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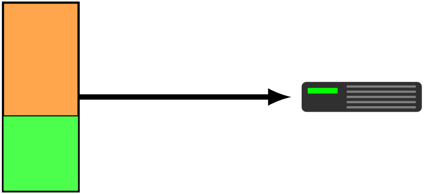

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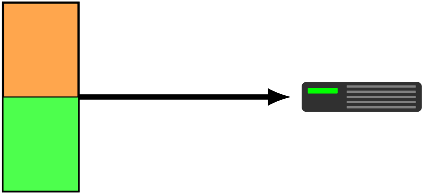

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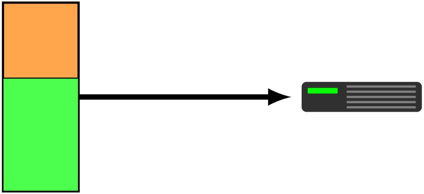

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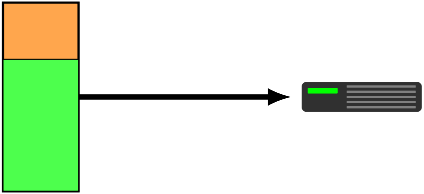

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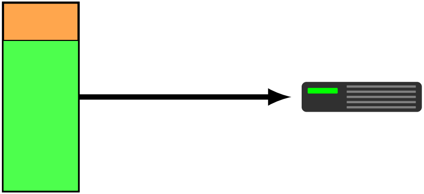

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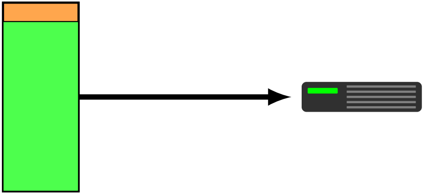

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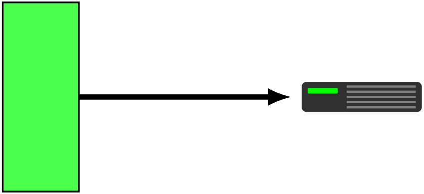

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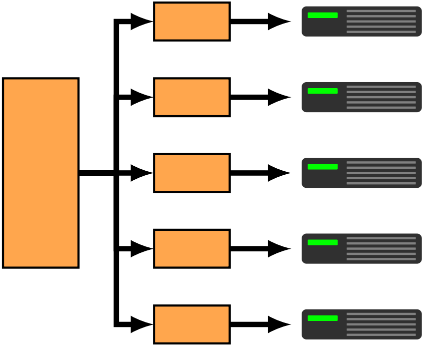

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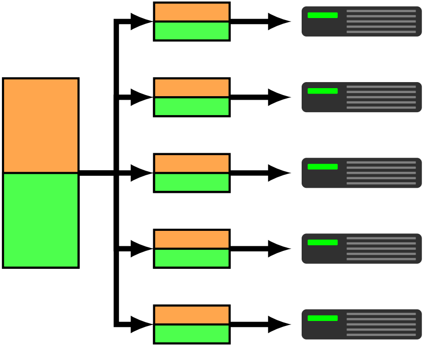

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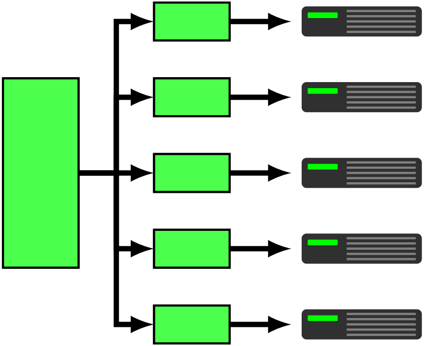

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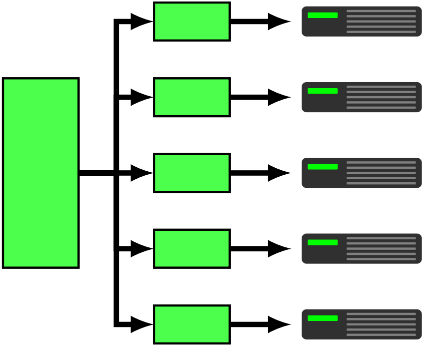

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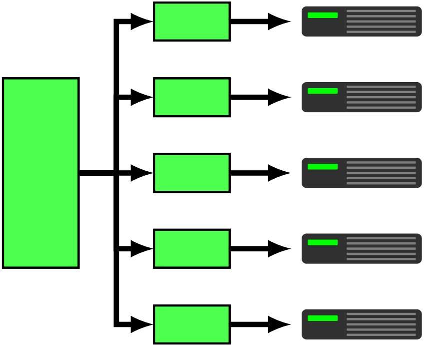

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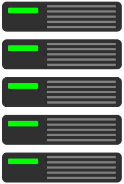
Note that software has to be specifically parallelized to run efficiently on HPC-Systems, which is not trivial!

HPC Cluster Components



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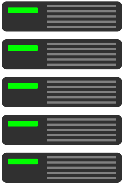

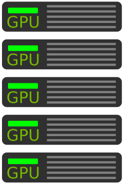

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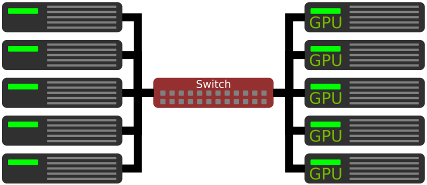

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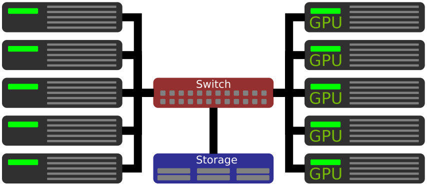

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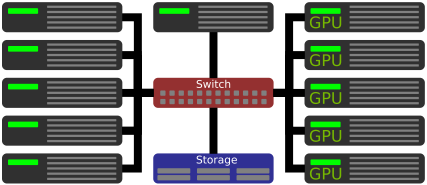

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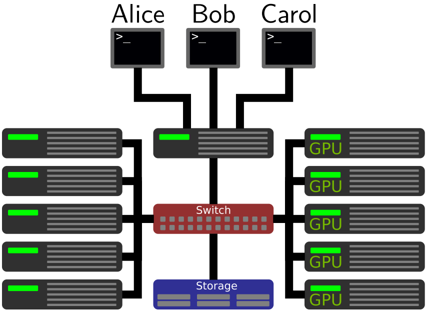

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- Serverrooms host delicate hardware and sensitive data
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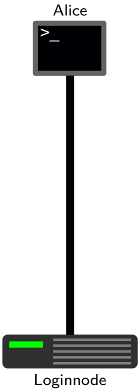
- HPC systems have hundreds of simultanious users
  $\Rightarrow$ Not enough physical space for local user access

How to Access an HPC Cluster?

Remote Access



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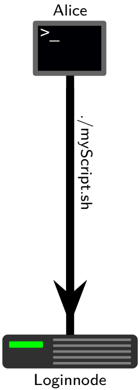

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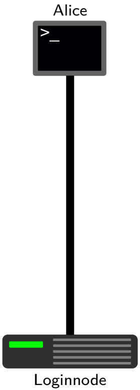

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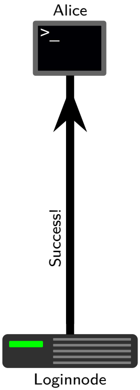
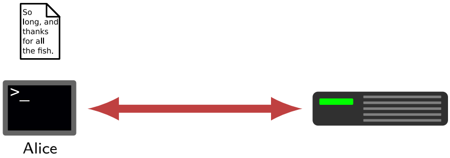


- Linux allows to connect terminals from remote.
- Commands are send over the network to the Cluster
- executed on the cluster
- and output is send back to the users terminal.

Is This Line Secure?



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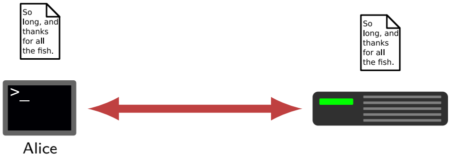

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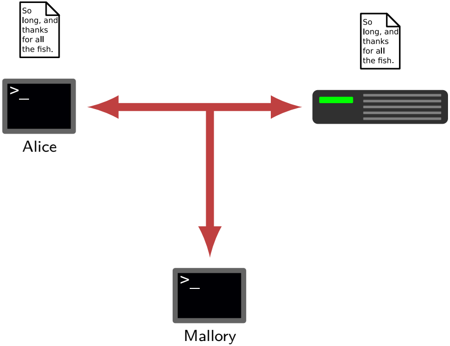

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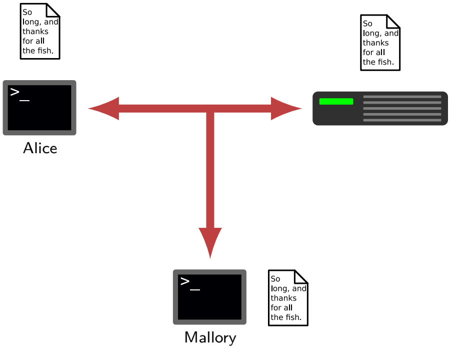

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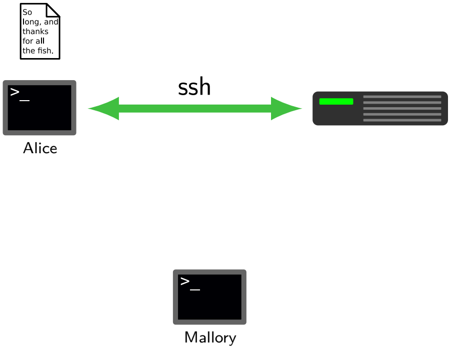

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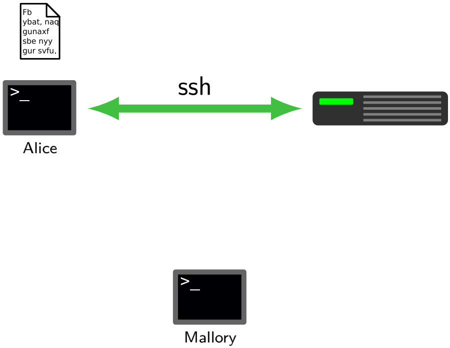

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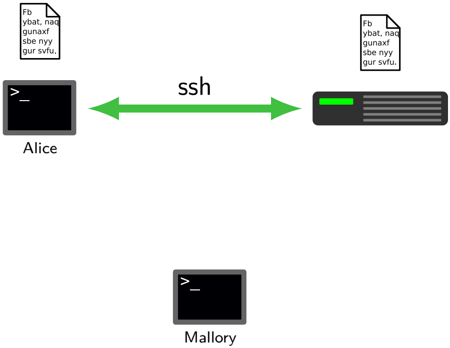

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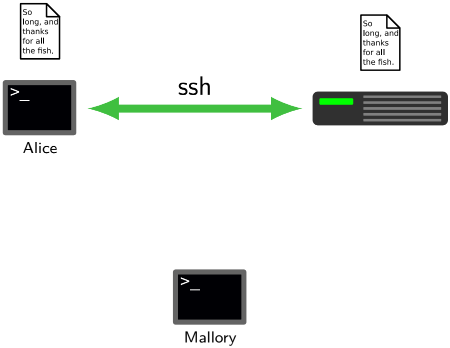

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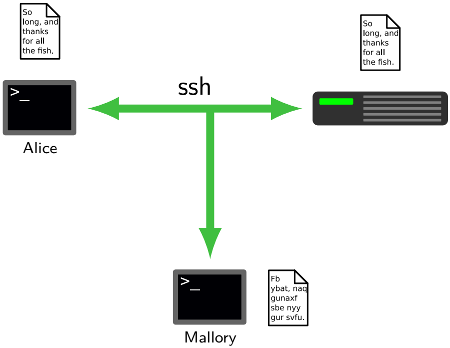

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- ssh copies the file to the cluster.
- ssh decrypts the file on the cluster.
- Mallory snoops the connection to get a copy of the data.
- Mallory cannot decrypt the file.

Access via SSH (Secure Shell)

An `ssh` connection can be established with

`ssh username@ip-address`

Terminal

```
alice@laptop:$ ssh alice@4.669.201.609
Password:
alice@hpc:$
```

Access via SSH (Secure Shell)

Alternatively:

`ssh username@hostname`

Terminal

```
alice@laptop:$ ssh alice@hpc.rub.de
Password:
alice@hpc:$
```

Access via SSH (Secure Shell)

For convenience a connection can be specified in `~/.ssh/config`

Terminal

```
alice@laptop:$ cat ~/.ssh/config
Host hpc-rub
    User alice
    Hostname hpc.rub.de
alice@laptop:$ ssh hpc-rub
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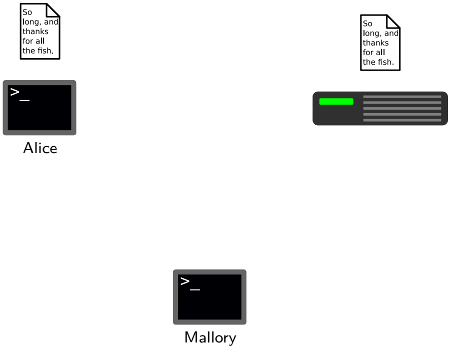

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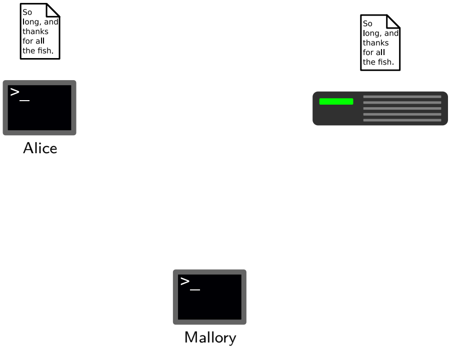

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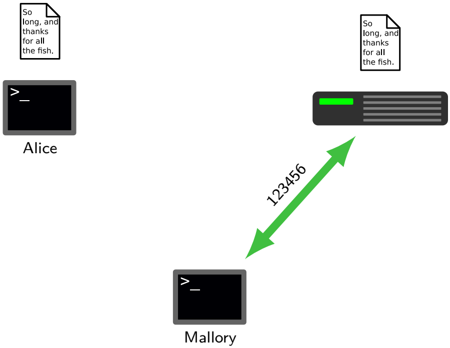

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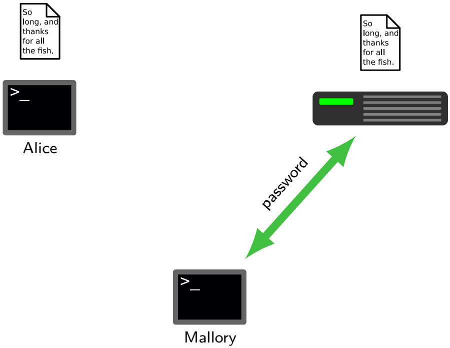

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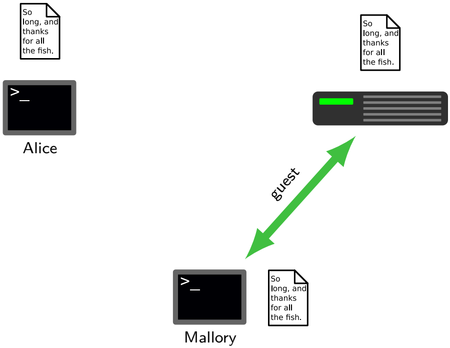

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- Mallory obtains an unencrypted copy of the data.

Public Key Authentication

- Alice generates an "elliptic-curve cryptography key-pair for asymmetric authentication"
  - Public key (green) can only encrypt!
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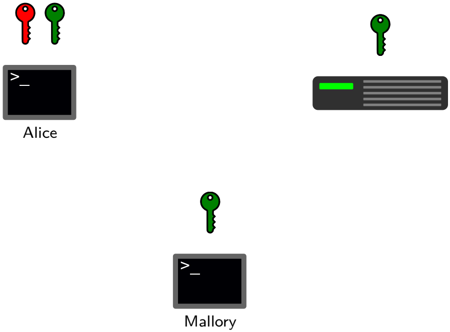

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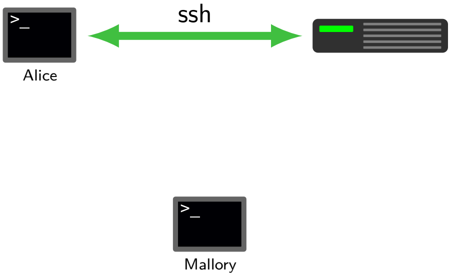

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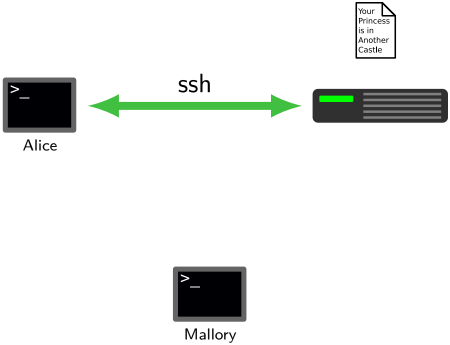

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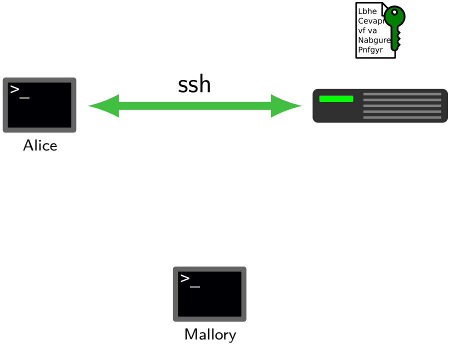

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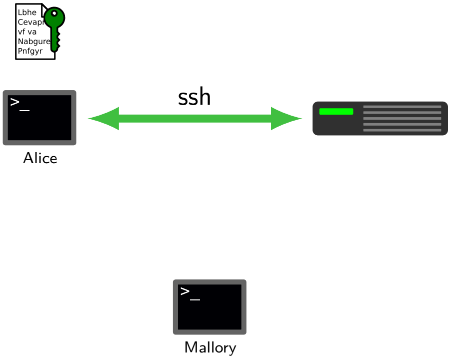

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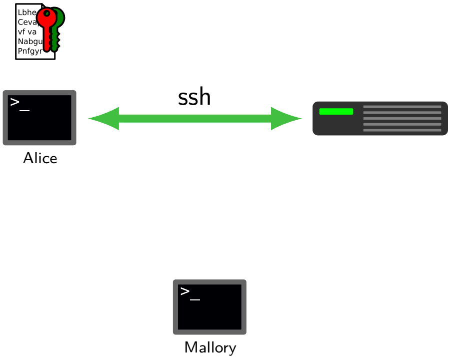

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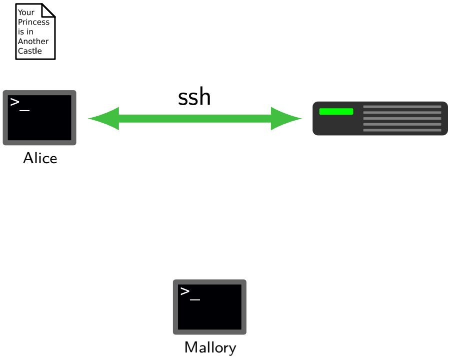
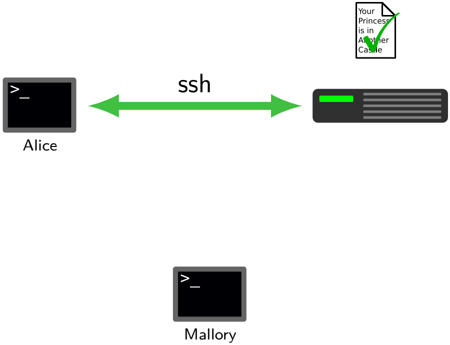
- Alice decrypts the text with her private key.

Public Key Authentication



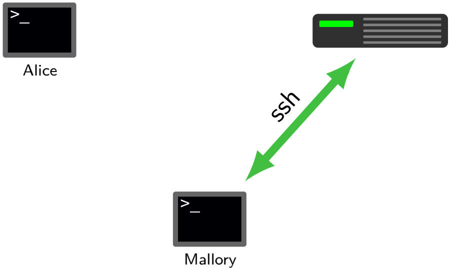
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster encrypts a random text with Alice's publick key and challenges Alice to decrypt it.
- Alice decrypts the text with her private key.

Public Key Authentication



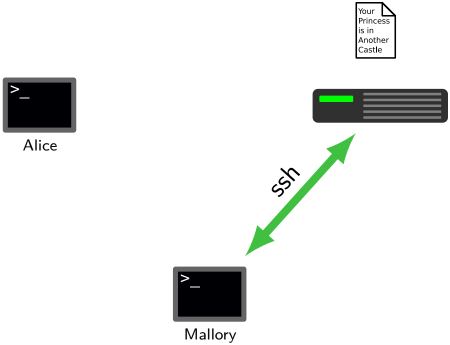
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster encrypts a random text with Alice's publick key and challenges Alice to decrypt it.
- Alice decrypts the text with her private key.
- Alice proved her identity.

Public Key Authentication



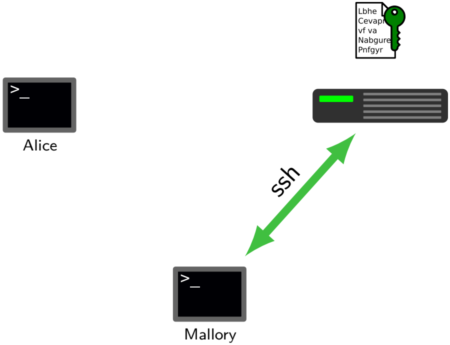
- Mallory establishes an ssh-connection with the HPC cluster.

Public Key Authentication



- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster encrypts a random text with Alice's publick key and challenges Mallory to decrypt it.

Public Key Authentication



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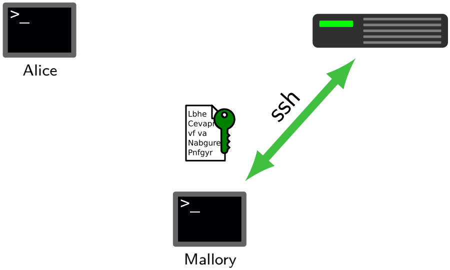
Public Key Authentication



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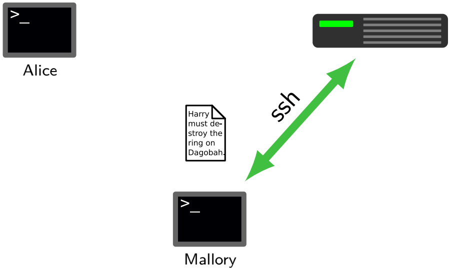
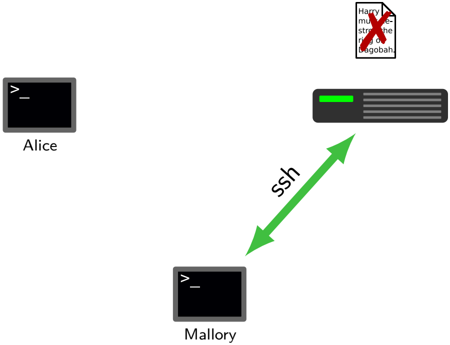
Public Key Authentication



- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster encrypts a random text with Alice's publick key and challenges Mallory to decrypt it.
- Mallory cannot decrypt the text.

Public Key Authentication



- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster encrypts a random text with Alice's publick key and challenges Mallory to decrypt it.
- Mallory cannot decrypt the text.
- Mallory is denied access.

Public Key Authentication

Generating and using an "elliptic-curve cryptography key-pair for asymmetric authentication" sounds hard, but is actually quite easy:

Terminal

```
alice@laptop:$ ssh-keygen -t ed25519 -N "password123!"
```

Public Key Authentication

Linux provides a key generator: `ssh-keygen`

`-t` selects the key-type (e.g.: ed25519 = elliptic curve key).

`-f` specify the filename for the key pair.

`-N` specifies additional passphrase.

Terminal

```
alice@laptop:$ ssh-keygen -t ed25519 -N "password123!"
Generating public/private ed25519 key pair.
Your identification has been saved in /home/alice/.ssh/id_ed25519
Your public key has been saved in /home/alice/.ssh/id_ed25519.pub
The key fingerprint is:
SHA256:yNhMofaDvRHn6AsgI8BNY17yWPRrxGtieQoRa479+SY alice@laptop
...
```

Public Key Authentication

You will find two new files in your `~/.ssh/` directory:

Terminal

```
alice@laptop:$ ls ~/.ssh/
config id_ed25519 id_ed25519.pub
```

Public Key Authentication

RUB

You will find two new files in your `~/.ssh/` directory:

id_ed25519 is your private key.

Terminal

```
alice@laptop:$ ls ~/.ssh/
config id_ed25519 id_ed25519.pub
```

Warning!

Never share your private key!
Not with your coworkers, admins, spouse, or even grandma!

Public Key Authentication

You will find two new files in your `~/.ssh/` directory:

id_ed25519 is your private key.

Terminal

```
alice@laptop:$ cat ~/.ssh/id_ed25519 #(THIS IS NOT MY ACTUAL KEY)
-----BEGIN OPENSSH PRIVATE KEY-----
b3BlbnNzaC1rZXAAAABG5vbmUAAAAEbm9uZQAAAAAAAABAAAAMwAAAAtzc2gtZW
...
-----END OPENSSH PRIVATE KEY-----
```

Warning!

Never share your private key!
Not with your coworkers, admins, spouse, or even grandma!

Public Key Authentication

You will find two new files in your `~/.ssh/` directory:

id_ed25519 is your private key.

id_ed25519.pub is your public key.

Terminal

```
alice@laptop:$ ls ~/.ssh/
config id_ed25519 id_ed25519.pub
```

Not a Warning!

You may share your public key!
Give it to your coworkers, admins, spouse, or even grandma!
Put it on your business card, e-mail signature, t-shirt, billboard.

Public Key Authentication

RUB

You will find two new files in your `~/.ssh/` directory:

id_ed25519	is your private key.
id_ed25519.pub	is your public key.

Terminal

```
alice@laptop:$ cat ~/.ssh/id_ed25519.pub
ssh-ed25519 AAAAC3NzaC1lZDI1NTE5AAAAIOHvm993oC6kwohuHbV0T2xu/x2INIXS2GxFb84s1KbL
alice@laptop
```

Not a Warning!

You may share your public key!
Give it to your coworkers, admins, spouse, or even grandma!
Put it on your business card, e-mail signature, t-shirt, billboard.

Public Key Authentication

The key is automatically used by `ssh`.

Terminal

```
alice@laptop:$ ssh hpc-rub
alice@hpc:$
```

Public Key Authentication

If you have multiple keys, specify `IdentityFile` in your config to use the correct key for the connection.

Terminal

```
alice@laptop:$ cat ~/.ssh/config
Host hpc-rub
    User alice
    Hostname hpc.rub.de
    IdentityFile ~/.ssh/id_ed25519
alice@laptop:$ ssh hpc-rub
alice@hpc:$
```

Exercise 2

1. Generate an elliptic-curve cryptography key-pair for asymmetric authentication
   - Generate in folder `~/.ssh/`
   - Generate an ed25519 key without passphrase
2. Copy the public key to the cluster
   (This is not required for the real HPC-System)
   - use `ssh-copy-id`
   - or write the key in `~/.ssh/authorized_keys` with copy/paste
3. Validate the key usage by connecting to the testcluster again

Exercise 2

RUB

1. Generate an elliptic-curve cryptography key-pair for asymmetric authentication
   - Generate in folder `~/.ssh/`
   - Generate an ed25519 key without passphrase

Terminal

```
alice@laptop:$ ssh-keygen -t ed25519 -N "" -f ~/.ssh/testcluster
```

Exercise 2

2 Copy the public key to the cluster
(This is not required for the real HPC-System)
  - use `ssh-copy-id`

Terminal

```
alice@laptop:$ ssh-copy-id -i ~/.ssh/testcluster testuser@134.147.41.133
```

Exercise 2

2 Copy the public key to the cluster
(This is not required for the real HPC-System)
   - use `ssh-copy-id`
   - or write the key in `~/.ssh/authorized_keys` with copy/paste

Terminal

```
alice@laptop:$ ssh-copy-id -i ~/.ssh/testcluster testuser@134.147.41.133
alice@hpc:$ nano ~/.ssh/authorized_keys
```

3 Validate the key usage by connecting to the testcluster again

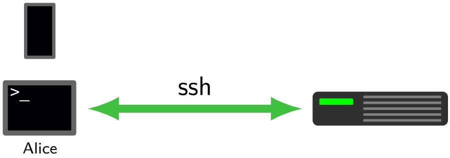
Terminal

```
alice@laptop:$ ssh testuser@134.147.41.133
alice@hpc:$
```

Two-Factor Authentication

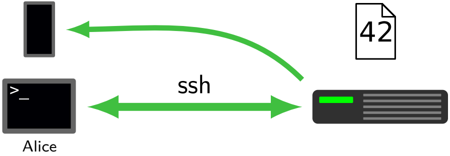
- Alice enables two-factor-authentication with her mobile phone.

Two-Factor Authentication



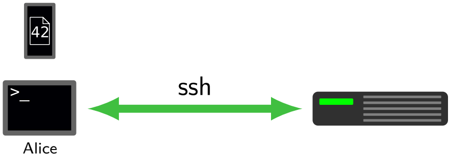
- Alice establishes an ssh-connection with the HPC cluster.

Two-Factor Authentication



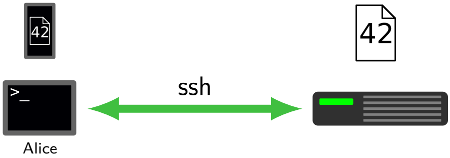
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.

Two-Factor Authentication



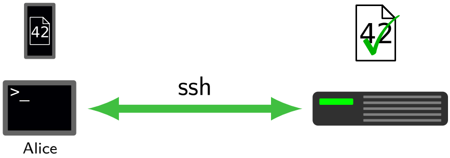
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.

Two-Factor Authentication



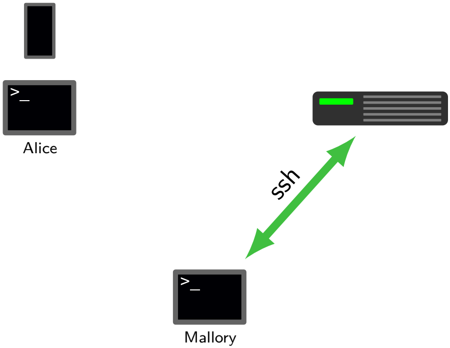
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.
- Alice sends the number to the cluster via ssh.

Two-Factor Authentication



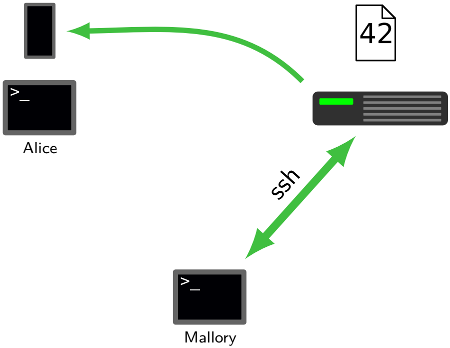
- Alice establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.
- Alice sends the number to the cluster via ssh.
- Alice proved her identity.

Two-Factor Authentication



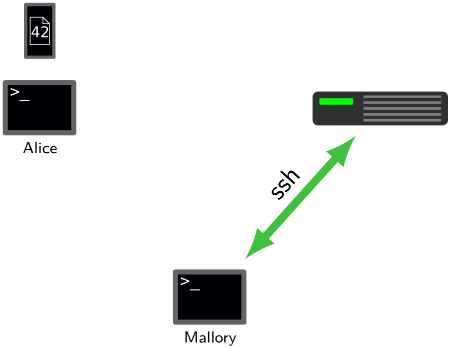
- Mallory establishes an ssh-connection with the HPC cluster.

Two-Factor Authentication



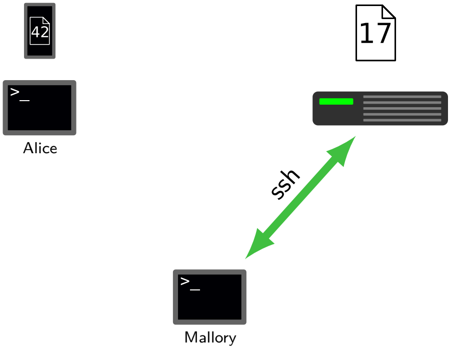
- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.

Two-Factor Authentication



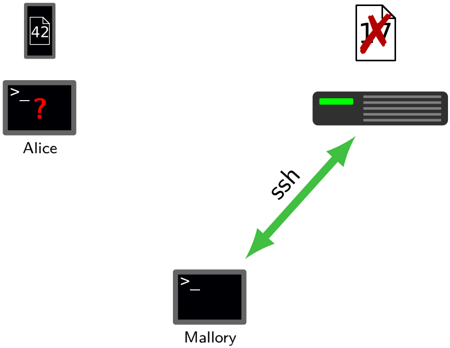
- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.

Two-Factor Authentication



- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.
- Mallory guesses the number.

Two-Factor Authentication



- Mallory establishes an ssh-connection with the HPC cluster.
- The cluster sends a random number to Alice's mobile phone.
- Mallory guesses the number.
- Mallory is denied access (and Alice is left confused).

Datatransfer from/to HPC Clusters

Review of cp

Terminal

```
alice@laptop:$ cp source destination
```

- The `cp` command copies a file given by `source` to `destination`

Review of cp

Terminal

```
alice@laptop:$ cp -r source destination
```

- The `cp` command copies a file given by `source` to `destination`
- The `-r` flag copies recursively, thus allowing copying of directories and their content

Review of cp

Terminal

```
alice@laptop:$ cp --help
```

- The `cp` command copies a file given by `source` to `destination`
- The `-r` flag copies recursively, thus allowing copying of directories and their content
- Consult the `--help` flag for more available options

SSH-copy

Terminal

```
alice@laptop:$ scp source destination
```

- Prepending an “s” to the `cp` command enables copies from/to remote machines

SSH-copy

Terminal

```
alice@laptop:$ scp myData username@ip-address:~/myProject/
```

- Prepending an "s" to the cp command enables copies from/to remote machines
- Remote locations are prefixed by the username and IP/hostname

SSH-copy

Terminal

```
alice@laptop:$ scp username@ip-address:~/myProject/myData .
```

- Prepending an “s” to the cp command enables copies from/to remote machines
- Remote locations are prefixed by the username and IP/hostname

SSH-copy

Terminal

```
alice@laptop:$ scp -r username@ip-address:~/myProject .
```

- Prepending an "`s`" to the `cp` command enables copies from/to remote machines
- Remote locations are prefixed by the username and IP/hostname
- The `-r` flag copies recursively, thus allowing copying of directories and their content

SSH-copy

Terminal

```
alice@laptop:$ scp --help
```

- Prepending an "`s`" to the `cp` command enables copies from/to remote machines
- Remote locations are prefixed by the username and IP/hostname
- The `-r` flag copies recursively, thus allowing copying of directories and their content
- Consult the `--help` flag for more available options

Terminal

```
alice@laptop:$ rsync source destination
```

- `rsync` functions similarly to `scp`, but adds many quality of life features

Terminal

```
alice@laptop:$ rsync -r username@ip-address:~/myProject .
```

- `rsync` functions similarly to `scp`, but adds many quality of life features

rsync

Terminal

```
alice@laptop:$ rsync --bwlimit=1024 username@ip-address:~/myProject .
```

- `rsync` functions similarly to `scp`, but adds many quality of life features
- `--bwlimit=RATE` limits the transfer speed by RATE KiBit/s

Terminal

```
alice@laptop:$ rsync --progress username@ip-address:~/myProject .
```

- `rsync` functions similarly to `scp`, but adds many quality of life features
- `--bwlimit=RATE` limits the transfer speed by RATE KiBit/s
- `--progress` gives live updates on copy

Terminal

```
alice@laptop:$ rsync --compress username@ip-address:~/myProject .
```

- `rsync` functions similarly to `scp`, but adds many quality of life features
- `--bwlimit=RATE` limits the transfer speed by RATE KiBit/s
- `--progress` gives live updates on copy
- `--compress` compresses data for transfer

rsync

Terminal

```
alice@laptop:$ rsync --checksum username@ip-address:~/myProject .
```

- `rsync` functions similarly to `scp`, but adds many quality of life features
- `--bwlimit=RATE` limits the transfer speed by RATE KiBit/s
- `--progress` gives live updates on copy
- `--compress` compresses data for transfer
- `--checksum` checks if data was already transferred with checksums

Terminal

```
alice@laptop:$ rsync --help
```

- `rsync` functions similarly to `scp`, but adds many quality of life features
- `--bwlimit=RATE` limits the transfer speed by RATE KiBit/s
- `--progress` gives live updates on copy
- `--compress` compresses data for transfer
- `--checksum` checks if data was already transferred with checksums
- Consult the `--help` flag for more available options

How to Inefficiently Transfer Files

RUB

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$
```

- Alice has a lot of files

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ for i in *; do rsync ${i} alice@141.421.356.23:~/ ;done
```

- Alice has a lot of files
- Alice loops over the files and starts an `rsync` for each

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

RUB

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ for i in *; do rsync ${i} alice@141.421.356.23:~/ ;done
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- Alice has a lot of files
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- Each file transfer requires:

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- Each file transfer requires:
  - establishing connection

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How to Inefficiently Transfer Files

Terminal

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alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ for i in *; do rsync ${i} alice@141.421.356.23:~/ ;done
```

- Alice has a lot of files
- Alice loops over the files and starts an `rsync` for each
- Each file transfer requires:
  - establishing connection
  - key exchange and key authentication

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ for i in *; do rsync ${i} alice@141.421.356.23:~/ ;done
```

- Alice has a lot of files
- Alice loops over the files and starts an `rsync` for each
- Each file transfer requires:
  - establishing connection
  - key exchange and key authentication
  - file transfer initialization and finalization

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ rsync * alice@141.421.356.23:~/
```

- Alice has a lot of files

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

RUB

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ rsync * alice@141.421.356.23:~/
```

- Alice has a lot of files
- Alice starts rsync with a wildcard for the files

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

RUB

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ rsync * alice@141.421.356.23:~/
```

- Alice has a lot of files
- Alice starts rsync with a wildcard for the files
- Each file transfer requires:

Warning!

Do not do this, as it is inefficient!

How to Inefficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ rsync * alice@141.421.356.23:~/
```

- Alice has a lot of files
- Alice starts rsync with a wildcard for the files
- Each file transfer requires:
  - file transfer initialization and finalization

Warning!

Do not do this, as it is inefficient!

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$
```

- Alice has a lot of files

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
alice@laptop:$ rsync files.tar alice@141.421.356.23:~/
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files
- Alice transfers one big file

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
alice@laptop:$ rsync files.tar alice@141.421.356.23:~/
alice@laptop:$ ssh alice@141.421.356.23
alice@hpc:$ tar -xvf files.tar
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files
- Alice transfers one big file

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
alice@laptop:$ rsync files.tar alice@141.421.356.23:~/
alice@laptop:$ ssh alice@141.421.356.23
alice@hpc:$ tar -xvf files.tar
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files
- Alice transfers one big file and extracts it on the cluster
- This is efficient because:

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
alice@laptop:$ rsync files.tar alice@141.421.356.23:~/
alice@laptop:$ ssh alice@141.421.356.23
alice@hpc:$ tar -xvf files.tar
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files
- Alice transfers one big file and extracts it on the cluster
- This is efficient because:
  - Minimizes `rsync` and file transfer overhead

How to Efficiently Transfer Files

Terminal

```
alice@laptop:$ ls -l | wc -l
65537
alice@laptop:$ tar -cvf files.tar *
alice@laptop:$ rsync files.tar alice@141.421.356.23:~/
alice@laptop:$ ssh alice@141.421.356.23
alice@hpc:$ tar -xvf files.tar
```

- Alice has a lot of files
- Alice creates a `tar` archive with her files
- Alice transfers one big file and extracts it on the cluster
- This is efficient because:
  - Minimizes `rsync` and file transfer overhead
  - Enables cross-file compression

SLURM: Simple Linux Utility for Resource Management

What is SLURM?

SLURM is:

https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Slurm_logo.svg/2238px-Slurm_logo.svg.png

What is SLURM?

SLURM is:

- A resource manager.

https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Slurm_logo.svg/2238px-Slurm_logo.svg.png

What is SLURM?

SLURM is:

- A resource manager.
- A scheduler.

https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Slurm_logo.svg/2238px-Slurm_logo.svg.png

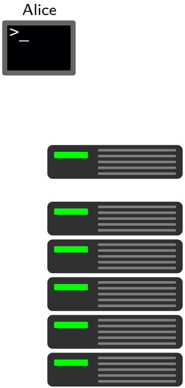
What is SLURM?

SLURM is:

- A resource manager.
- A scheduler.
- An accountant.

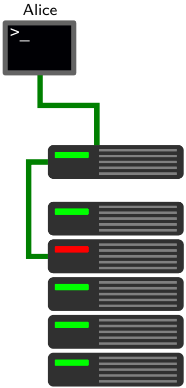
https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Slurm_logo.svg/2238px-Slurm_logo.svg.png

SLURM as Resource Manager



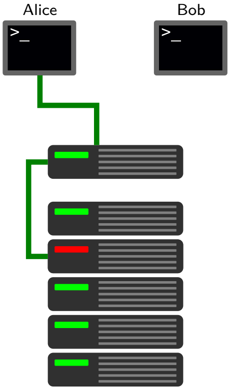
Alice is conducting Research on an HPC cluster.

SLURM as Resource Manager



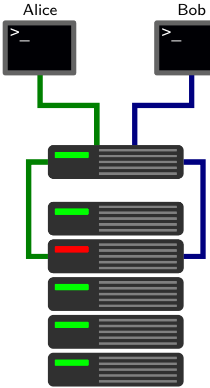
Alice connects to a compute node.

SLURM as Resource Manager



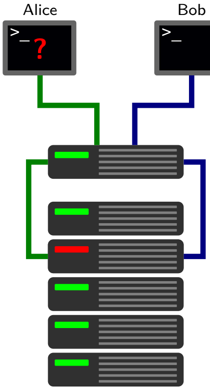
Bob is conducting Research on an HPC cluster.

SLURM as Resource Manager



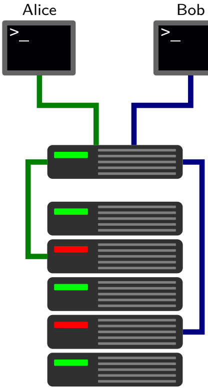
Bob forgets which node was dedicated to him and accidentially connects to the same one as Alice.

SLURM as Resource Manager



Alice wonders why her calculation slows down. Bob accidentially interferes with Alice's research.

SLURM as Resource Manager



Solution:
Alice and Bob request a free node from the SLURM resource manager on the login node.

SLURM as Resource Manager: Available Nodes?

`sinfo` gives a list of all nodes and their status:

Terminal

```
alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
first-nodes    up 2-00:00:00     2  idle  cpu01,gpu01
cpu-nodes      up 2-00:00:00     3  idle  cpu[01,02,04]
cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

SLUMR as Resource Manager: Available Nodes?

RUB

`sinfo` gives a list of all nodes and their status:

Terminal

```
alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
first-nodes    up 2-00:00:00     2  idle  cpu01,gpu01
cpu-nodes      up 2-00:00:00     3  idle  cpu[01,02,04]
cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

PARTITION — Name of a set of nodes of similar type. Allows for hardware specific requests.
A node can be part of multiple partitions.

SLURM as Resource Manager: Available Nodes?

`sinfo` gives a list of all nodes and their status:

Terminal

```
alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
first-nodes    up 2-00:00:00     2  idle  cpu01,gpu01
cpu-nodes      up 2-00:00:00     3  idle  cpu[01,02,04]
cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

AVAIL Availability of a partition (Up, down, ...).

SLURM as Resource Manager: Available Nodes?

`sinfo` gives a list of all nodes and their status:

Terminal

```
alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
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cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

TIMELIMIT
: Maximum time for a resource request (job) in in this partition. Format: dd-hh:mm:ss

SLURM as Resource Manager: Available Nodes?

RUB

`sinfo` gives a list of all nodes and their status:

Terminal

```
alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
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cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

NODES Number of nodes in this partition.

SLURM as Resource Manager: Available Nodes?

`sinfo` gives a list of all nodes and their status:

Terminal

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alice@hpc:$ sinfo
PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
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cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

STATE Current operation status of nodes in this partition:
idle: Node is waiting for work.
alloc: Node is allocated and busy.
down: Node is unreachable.

SLURM as Resource Manager: Available Nodes?

`sinfo` gives a list of all nodes and their status:

Terminal

```
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PARTITION   AVAIL  TIMELIMIT NODES STATE  NODELIST
first-nodes    up 2-00:00:00     2  idle  cpu01,gpu01
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cpu-nodes      up 2-00:00:00     1  alloc cpu03
gpu-nodes      up 2-00:00:00     2  idle  gpu[01-02]
```

NODELIST List of nodes in the partition in compressed form.
node[1-3,6-7]: node1, node2, node3, node6, node7

SLURM as Resource Manager: Requesting Interactive Jobs

`srun` can be used to request resources for an interactive session:

Terminal

```
alice@hpc:$ srun -p gpu-nodes --time=30:00 --pty bash
alice@gpu1:$
```

SLURM as Resource Manager: Requesting Interactive Jobs

`srun` can be used to request resources for an interactive session:

Terminal

```
alice@hpc:$ srun -p gpu-nodes --time=30:00 --pty bash
alice@gpu1:$
```

-p/--partition Partition to request a node from.

SLURM as Resource Manager: Requesting Interactive Jobs

`srun` can be used to request resources for an interactive session:

Terminal

```
alice@hpc:$ srun -p gpu-nodes --time=30:00 --pty bash
alice@gpu1:$
```

-p/--partition Partition to request a node from.

-t/--time Maximum time the job will run.

SLURM as Resource Manager: Requesting Interactive Jobs

`srun` can be used to request resources for an interactive session:

Terminal

```
alice@hpc:$ srun -p gpu-nodes --time=30:00 --pty bash
alice@gpu1:$
```

-p/--partition	Partition to request a node from.
-t/--time	Maximum time the job will run.
--pty	Run with pseudoterminal

SLURM as Resource Manager: Requesting Interactive Jobs

`srun` can be used to request resources for an interactive session:

Terminal

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```

-p/--partition	Partition to request a node from.
-t/--time	Maximum time the job will run.
--pty	Run with pseudoterminal
bash	run a bash shell

SLURM as Resource Manager: Requesting Interactive Jobs

RUB

`srun` can be used to request resources for an interactive session:

Terminal

```
alice@hpc:$ srun -p gpu-nodes --time=30:00 --pty bash
alice@gpu1:$
```

-p/--partition	Partition to request a node from.
-t/--time	Maximum time the job will run.
--pty	Run with pseudoterminal
bash	run a bash shell
	All flags at https://slurm.schedmd.com/srun.html

SLURM as Resource Manager: Requesting Batch Jobs

`sbatch` can be used to request resources for scripted job.

Terminal

```
alice@hpc:$ sbatch -p gpu-nodes --time=30:00 myscript.sh
Submitted batch job 1337
```

SLURM as Resource Manager: Requesting Batch Jobs

`sbatch` can be used to request resources for scripted job.

Terminal

```
alice@hpc:$ sbatch -p gpu-nodes --time=30:00 myscript.sh
Submitted batch job 1337
```

- `myscript.sh` will be executed on the nodes.

SLURM as Resource Manager: Requesting Batch Jobs

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Submitted batch job 1337
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- `myscript.sh` will be executed on the nodes.
- Each batch job is assigned a unique ID (e.g. 1337).

SLURM as Resource Manager: Requesting Batch Jobs

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Submitted batch job 1337
```

- `myscript.sh` will be executed on the nodes.
- Each batch job is assigned a unique ID (e.g. 1337).
- Output and errors will be written to `slurm-${SLURM_JOB_ID}.out/err`

SLURM as Resource Manager: Requesting Batch Jobs

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Terminal

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Submitted batch job 1337
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- `myscript.sh` will be executed on the nodes.
- Each batch job is assigned a unique ID (e.g. 1337).
- Output and errors will be written to `slurm-${SLURM_JOB_ID}.out/err`
- Set output/error files with `--output=`/`--error=` flags.

SLURM as Resource Manager: Requesting Batch Jobs

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Terminal

```
alice@hpc:$ sbatch -p gpu-nodes --time=30:00 myscript.sh
Submitted batch job 1337
```

- `myscript.sh` will be executed on the nodes.
- Each batch job is assigned a unique ID (e.g. 1337).
- Output and errors will be written to `slurm-${SLURM_JOB_ID}.out/err`
- Set output/error files with `--output=`/`--error=` flags.
- All flags at https://slurm.schedmd.com/sbatch.html

All valid `sbatch`-flags can also be incorporated into the script itself:

Terminal

```
alice@hpc:$ cat myscript.sh
#!/bin/bash
#SBATCH --output=TestJob.out
#SBATCH --error=TestJob.err
#SBATCH --time=00:10:00
#SBATCH --partition=cpu-nodes
...
alice@hpc:$ sbatch myscript.sh
```

SLURM as Resource Manager: Requesting Batch Jobs

All valid `sbatch`-flags can also be incorporated into the script itself:

Terminal

```
alice@hpc:$ cat myscript.sh
#!/bin/bash
#SBATCH --output=TestJob.out
#SBATCH --error=TestJob.err
#SBATCH --time=00:10:00
#SBATCH --partition=cpu-nodes
...
alice@hpc:$ sbatch myscript.sh
```

This is called the SLURM-Header.

SLURM as Resource Manager: Requesting Batch Jobs

All valid `sbatch`-flags can also be incorporated into the script itself:

Terminal

```
alice@hpc:$ cat myscript.sh
#!/bin/bash
#SBATCH --output=TestJob.out
#SBATCH --error=TestJob.err
#SBATCH --time=00:10:00
#SBATCH --partition=cpu-nodes
...
alice@hpc:$ sbatch myscript.sh
```

This is called the SLURM-Header.

`#!/bin/bash` The script interpreter should be `bash`.

SLURM as Resource Manager: Requesting Batch Jobs

All valid `sbatch`-flags can also be incorporated into the script itself:

Terminal

```
alice@hpc:$ cat myscript.sh
#!/bin/bash
#SBATCH --output=TestJob.out
#SBATCH --error=TestJob.err
#SBATCH --time=00:10:00
#SBATCH --partition=cpu-nodes
...
alice@hpc:$ sbatch myscript.sh
```

This is called the SLURM-Header.

`#!/bin/bash` The script interpreter should be `bash`.

`#SBATCH` Ignored by the interpreter, but parsed by `sbatch`.

SLURM as Resource Manager: Canceling/Deleting Jobs

Mistakes happen to everyone!
If you accidentially submitted a job and want to cancel it (running or pending) you can use the `scancel` command.

Terminal

```
alice@hpc:$ scancel 1337
alice@hpc:$
```

SLURM as Resource Manager: Canceling/Deleting Jobs

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If you accidentially submitted a job and want to cancel it (running or pending) you can use the `scancel` command.

Terminal

```
alice@hpc:$ scancel 1337
alice@hpc:$
```

- Job with the jobid 1337 will be stopped (if possible)

SLURM as Resource Manager: Canceling/Deleting Jobs

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If you accidentially submitted a job and want to cancel it (running or pending) you can use the `scancel` command.

Terminal

```
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- Job with the jobid 1337 will be stopped (if possible)
- You can only cancel your own jobs!

Mistakes happen to everyone!
If you accidentially submitted a job and want to cancel it (running or pending) you can use the `scancel` command.

Terminal

```
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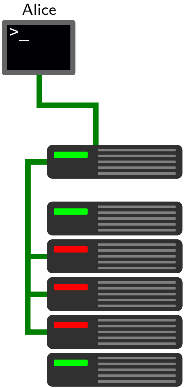
alice@hpc:$
```

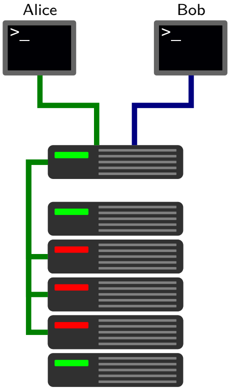
- Job with the jobid 1337 will be stopped (if possible)
- You can only cancel your own jobs!
- All flags at https://slurm.schedmd.com/scancel.html

SLURM as Scheduler



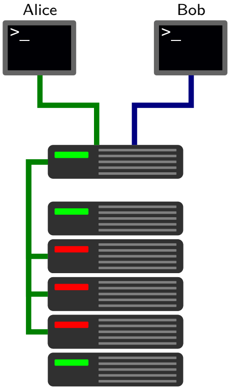
Alice' job occupies several nodes.

SLURM as Scheduler



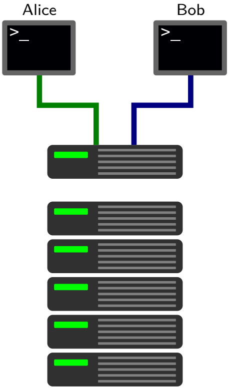
There are not enough free nodes left for Bob's job.

SLURM as Scheduler



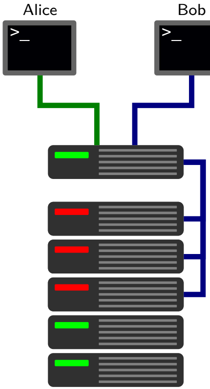
SLURM put Bob's job on hold until the required resources are available.

SLURM as Scheduler



SLURM put Bob's job on hold until the required resources are available.

SLURM as Scheduler



SLURM put Bob's job on hold until the required resources are available.

SLURM as Scheduler: Job-Queue

`squeue` gives a list of all running and pending jobs:

Terminal

```
alice@hpc:$ squeue
JOBID PARTITION NAME  USER  ST TIME NODES NODELIST(REASON)
6886  cpu-nodes check bob   PD 0:00     1 (Resources)
6882  cpu-nodes sim   alice  R 1:37     1 cpu01
6883  cpu-nodes calc  carol  R 0:42     1 cpu02 ...
```

SLURM as Scheduler: Job-Queue

`squeue` gives a list of all running and pending jobs:

Terminal

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JOBID PARTITION NAME  USER  ST TIME NODES NODELIST(REASON)
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6883  cpu-nodes calc  carol  R 0:42     1 cpu02 ...
```

JOBID Unique ID for this job

SLURM as Scheduler: Job-Queue

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Terminal

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6883  cpu-nodes calc  carol  R 0:42     1 cpu02 ...
```

PARTITION Partition the job is running on.

SLURM as Scheduler: Job-Queue

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```

NAME Name given to job by user via the `--job-name=` flag.

SLURM as Scheduler: Job-Queue

squeue gives a list of all running and pending jobs:

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JOBID PARTITION NAME  USER  ST TIME NODES NODELIST(REASON)
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6882  cpu-nodes sim   alice  R 1:37     1 cpu01
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```

USER User who submitted/started the job.

SLURM as Scheduler: Job-Queue

`squeue` gives a list of all running and pending jobs:

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```

ST Status of the Job. Most important statuses are:

- **R** Running
- **PD** Pending
- **CG** Completing

SLURM as Scheduler: Job-Queue

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```

TIME Time the job is already running.

SLURM as Scheduler: Job-Queue

`squeue` gives a list of all running and pending jobs:

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```

NODES Number of nodes allocated to this job.

SLURM as Scheduler: Job-Queue

`squeue` gives a list of all running and pending jobs:

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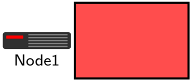
```

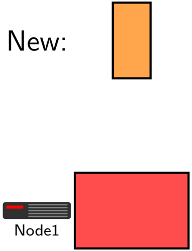
NODELIST(REASON) List of nodes allocated to the job.
Or reason why the job is not running (e.g. Resources).

New:



Backfill-Scheduling for one node:

SLURM as Scheduler: Singlenode Scheduling

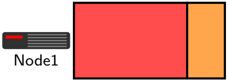


Backfill-Scheduling for one node:

- Append new jobs as they come in.

SLURM as Scheduler: Singlenode Scheduling

New:



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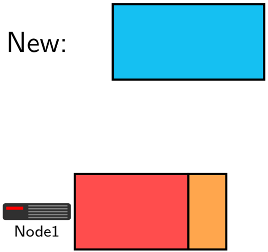
SLURM as Scheduler: Singlenode Scheduling



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SLURM as Scheduler: Singlenode Scheduling

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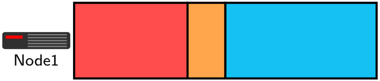

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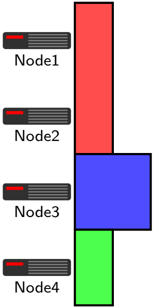
SLURM as Scheduler: Multinode Scheduling

New:



Backfill-Scheduling for multiple nodes:

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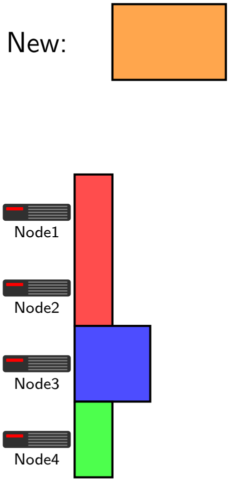
SLURM as Scheduler: Multinode Scheduling



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SLURM as Scheduler: Multinode Scheduling

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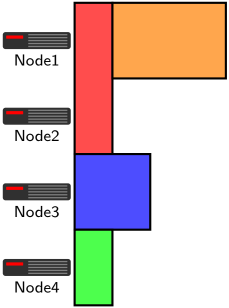

Backfill-Scheduling for multiple nodes:

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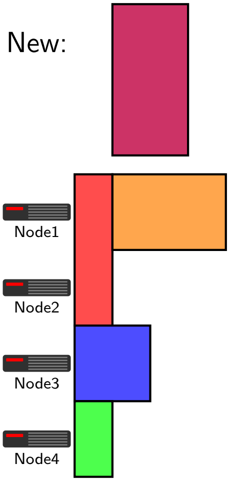
SLURM as Scheduler: Multinode Scheduling



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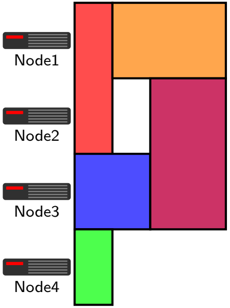

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SLURM as Scheduler: Multinode Scheduling

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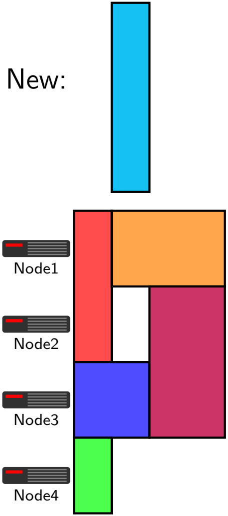

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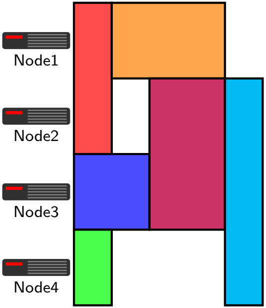
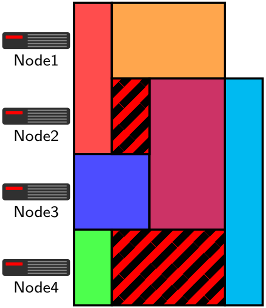


Backfill-Scheduling for multiple nodes:

- Append new jobs as they come in.

SLURM as Scheduler: Multinode Scheduling

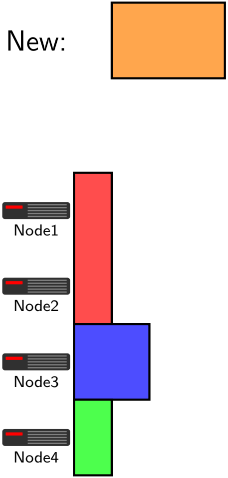
New:



Backfill-Scheduling for multiple nodes:

- Append new jobs as they come in.
- This can leave gaps in the schedule and lead to idle times.

SLURM as Scheduler: Multinode Scheduling

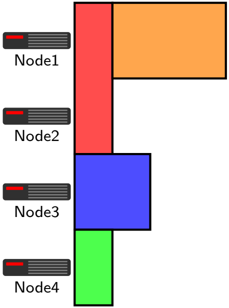


Intelligent scheduling for multiple nodes:

- Append new jobs as they come in.

SLURM as Scheduler: Multinode Scheduling

New:



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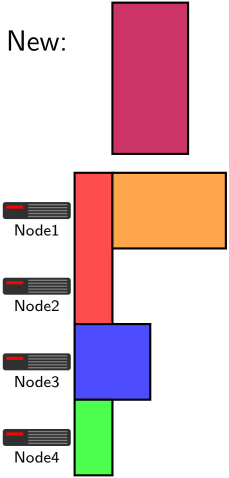
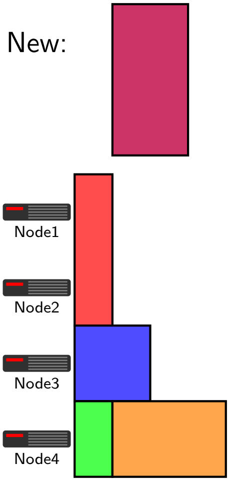
SLURM as Scheduler: Multinode Scheduling



Intelligent scheduling for multiple nodes:

- Append new jobs as they come in.
- Reorganize queued jobs to minimize idle times.

SLURM as Scheduler: Multinode Scheduling



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SLURM as Scheduler: Multinode Scheduling

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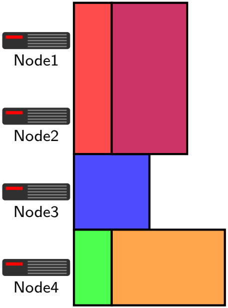

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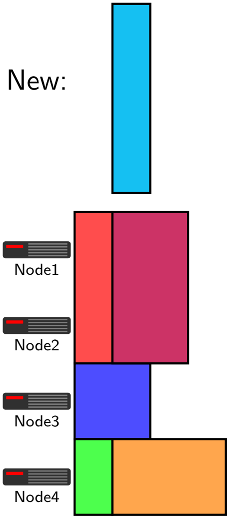

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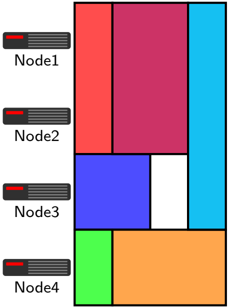

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SLURM as Scheduler: Multinode Scheduling

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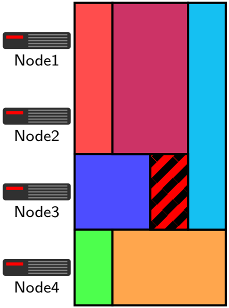
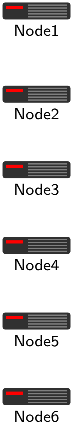


Intelligent scheduling for multiple nodes:

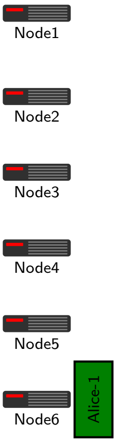
- Append new jobs as they come in.
- Reorganize queued jobs to minimize idle times.
- Leaves fewer and smaller gaps than Backfilling.
- Relies on realistic runtime estimates by users.

SLURM as Accountant: Sharing Computing Time



Alice submits a huge amount of jobs.

SLURM as Accountant: Sharing Computing Time



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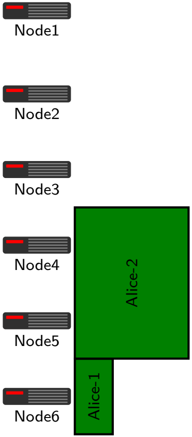

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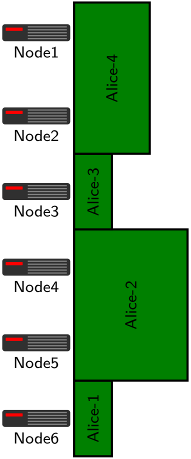

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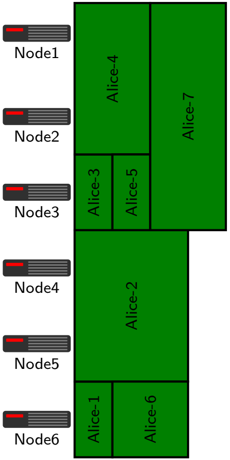

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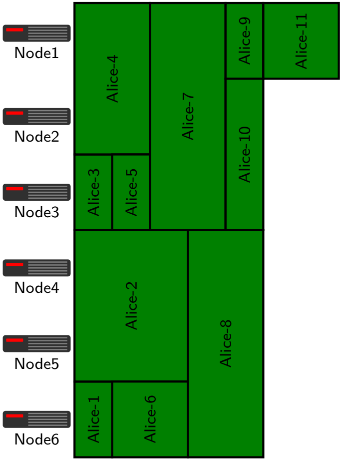

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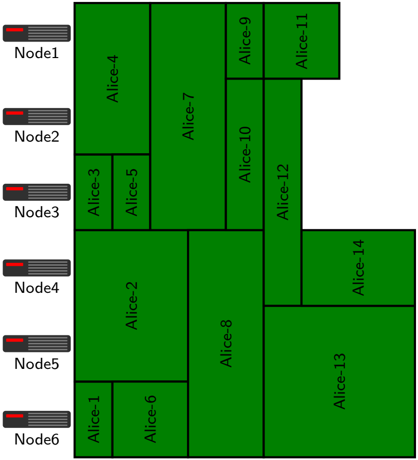

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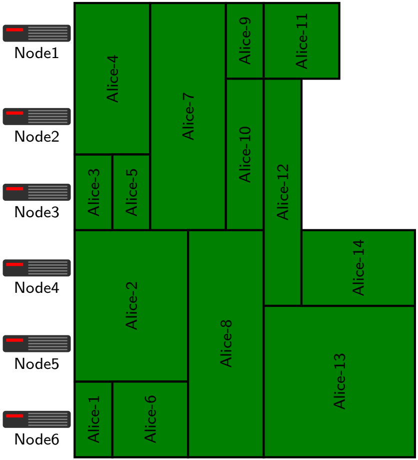
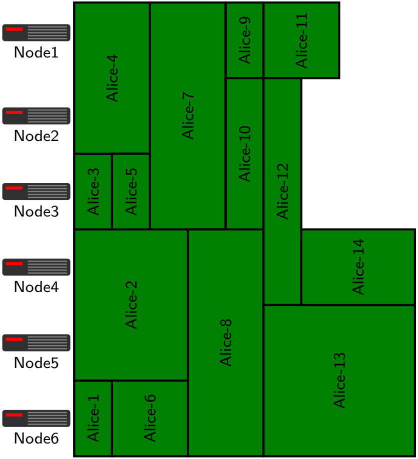
SLURM as Accountant: Sharing Computing Time



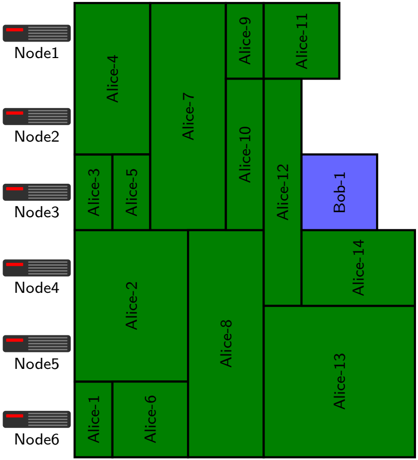
Alice submits a huge amount of jobs.
She filled the cluster and queue.

SLURM as Accountant: Sharing Computing Time



Bob submits some jobs.

SLURM as Accountant: Sharing Computing Time



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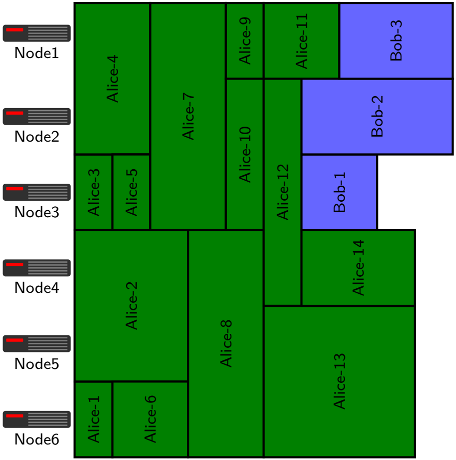
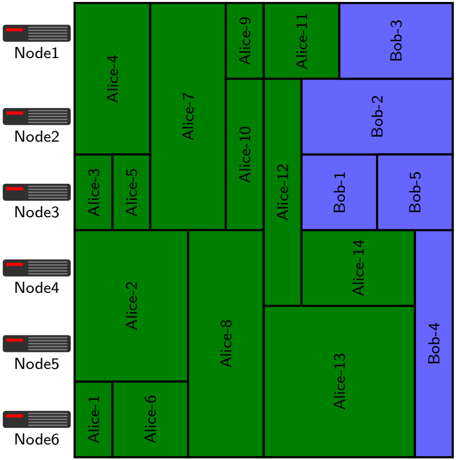
SLURM as Accountant: Sharing Computing Time



Bob submits some jobs.

SLURM as Accountant: Sharing Computing Time



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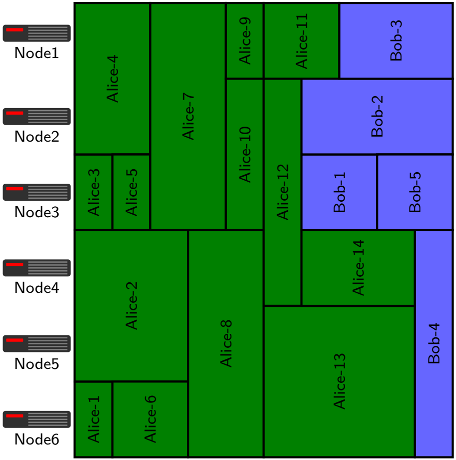
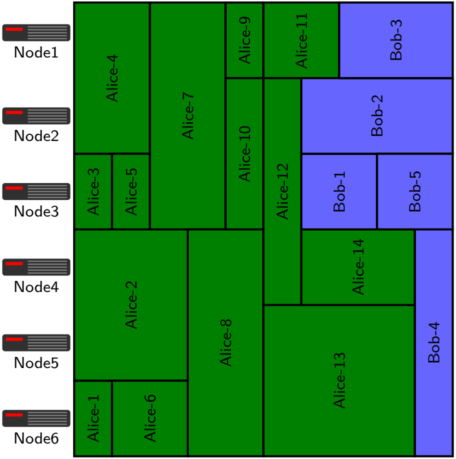
SLURM as Accountant: Sharing Computing Time



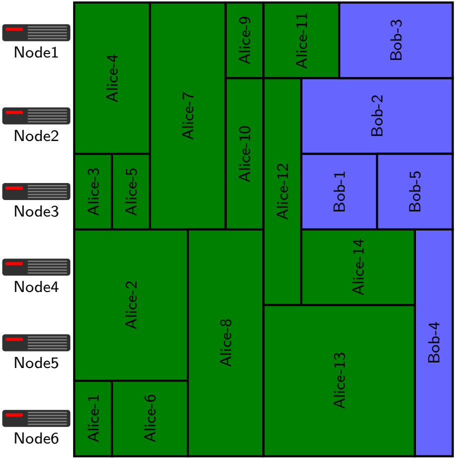
The cluster is not shared fairly, just because Alice spammed jobs quickly and early enough.

SLURM as Accountant: Sharing Computing Time



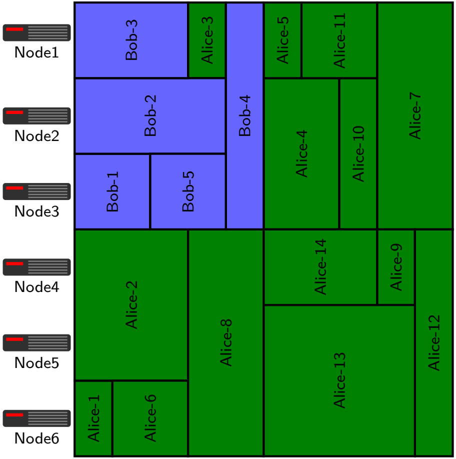
SLURM assigns a priority to each job, based on the users past resource usage.

SLURM as Accountant: Sharing Computing Time



Users who used the cluster less have a higher job priority.

SLURM as Accountant: Sharing Computing Time



SLURM reorganizes the queue based on the priorities to ensure a fair share of the cluster.

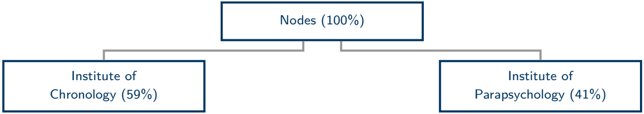
Already running jobs are not stoped!

SLURM as Accountant: Hierarchical Accounting

Nodes (100%)

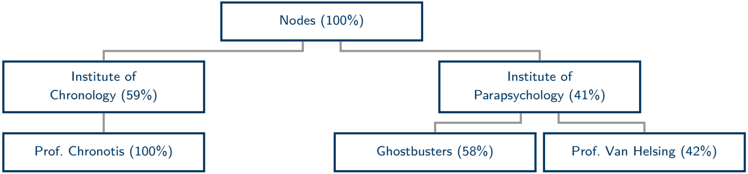
The accounting is done in a tree-like structure.

SLURM as Accountant: Hierarchical Accounting



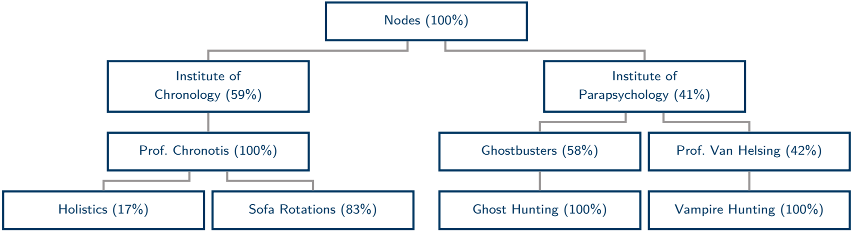
All nodes are shared between all institutes with individual shares.

SLURM as Accountant: Hierarchical Accounting



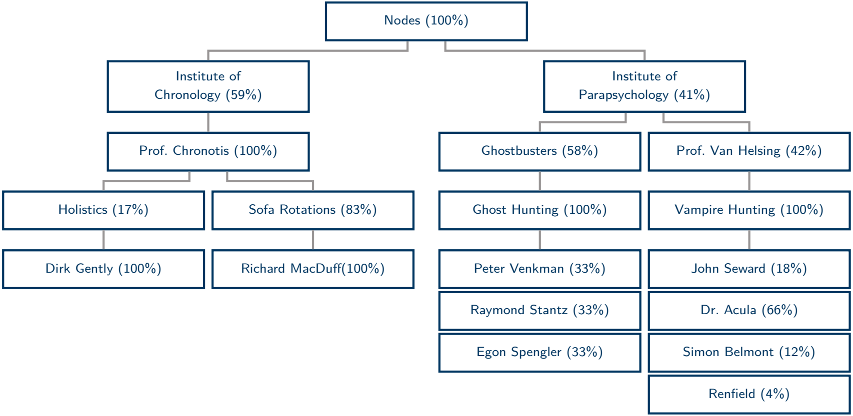
An institutes share is further shared between different groups.

SLURM as Accountant: Hierarchical Accounting



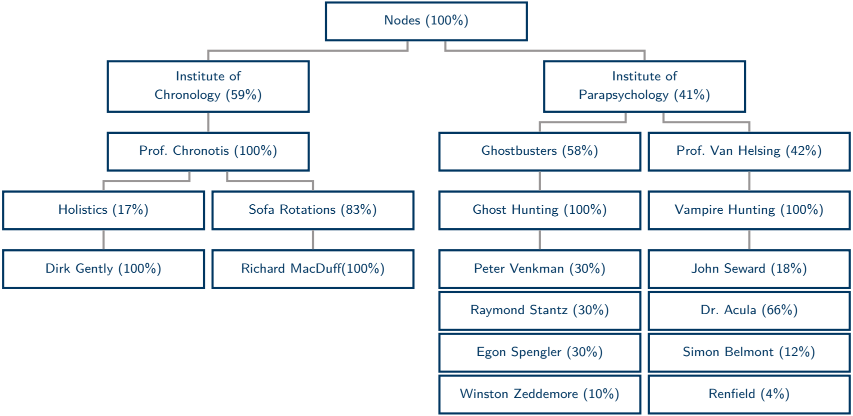
A group can have multiple projects that share the groups share.

SLURM as Accountant: Hierarchical Accounting



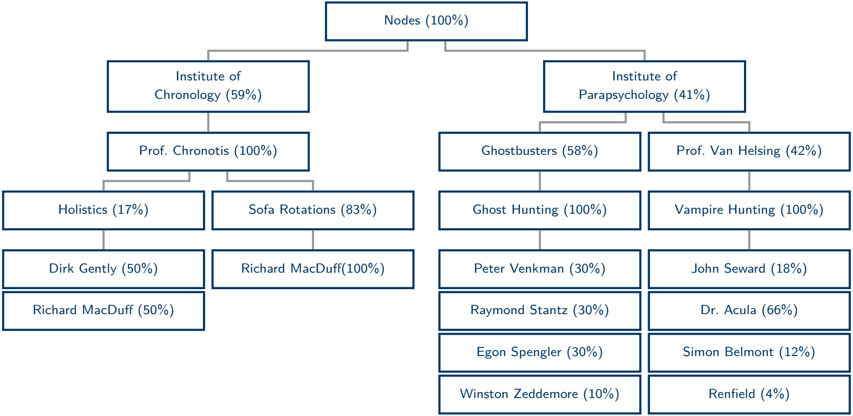
A project can have multiple users, that share the projects share.

SLURM as Accountant: Hierarchical Accounting



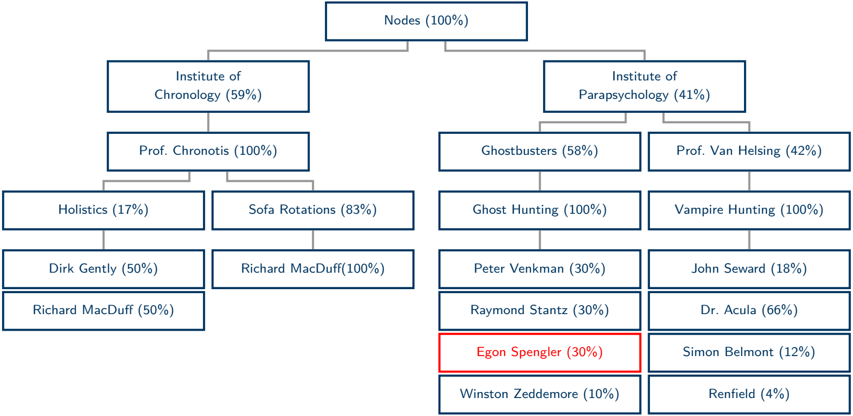
Adding a new user renormalizes the shares of the users in the same project.

SLURM as Accountant: Hierarchical Accounting



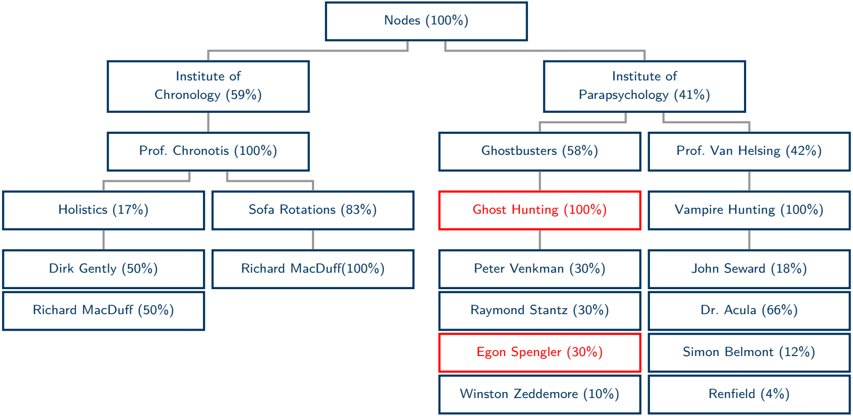
Users can be members of multiple projects. The project needs to be specified during job submission (e.g. SLURM-header).

SLURM as Accountant: Hierarchical Accounting



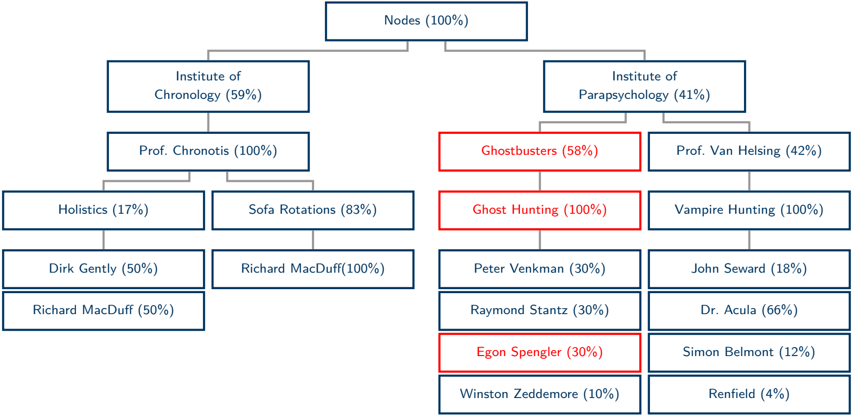
Example: User “Egon Spengler”

SLURM as Accountant: Hierarchical Accounting



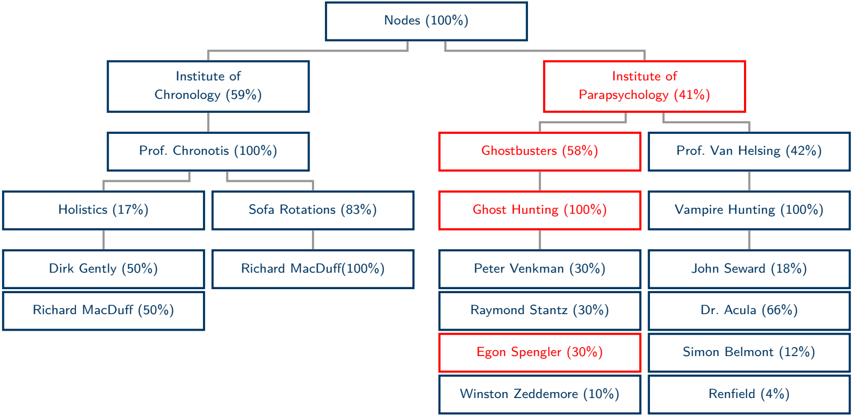
Example: User “Egon Spengler” of the “Ghost Hunting” project

SLURM as Accountant: Hierarchical Accounting



Example: User "Egon Spengler" of the "Ghost Hunting" project of the "Ghostbusters" group

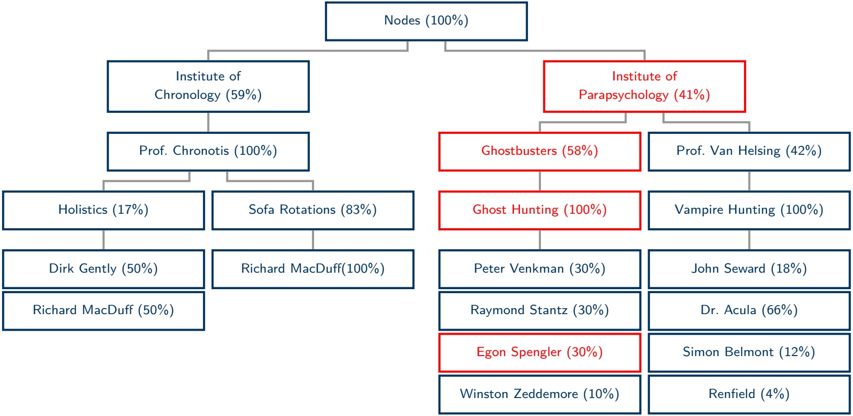
SLURM as Accountant: Hierarchical Accounting



Example: User “Egon Spengler” of the “Ghost Hunting“ project of the “Ghostbusters” group in the “Chair of Parapsychology”

SLURM as Accountant: Hierarchical Accounting

RUB



Example: User “Egon Spengler” has a real share of:
$30\% \times 100\% \times 58\% \times 41\% = 7\%$ of the Nodes.

SLURM as Accountant: sshare

Terminal

```
root@hpc:$ sshare
Account                User RawShares NormShares RawUsage EffectvUsage FairShare
-------------------------------------------------------------------------------
...
parapsy                            41   0.525641  1432063     0.737318  0.000000
 ghostbusters                      58   0.580000   917609     0.640760  0.000000
  ghosthunting                    100   1.000000   917609     1.000000  0.000000
   ghosthunting  pvenkman          30   0.300000     3365     0.003667  0.272727
   ghosthunting   rstantz          30   0.300000   186275     0.203000  0.181818
   ghosthunting  espengle          30   0.300000   727422     0.792736  0.090909
   ghosthunting  wzeddemo          10   0.100000      547     0.000596  0.363636
 vanhelsing                        42   0.420000   514454     0.359240  0.000000
  vamphunting                     100   1.000000   514454     1.000000  0.000000
   vamphunting    jseward          18   0.180000    72698     0.141311  0.545455
   vamphunting      acula          66   0.660000      666     0.001295  0.636364
   vamphunting   sbelmont          12   0.120000   441050     0.857317  0.454545
   vamphunting   renfield           4   0.040000       40     0.000078  0.727273
```

SLURM as Accountant: sshare

`sshare` shows only own shares and usage (privacy reasons):

Terminal

```
rmduff@hpc:$ sshare
Account     User RawShares NormShares RawUsage EffectvUsage FairShare
-------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

SLURM as Accountant: sshare

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rmduff@hpc:$ sshare
Account     User RawShares NormShares RawUsage EffectvUsage FairShare
--------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

Account Name of the account.

SLURM as Accountant: sshare

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Account     User RawShares NormShares RawUsage EffectvUsage FairShare
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sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

User Name of the user.

SLURM as Accountant: sshare

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Terminal

```
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Account      User RawShares NormShares RawUsage EffectvUsage FairShare
-------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

RawShares User's share of the account.

NormShares User's share of the account relative to other members of the same account $\left(S_{norm} = \frac{S_{raw,user}}{\sum S_{raw,siblings}}\right)$.

SLURM as Accountant: sshare

`sshare` shows only own shares and usage (privacy reasons):

Terminal

```
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Account     User RawShares NormShares RawUsage EffectvUsage FairShare
--------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

RawUsage Time in seconds nodes were used.

EffectvUsage Resource usage relative to other members of the same account $\left(U_{eff} = \frac{U_{raw,user}}{\sum U_{raw,siblings}}\right)$

SLURM as Accountant: sshare

`sshare` shows only own shares and usage (privacy reasons):

Terminal

```
rmduff@hpc:$ sshare
Account     User RawShares NormShares RawUsage EffectvUsage FairShare
------------------------------------------------------------------
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sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

FairShare $[0, 1]$ Priority rank with which jobs will be scheduled. The closer to 1.0 the more the jobs are prioritized.

SLURM as Accountant: sshare

`sshare` shows only own shares and usage (privacy reasons):

Terminal

```
rmduff@hpc:$ sshare
Account     User RawShares NormShares RawUsage EffectvUsage FairShare
--------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

On If a user belongs to multiple accounts the account must be specified at job submission with the `--account` flag.
(On the RUB cluster the flag is always required)

SLURM as Accountant: Account Lists

If a user participates in multiple projects with cryptic account names it can be cumbersome to figure out which project to select for a job.

Terminal

```
rmduff@hpc:$ sshare
Account     User RawShares NormShares RawUsage EffectvUsage FairShare
---------------------------------------------------------------------
holistics rmduff        50   0.500000    24799     0.321122  1.000000
sofarot   rmduff       100   1.000000   432971     1.000000  0.818182
```

SLURM as Accountant: Account Lists

If a user participates in multiple projects with cryptic account names it can be cumbersome to figure out which project to select for a job.

Terminal

```
rmduff@hpc:$ rub-acclist
Project ID    | Project Description
--------------+-----------------------------------------------------
holistics     | The fundamental interconnectedness of all things
sofarot       | The translated quaternion for optimal pivoting
```

The `rub-acclist` (RUB exclusive) lists all projects a user is part of, as well as the description provided by the project manager.

SLURM as Accountant: Fair Share Through Prioritization

FairShare Assignment:

- Sibling accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.

SLURM as Accountant: Fair Share Through Prioritization

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- Sibling accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.
- $R = \frac{S_{norm}}{U_{eff}} > 1$: Used less than entitled to

SLURM as Accountant: Fair Share Through Prioritization

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- Sibling accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.
- $R = \frac{S_{norm}}{U_{eff}} > 1$: Used less than entitled to
- $R = \frac{S_{norm}}{U_{eff}} < 1$: Used more than entitled to

SLURM as Accountant: Fair Share Through Prioritization

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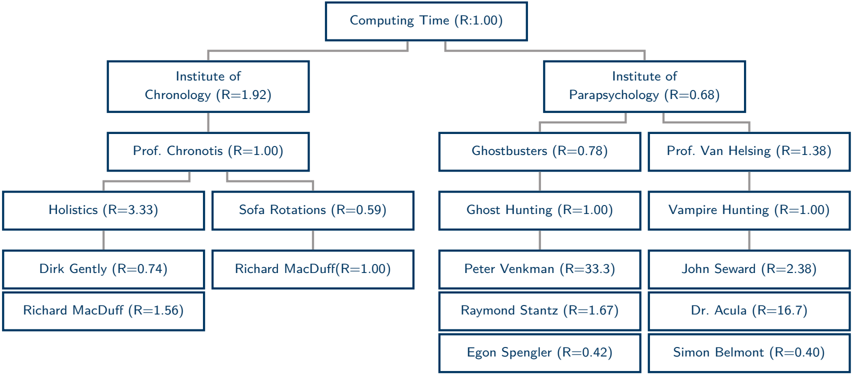
- $R = \frac{S_{norm}}{U_{eff}} > 1$: Used less than entitled to
- $R = \frac{S_{norm}}{U_{eff}} < 1$: Used more than entitled to
- Parent accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.

FairShare Assignment:

- Sibling accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.
- $R = \frac{S_{norm}}{U_{eff}} > 1$: Used less than entitled to
- $R = \frac{S_{norm}}{U_{eff}} < 1$: Used more than entitled to
- Parent accounts are ranked by their $R = \frac{S_{norm}}{U_{eff}}$ value.
- Child rankings are concatenated accordingly.

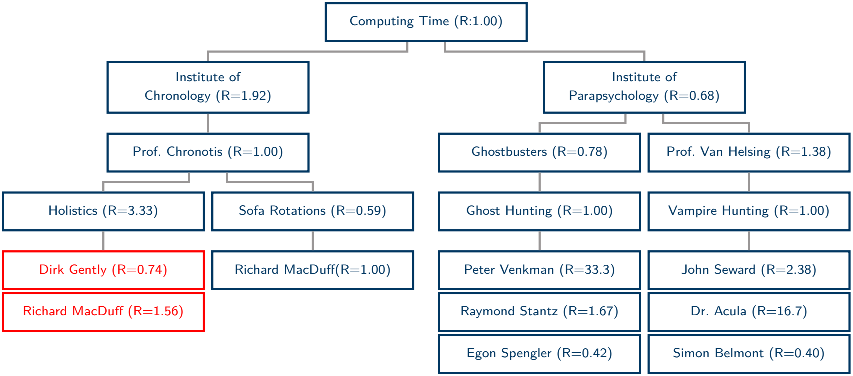
SLURM as Accountant: Prioritization Example



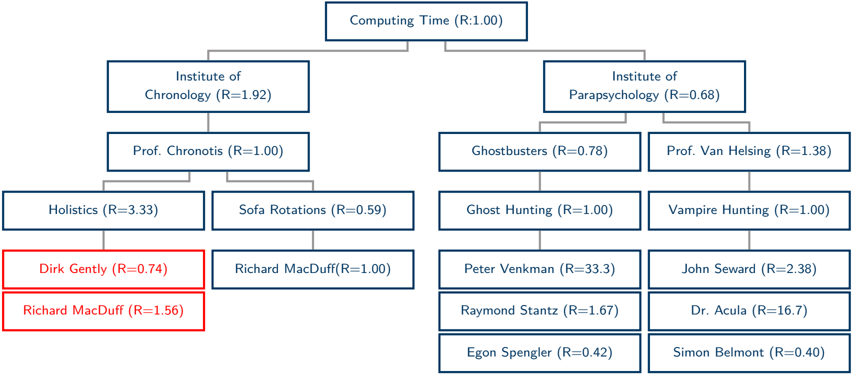
$R = \frac{S_{norm}}{U_{eff}} > 1$: used fewer ressources than entitled to

$R = \frac{S_{norm}}{U_{eff}} < 1$: used more ressources than entitled to

SLURM as Accountant: Prioritization Example

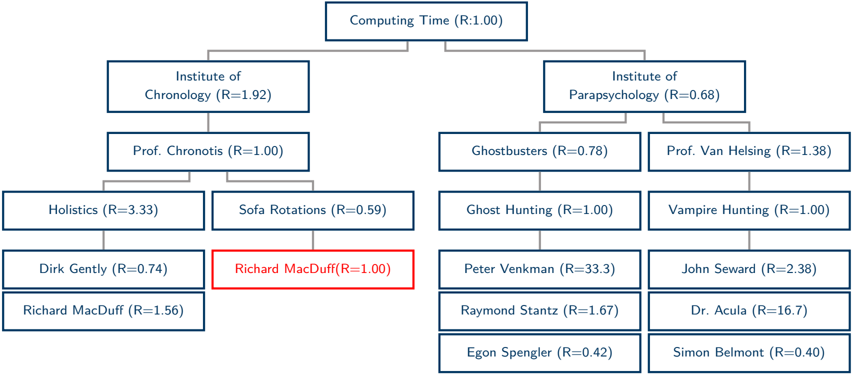


SLURM as Accountant: Prioritization Example



McDuff(Holistics) > Gently

SLURM as Accountant: Prioritization Example



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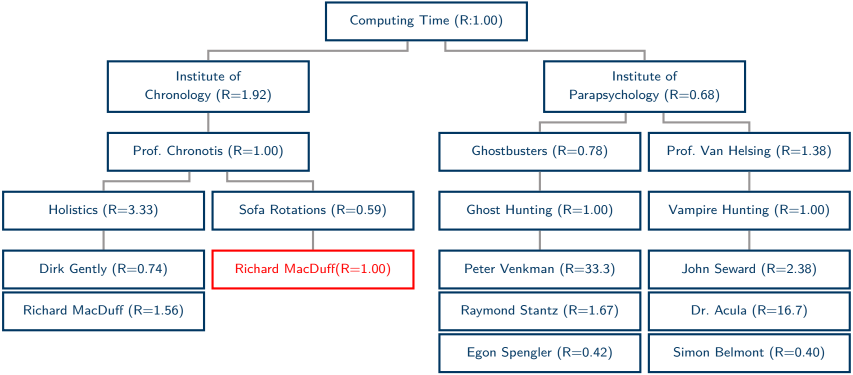
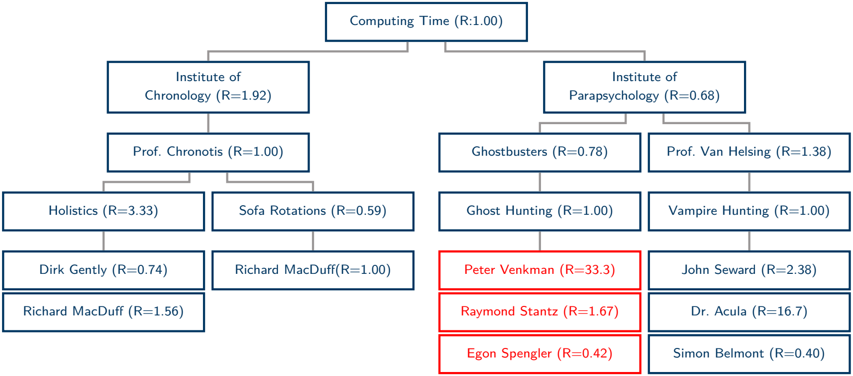
SLURM as Accountant: Prioritization Example



McDuff(Holistics) > Gently

McDuff(SofaRot)

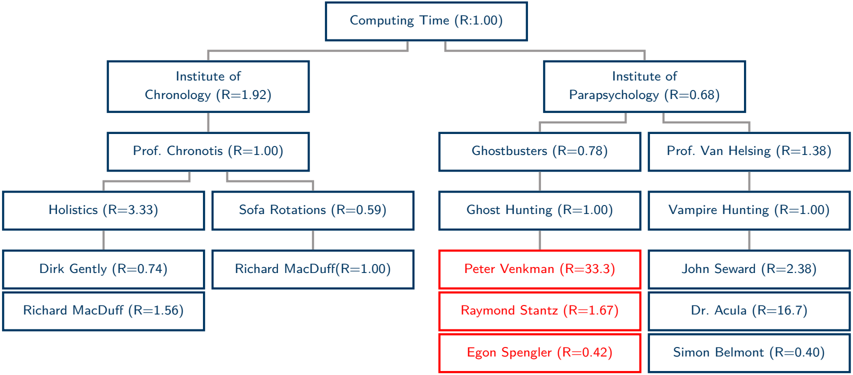
SLURM as Accountant: Prioritization Example



McDuff(Holistics) > Gently

McDuff(SofaRot)

SLURM as Accountant: Prioritization Example

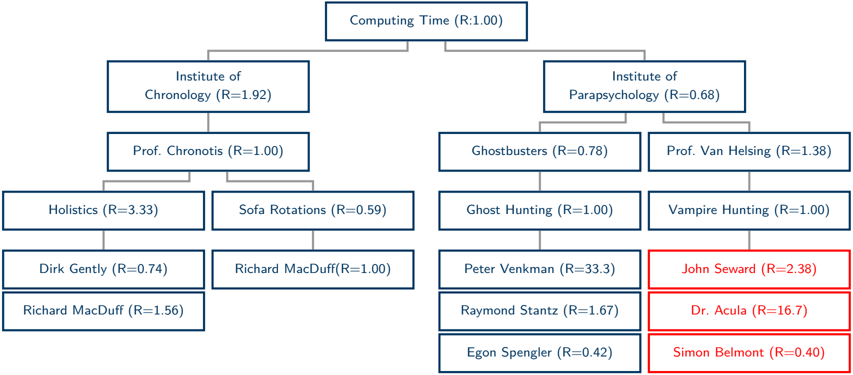


McDuff(Holistics) > Gently

McDuff(SofaRot)

Venkman > Stantz > Spengler

SLURM as Accountant: Prioritization Example

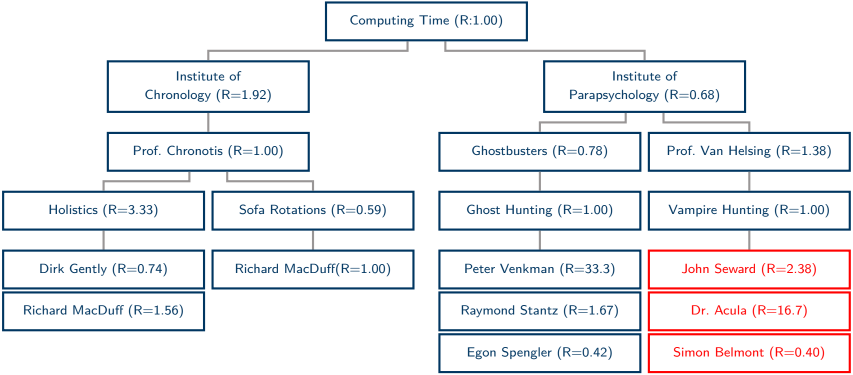


McDuff(Holistics) > Gently

McDuff(SofaRot)

Venkman > Stantz > Spengler

SLURM as Accountant: Prioritization Example



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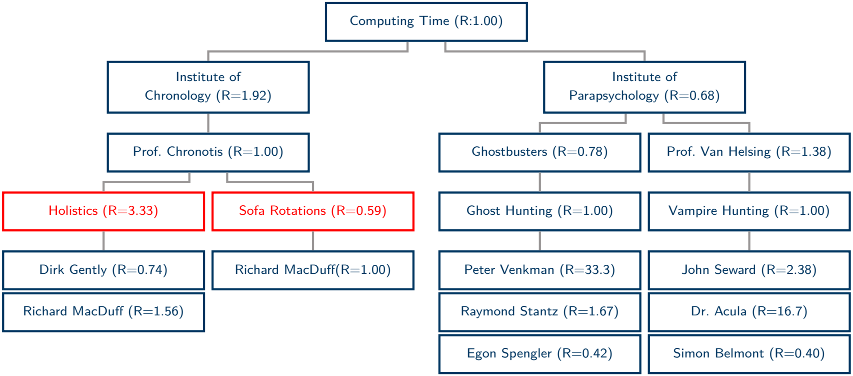

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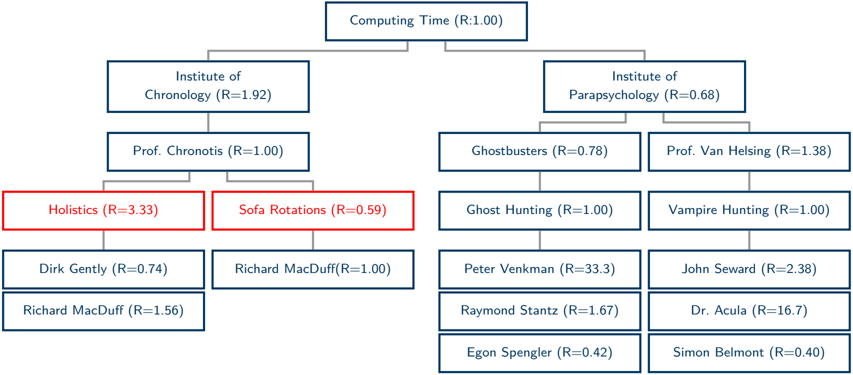

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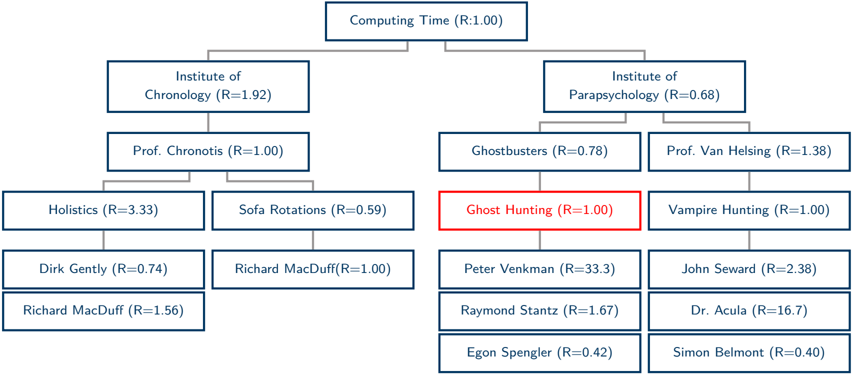

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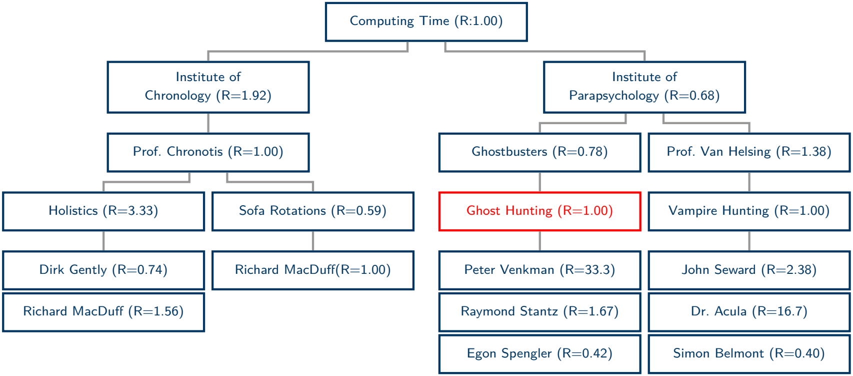

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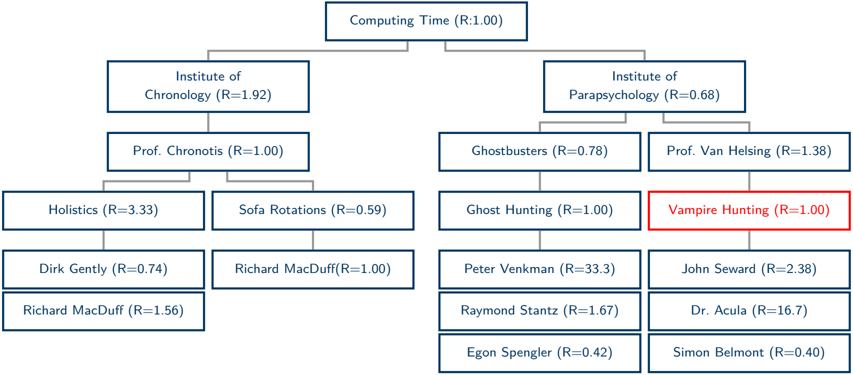

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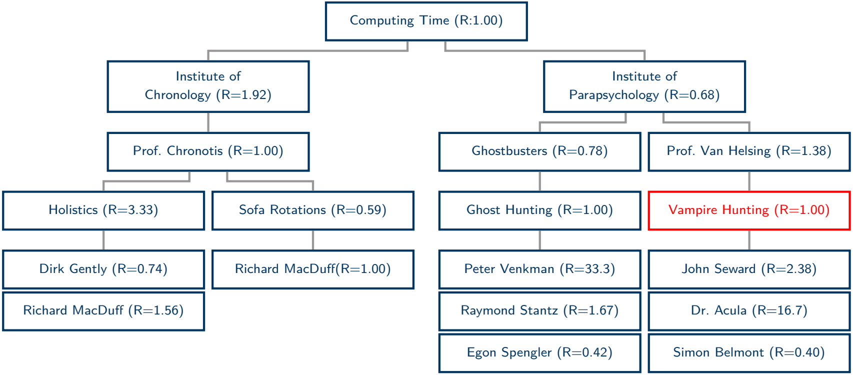
SLURM as Accountant: Prioritization Example

RUB



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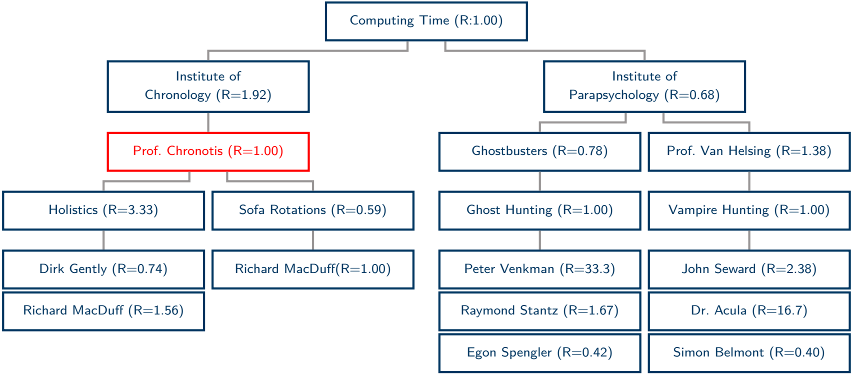
SLURM as Accountant: Prioritization Example



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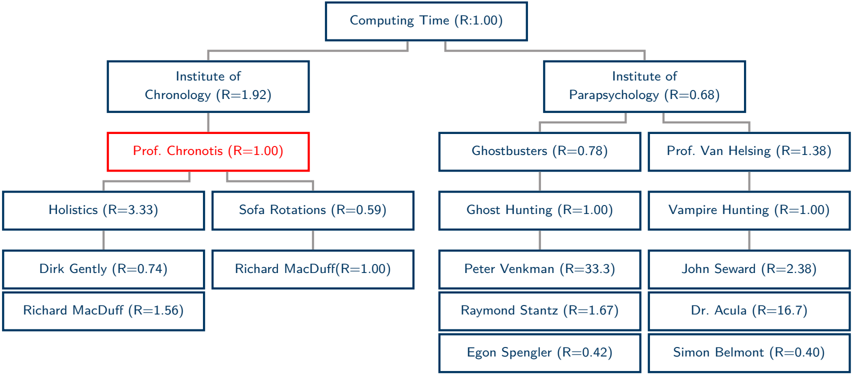
SLURM as Accountant: Prioritization Example



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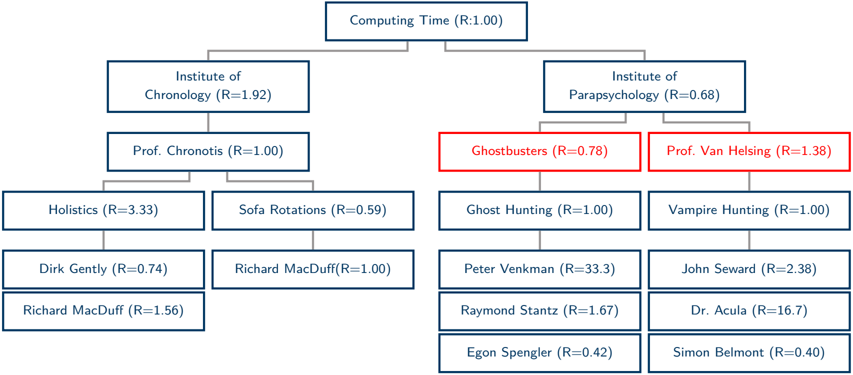
SLURM as Accountant: Prioritization Example



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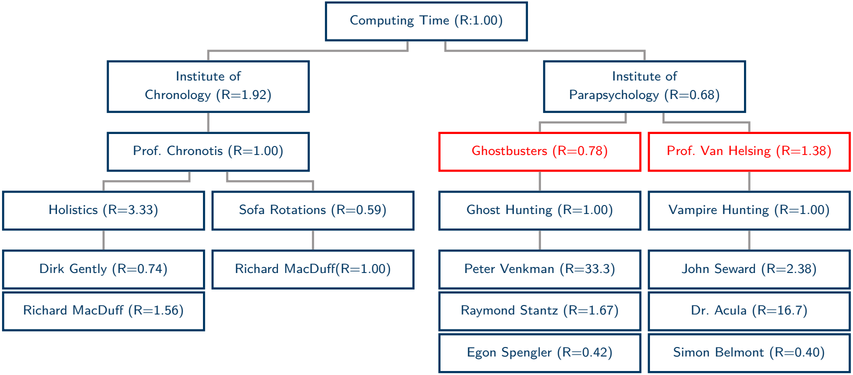

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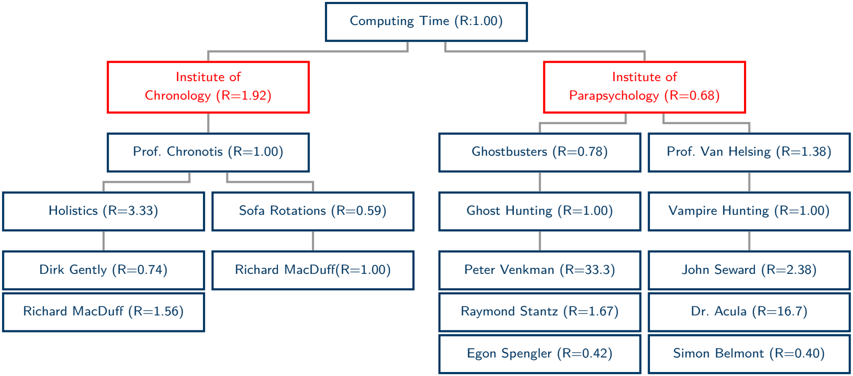
SLURM as Accountant: Prioritization Example



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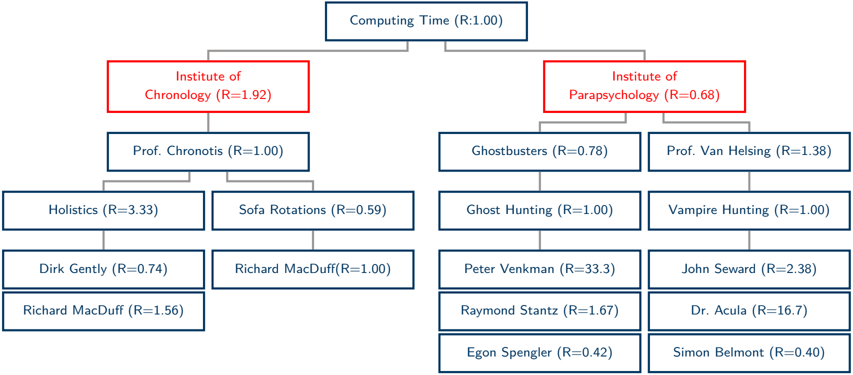
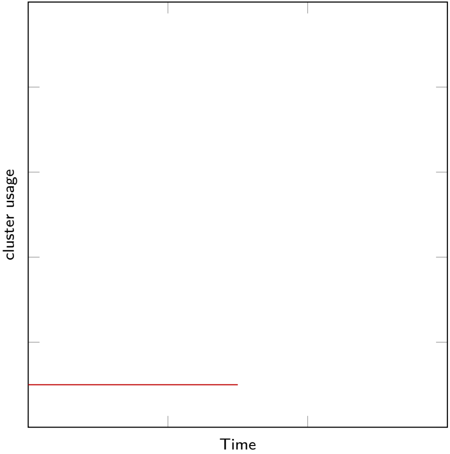
SLURM as Accountant: Prioritization Example



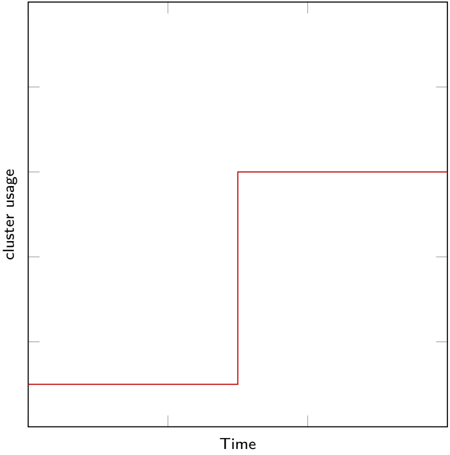
McDuff(Holistics) > Gently > McDuff(SofaRot) >
Acula > Seward > Belmont > Venkman > Stantz > Spengler

SLURM: Usage Accumulation



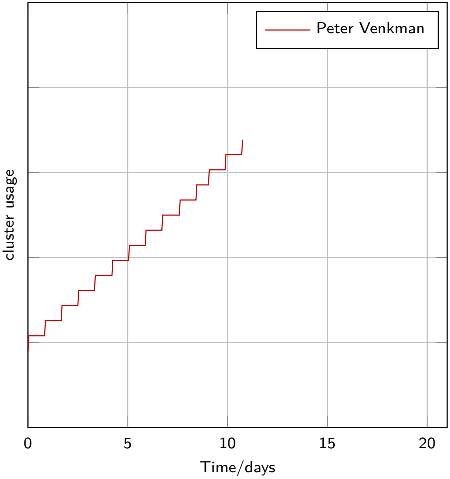
The user's `rawUsage` is tracked by SLURM over time.

SLURM: Usage Accumulation



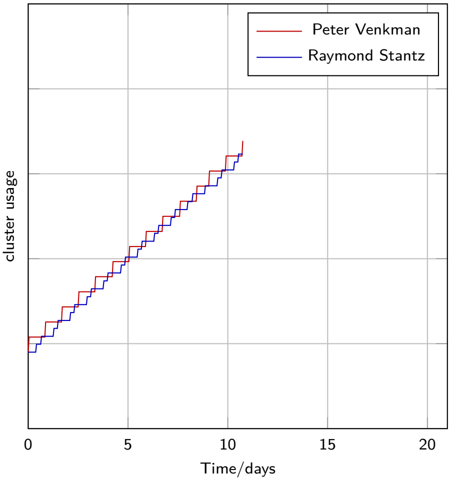
If a job is executed the jobs runtime (multiplied with the number cores/GPUs) is added to the users `rawUsage`.

SLURM: Usage Accumulation



Example: Peter Venkman submits jobs.
The runtime is added to his `rawUsage`.

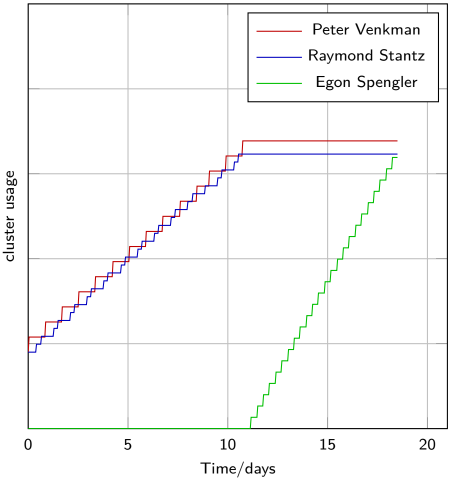
SLURM: Usage Accumulation



Raymond Stantz also uses the cluster

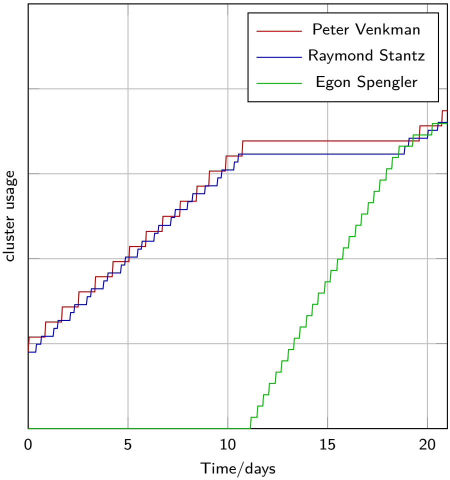
Their `rawUsage` is similar, their jobs take turns. The cluster is shared fairly.

SLURM: Usage Accumulation



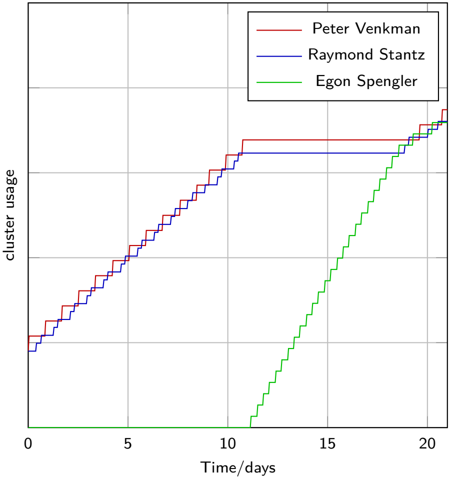
Egon Spengler starts to use the cluster.
His `rawUsage` is lowest, so he takes over and forces Peter's and Raymod's jobs to wait.

SLURM: Usage Accumulation



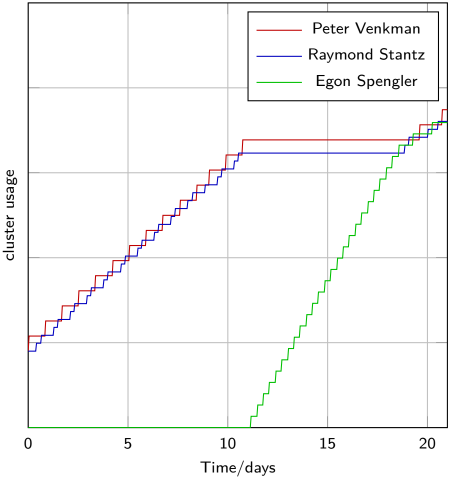
Finally Egon's `rawUsage` caught up with Peter's and Raymod's and everyone shares the cluster evenly.

SLURM: Usage Accumulation



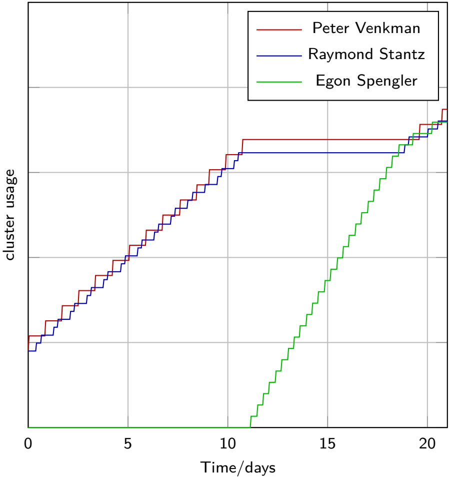
- All of a user's usage history is considered to prioritize jobs.

SLURM: Usage Accumulation



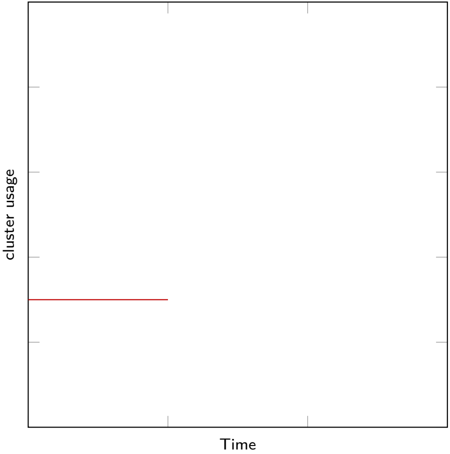
- All of a user's usage history is considered to prioritize jobs.
- This is unfair, especially as new users/groups could take over the complete cluster and block everyone until the `rawUsage` caught up with everyone else.

SLURM: Usage Accumulation



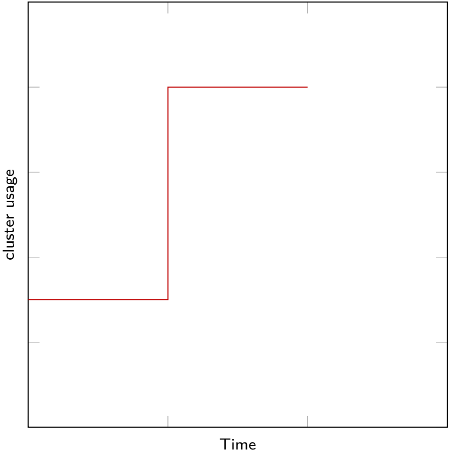
- All of a user's usage history is considered to prioritize jobs.
- This is unfair, especially as new users/groups could take over the complete cluster and block everyone until the `rawUsage` caught up with everyone else.
- Some way to "forget" the past is needed to ensure fair usage.

SLURM: Usage Accumulation and Reset



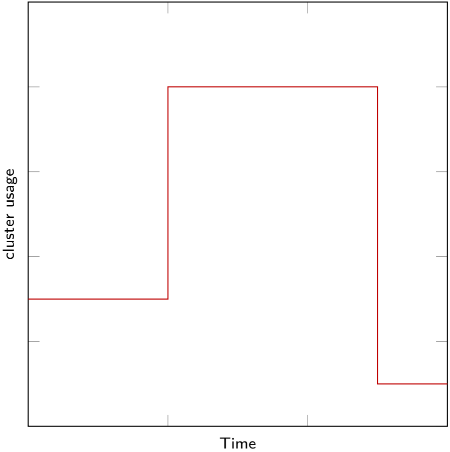
The user's `rawUsage` is tracked by SLURM over time.

SLURM: Usage Accumulation and Reset



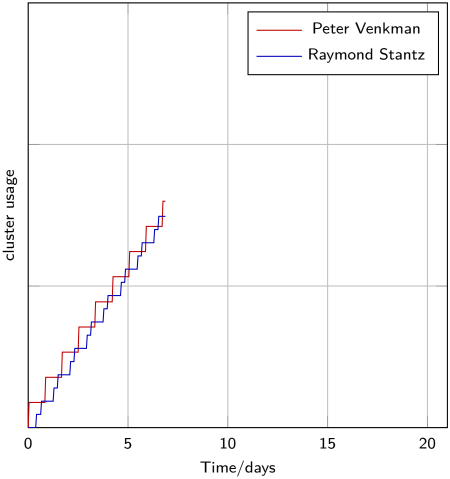
If a job is executed the jobs runtime (multiplied with the number of nodes) is added to the users `rawUsage`.

SLURM: Usage Accumulation and Reset



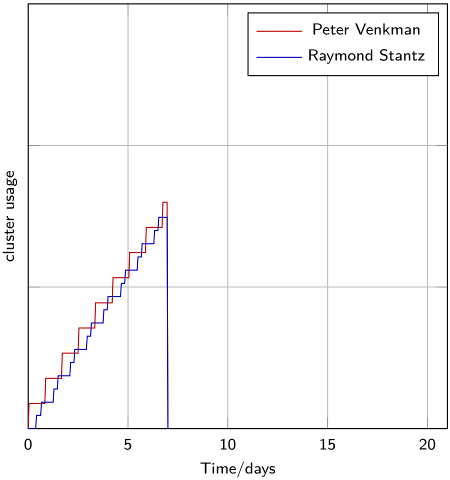
In regular intervals the `rawUsage` of all users is set to zero in order to ignore distant usage history.

SLURM: Usage Accumulation and Reset



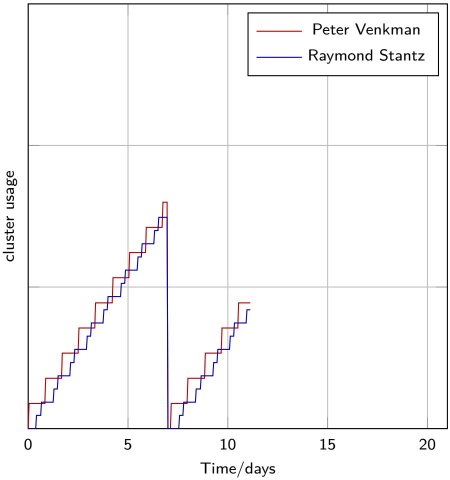
Example: Peter Venkman and Raymond Stantz share the cluster evenly.

SLURM: Usage Accumulation and Reset



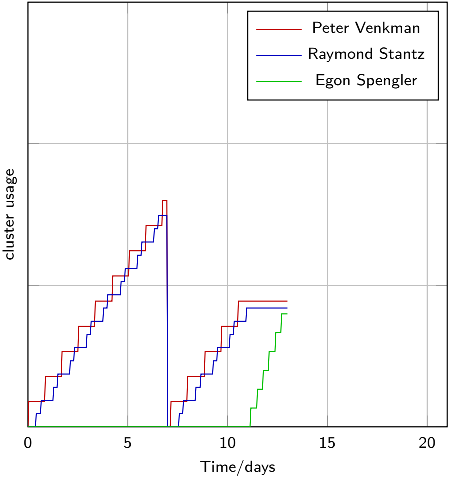
A reset point is reached and everyones `rawUsage` is cleared.

SLURM: Usage Accumulation and Reset



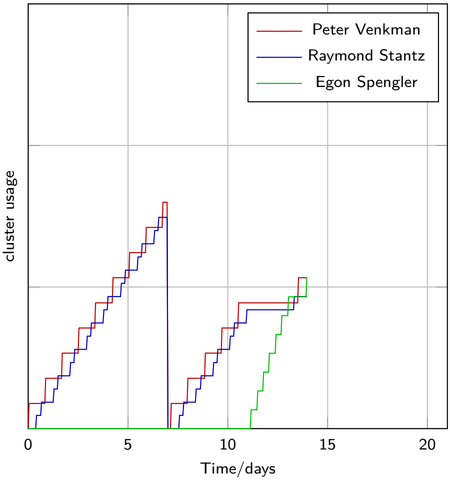
Peter and Raymond still share the cluster evenly.

SLURM: Usage Accumulation and Reset



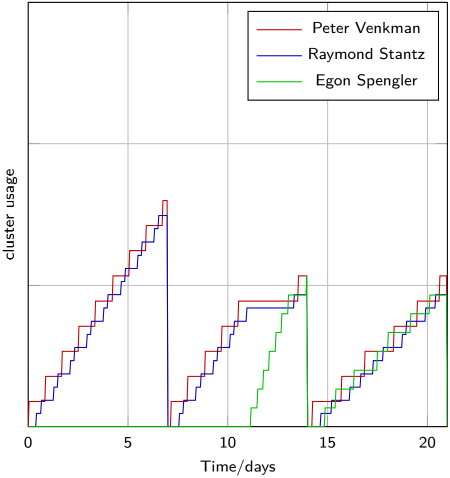
Egon Spengler starts to use the cluster.
His `rawUsage` is lowest, so he takes over and forces Peter's and Raymod's jobs to wait.

SLURM: Usage Accumulation and Reset



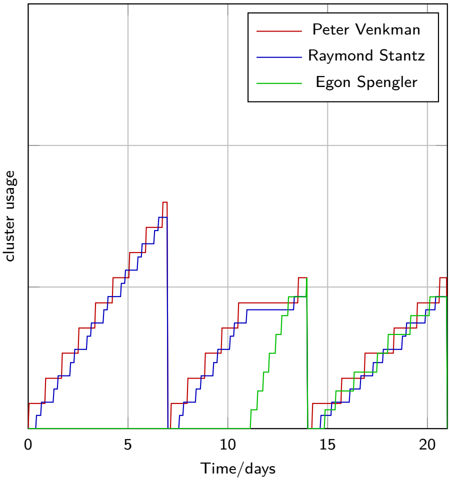
Egon's `rawUsage` overtakes Raymond's and Peter's `rawUsage` and they share the cluster fairly.

SLURM: Usage Accumulation and Reset



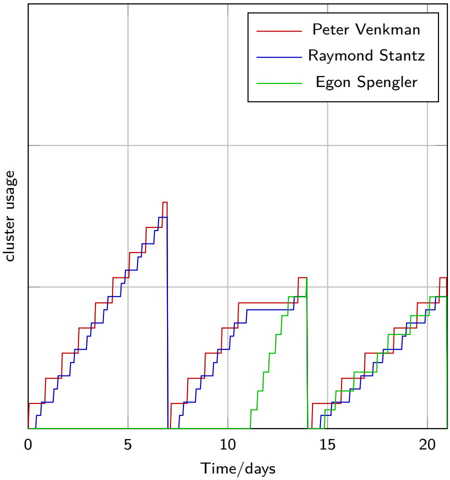
The next reset has no influence on the fair sharing of the cluster.

SLURM: Usage Accumulation and Reset



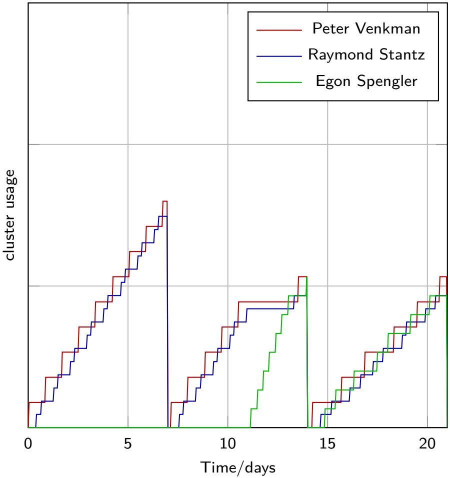
- New users cannot take over the cluster for extended periods of time.

SLURM: Usage Accumulation and Reset



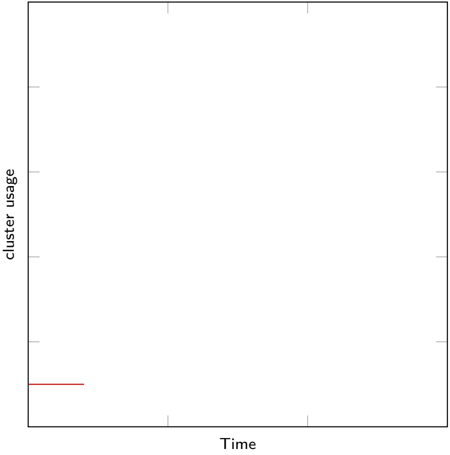
- New users cannot take over the cluster for extended periods of time.
- However, new users can aim at maximizing cluster blockage by choosing a clever starting point.

SLUMR: Usage Accumulation and Reset



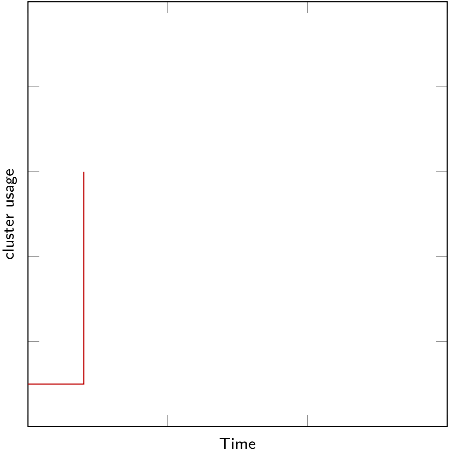
- New users cannot take over the cluster for extended periods of time.
- However, new users can aim at maximizing cluster blockage by choosing a clever starting point.
- Some way to make the distant past less relevant than the recent past is needed to ensure fair usage.

SLURM: Usage Accumulation and Decay



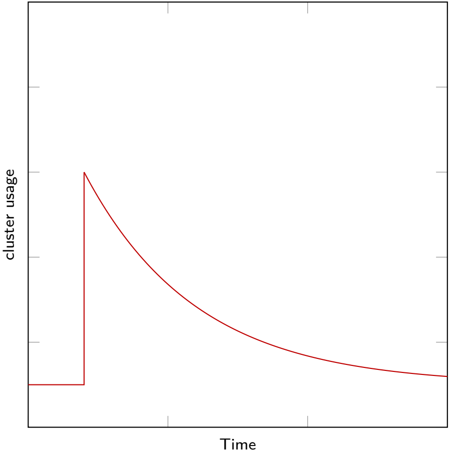
The user's `rawUsage` is tracked by SLURM over time.

SLURM: Usage Accumulation and Decay



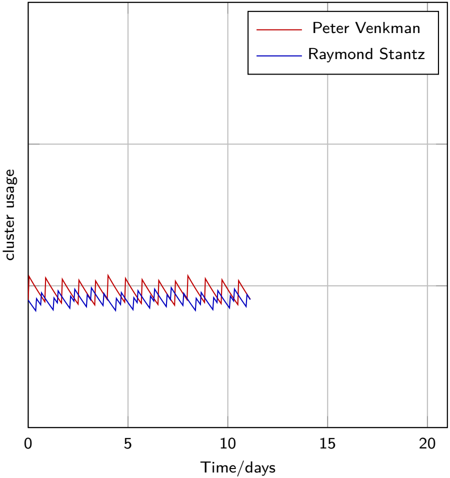
If a job is executed the jobs runtime (multiplied with the number of nodes) is added to the users `rawUsage`.

SLURM: Usage Accumulation and Decay



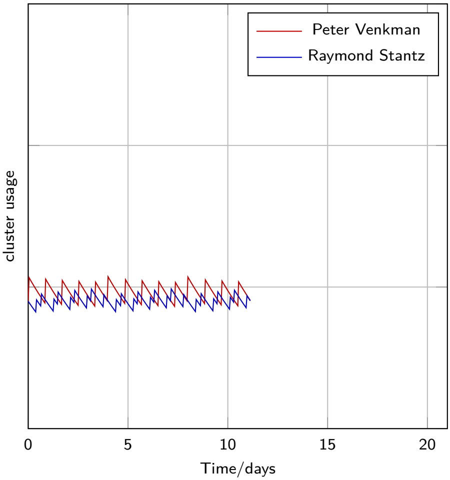
`rawUsage` is subject to constant exponential decay.

SLURM: Usage Accumulation and Decay



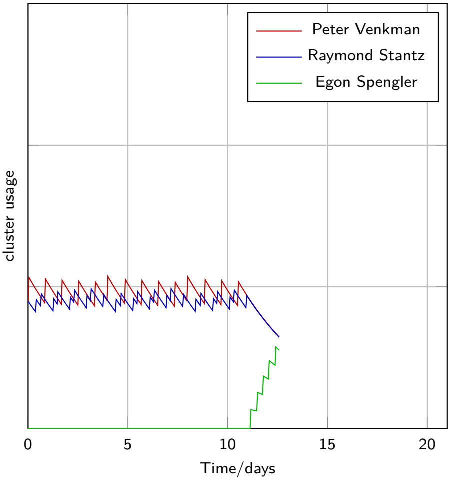
Example: Peter Venkman and Raymond Stantz share the cluster evenly.

SLURM: Usage Accumulation and Decay



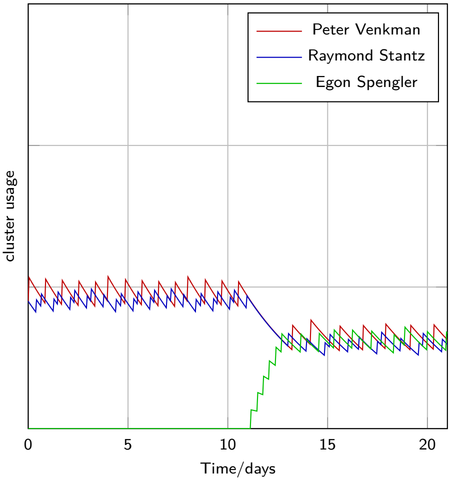
The exponential decay is already visible and ensures that the `rawUsage` dose not grow indefinetly.

SLURM: Usage Accumulation and Decay



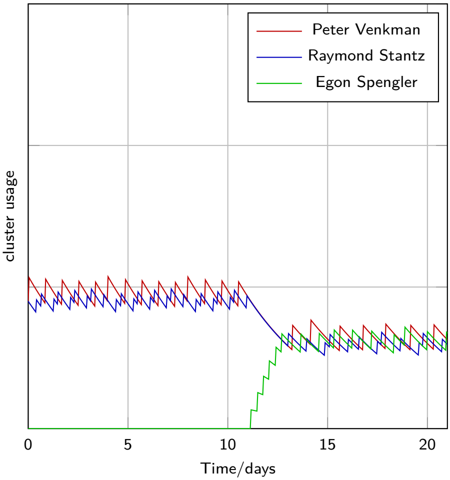
Egon Spengler starts to use the cluster.
His `rawUsage` is lowest, so he takes over and forces Peter's and Raymod's jobs to wait.

SLURM: Usage Accumulation and Decay



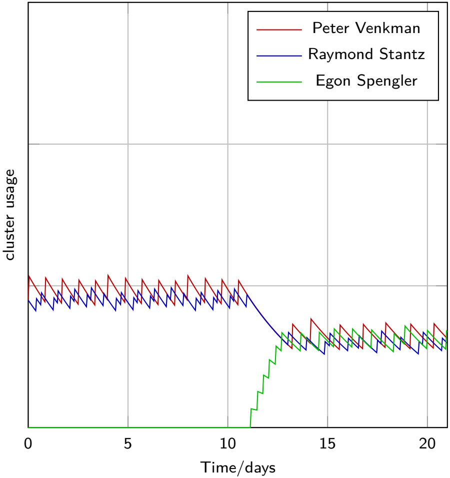
Egon's `rawUsage` quickly overtakes Raymond's and Peter's `rawUsage` and they share the cluster fairly.

SLURM: Usage Accumulation and Decay



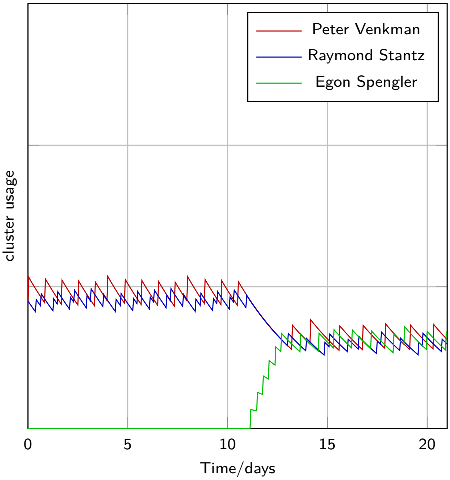
- Distant usage history is dampened and recent usage history preserved.

SLURM: Usage Accumulation and Decay



- Distant usage history is dampened and recent usage history preserved.
- New users cannot take over the cluster for extended periods of time.

SLURM: Usage Accumulation and Decay



- Distant usage history is dampened and recent usage history preserved.
- New users cannot take over the cluster for extended periods of time.
- Users are not punished for taking advantage of an empty cluster.

Exercise 3

RUB

1. Check the available partitions/queues with `sinfo`
2. Start an interactive session with `srun`, and exit again
3. Read the `sample_job_sleepter.sh` script and fill in all `FIX_ME`
4. Submit the `sample_job_sleepter.sh`
5. Check the jobs status with `squeue`

Exercise 3

1 Check the available partitions/queues with `sinfo`

Terminal

```
alice@hpc:$ sinfo
PARTITION        AVAIL  TIMELIMIT  NODES  STATE NODELIST
cpu-nodes           up 2-00:00:00      4   idle hpc-dev-cpu[01-04]
gpu-nodes           up 2-00:00:00      2   idle hpc-dev-gpu[01-02]
alice@hpc:$
```

Exercise 3

2 Start an interactive session with `srun`, and exit again

Terminal

```
alice@hpc:$ srun --partition=cpu-nodes --pty /bin/bash
alice@hpc-cpu01:$ hostname
hpc-dev-cpu01
alice@hpc-cpu01:$ exit
alice@hpc:$
```

Exercise 3

3 Read the `sample_job_sleepter.sh` script and fill in all `FIX_ME`

Terminal

```
#!/bin/bash

#SBATCH --nodes=1
#SBATCH --partition=                                 <= FIX_ME
#SBATCH --job-name=                                  <= FIX_ME
#SBATCH --time=hh:mm:ss                              <= FIX_ME
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err

# Do nothing for 10 seconds
sleep 10s
```

Exercise 3

3 Read the `sample_job_sleepter.sh` script and fill in all `FIX_ME`

Terminal

```
#!/bin/bash

#SBATCH --nodes=1
#SBATCH --partition=cpu-nodes
#SBATCH --job-name=                                   <= FIX_ME
#SBATCH --time=hh:mm:ss                               <= FIX_ME
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err

# Do nothing for 10 seconds
sleep 10s
```

Exercise 3

3 Read the `sample_job_sleepter.sh` script and fill in all `FIX_ME`

Terminal

```
#!/bin/bash

#SBATCH --nodes=1
#SBATCH --partition=cpu-nodes
#SBATCH --job-name=sleeper
#SBATCH --time=hh:mm:ss                                 <= FIX_ME
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err

# Do nothing for 10 seconds
sleep 10s
```

Exercise 3

3 Read the `sample_job_sleepter.sh` script and fill in all `FIX_ME`

Terminal

```
#!/bin/bash

#SBATCH --nodes=1
#SBATCH --partition=cpu-nodes
#SBATCH --job-name=sleeper
#SBATCH --time=00:05:00
#SBATCH --output=%x-%j.out
#SBATCH --error=%x-%j.err

# Do nothing for 10 seconds
sleep 10s
```

Exercise 3

4 Submit the `sample_job_sleepter.sh`

Terminal

```
alice@hpc:$ sbatch sample_job_sleepter.sh
Submitted batch job 13491
alice@hpc:$
```

Exercise 3

5 Check the jobs status with `squeue`

Terminal

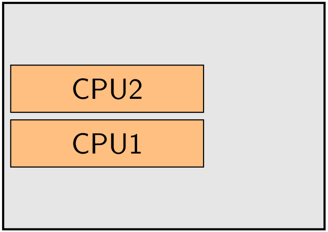
```
alice@hpc:$ squeue
JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
13491 cpu-nodes  sleeper    alice  R       0:07      1 hpc-cpu01
alice@hpc:$
```

Running Programs in Parallel

Compute Node Components

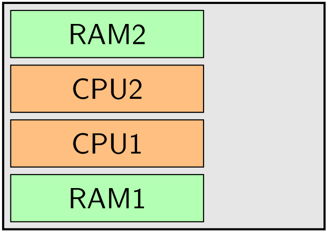
- The most important compute node components:

Compute Node Components



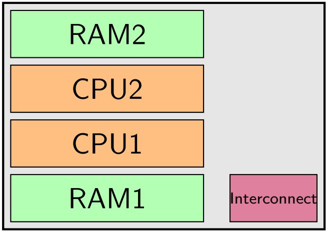
- The most important compute node components:
  - CPUs

Compute Node Components



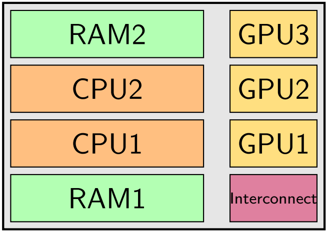
- The most important compute node components:
  - CPUs
  - Memory

Compute Node Components



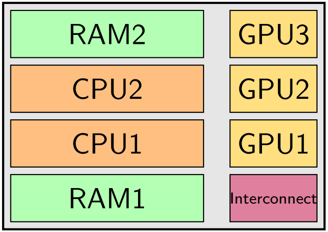
- The most important compute node components:
  - CPUs
  - Memory
  - Interconnect

Compute Node Components



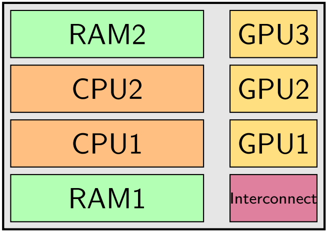
- The most important compute node components:
  - CPUs
  - Memory
  - Interconnect
  - Accelerator(GPU)

Compute Node Components



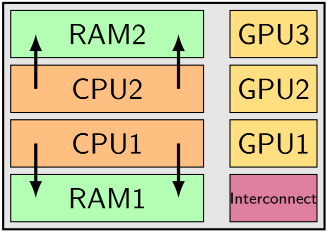
- CPU:

Compute Node Components



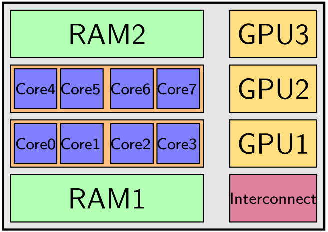
- CPU:
  - sits in a socket

Compute Node Components



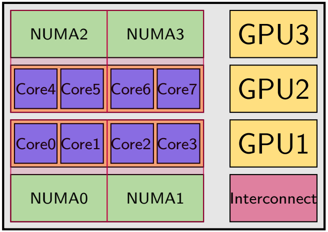
- CPU:
  - sits in a socket
  - only part of memory directly addressable

Compute Node Components



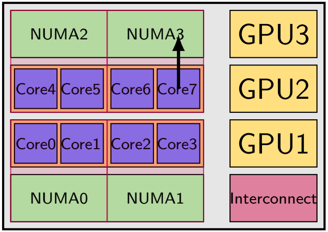
- CPU:
  - sits in a socket
  - only part of memory directly addressable
  - several (4-128) cores

Compute Node Components



- CPU:
  - sits in a socket
  - only part of memory directly addressable
  - several (4-128) cores
  - cores and memory portions are grouped (NUMA)

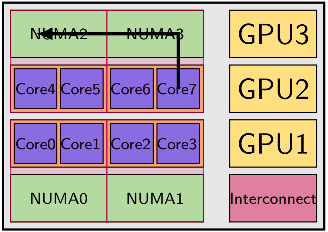
Compute Node Components



Data Location	Latency
Within NUMA	$\sim$20 ns

To ensure minimal latencies pin processes to cores.

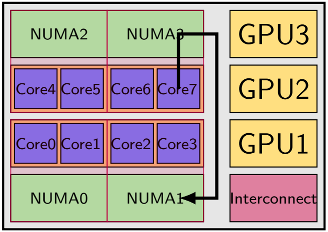
Compute Node Components



Data Location	Latency
Within NUMA	∼20 ns
Within Socket	∼100 ns

To ensure minimal latencies pin processes to cores.

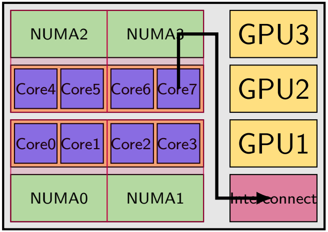
Compute Node Components



Data Location	Latency
Within NUMA	$\sim$20 ns
Within Socket	$\sim$100 ns
Other Socket	$\sim$200 ns

To ensure minimal latencies pin processes to cores.

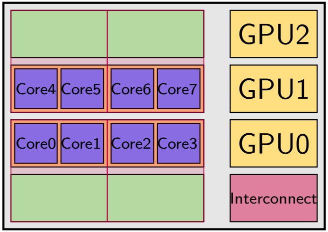
Compute Node Components



Data Location	Latency
Within NUMA	∼20 ns
Within Socket	∼100 ns
Other Socket	∼200 ns
Other Node	∼1200 ns

To ensure minimal latencies pin processes to cores.

Farming Jobs

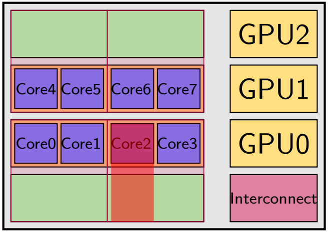


Terminal

```
alice@hpc:$
```

Farming Jobs

RUB

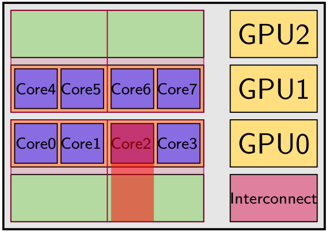


- A program is executed on a "randomly" selected core

Terminal

```
alice@hpc:$ ./myprog.x
```

Farming Jobs

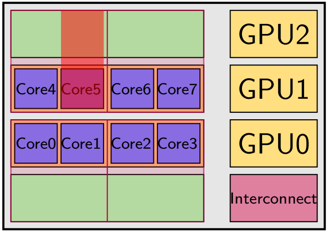


- A program is executed on a "randomly" selected core
- It accesses memory in its NUMA region

Terminal

```
alice@hpc:$ ./myprog.x
```

Farming Jobs

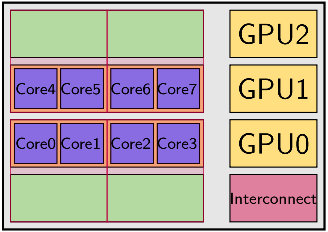


- A program is executed on a "randomly" selected core
- It accesses memory in its NUMA region
- The core assignment might switch during execution

Terminal

```
alice@hpc:$ ./myprog.x
```

Farming Jobs

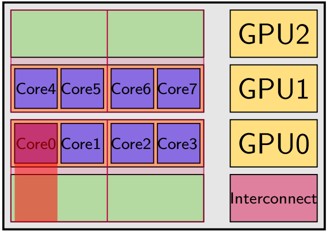


- A program is executed on a "randomly" selected core
- It accesses memory in its NUMA region
- The core assignment might switch during execution
- The terminal awaits its completion before it returns

Terminal

```
alice@hpc:$ ./myprog.x
alice@hpc:$
```

Farming Jobs

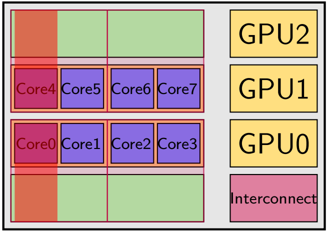


- An “&” starts the process in the background and returns immediately

Terminal

```
alice@hpc:$ ./myprog.x &
alice@hpc:$
```

Farming Jobs

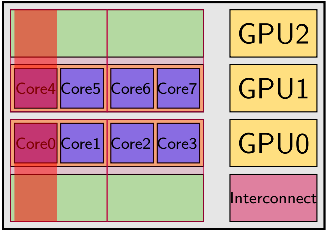


- An “&” starts the process in the background and returns immediately
- This allows for multiple parallel program executions

Terminal

```
alice@hpc:$ ./myprog.x &
alice@hpc:$ ./myprog.x &
alice@hpc:$
```

Farming Jobs

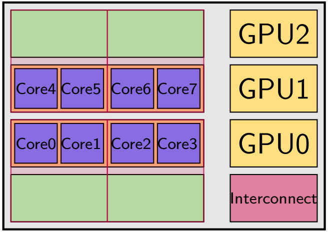


- An “&” starts the process in the background and returns immediately
- This allows for multiple parallel program executions
- `wait` returns as soon as all background processes have returned

Terminal

```
alice@hpc:$ ./myprog.x &
alice@hpc:$ ./myprog.x &
alice@hpc:$ wait
```

Farming Jobs

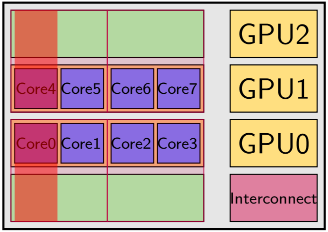


- An “&” starts the process in the background and returns immediately
- This allows for multiple parallel program executions
- `wait` returns as soon as all background processes have returned

Terminal

```
alice@hpc:$ ./myprog.x &
alice@hpc:$ ./myprog.x &
alice@hpc:$ wait
alice@hpc:$
```

Farming Jobs

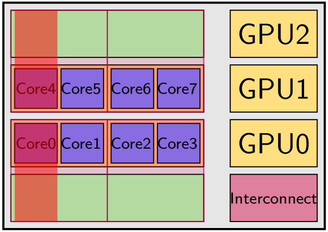


- `taskset -c <coreid>` pinns a process to a core and prevents core switching

Terminal

```
alice@hpc:$ taskset -c 0 ./myprog.x &
alice@hpc:$ taskset -c 4 ./myprog.x &
alice@hpc:$ wait
```

Farming Jobs

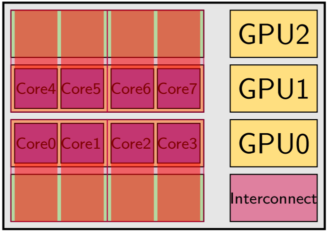


- `taskset -c <coreid>` pinns a process to a core and prevents core switching
- this allows for optimal process placement for memory access

Terminal

```
alice@hpc:$ taskset -c 0 ./myprog.x &
alice@hpc:$ taskset -c 4 ./myprog.x &
alice@hpc:$ wait
```

Farming Jobs

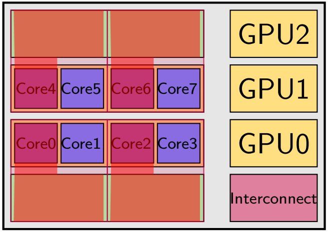


- Loops can be used to start and pin huge amounts of processes

Terminal

```
alice@hpc:$ for i in $(seq 0 1 7); do taskset -c ${i} ./myprog.x & done
alice@hpc:$ wait
```

Farming Jobs



- Loops can be used to start and pin huge amounts of processes
- For memory intensive jobs cores can be skipped

Terminal

```
alice@hpc:$ for i in $(seq 0 2 7); do taskset -c ${i} ./myprog.x & done
alice@hpc:$ wait
```

Exercise 3

1. Read the `farming_job.sh` script and fill in all `FIX_ME`
2. Read the farming outputfile and check the pinning

Exercise 3

1 Read the `farming_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
# loop to pin processes to different cores
for icore in $(seq <FIX_ME>)
do
    taskset -c <FIX_ME> ${pinnalizer} > farming_${icore}.tmpout &
done
...
```

Exercise 3

1 Read the `farming_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
# loop to pin processes to different cores
for icore in $(seq 4)
do
    taskset -c <FIX_ME> ${pinnalizer} > farming_${icore}.tmpout &
done
...
```

Exercise 3

1. Read the `farming_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
# loop to pin processes to different cores
for icore in $(seq 4)
do
    taskset -c ${icore} ${pinnalizer} > farming_${icore}.tmpout &
done
...
```

Exercise 3

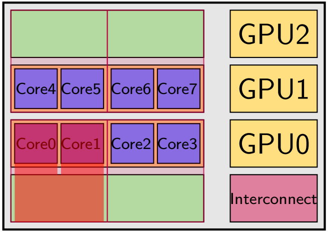
RUB

2 Read the farming outputfile and check the pinning

Terminal

```
alice@hpc:$ cat farming-1234.out
Running process  0/1 on cpu  1/48 on hpc-cpu01
Running process  0/1 on cpu  2/48 on hpc-cpu01
Running process  0/1 on cpu  3/48 on hpc-cpu01
Running process  0/1 on cpu  4/48 on hpc-cpu01
```

Shared Memory Jobs

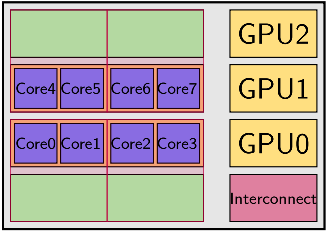


- In shared memory parallelized (or threaded) programs the process can spawn threads running on other cores, but accessing the same memory regions

Terminal

```
alice@hpc:$ ./myprog.x
```

Shared Memory Jobs

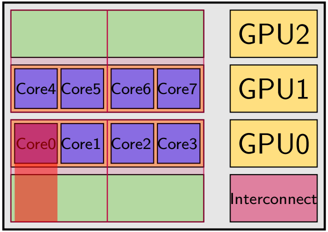


- In shared memory parallelized (or threaded) programs the process can spawn threads running on other cores, but accessing the same memory regions
- Threading is usually done via OpenMP or pthreads

Terminal

```
alice@hpc:$
```

Shared Memory Jobs

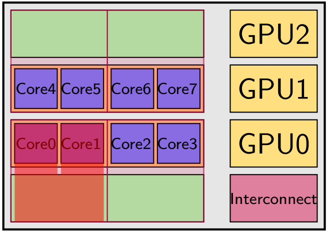


- In pthreaded programs the threading behaviour is part of the program

Terminal

```
alice@hpc:$ ./my_single_thread_prog.x
```

Shared Memory Jobs

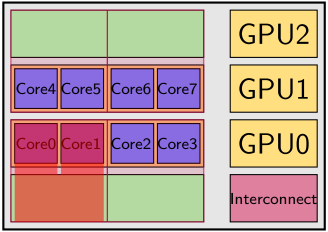


- In pthreaded programs the threading behaviour is part of the program

Terminal

```
alice@hpc:$ ./my_dual_thread_prog.x
```

Shared Memory Jobs

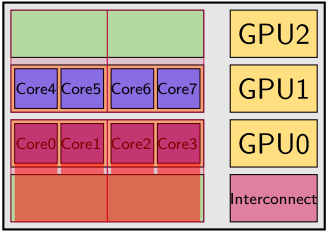


- In pthreaded programs the threading behaviour is part of the program

Terminal

```
alice@hpc:$ taskset -c 0,1 ./my_dual_thread_prog.x
```

Shared Memory Jobs

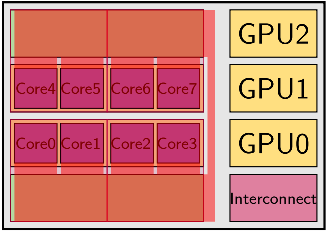


- In pthreaded programs the threading behaviour is part of the program

Terminal

```
alice@hpc:$ ./my_quad_thread_prog.x
```

Shared Memory Jobs

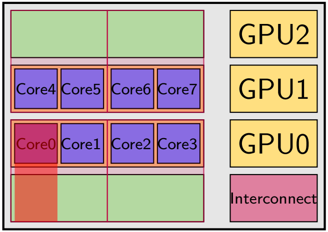


- In pthreaded programs the threading behaviour is part of the program

Terminal

```
alice@hpc:$ ./my_oct_thread_prog.x
```

Shared Memory Jobs

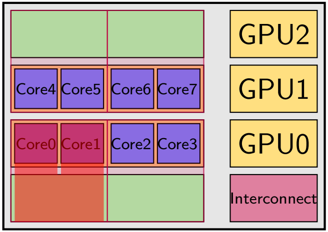


- OMP uses the `OMP_NUM_THREADS` environment variable to set the number of threads

Terminal

```
alice@hpc:$ export OMP_NUM_THREADS=1
alice@hpc:$ ./my_omp_prog.x
```

Shared Memory Jobs

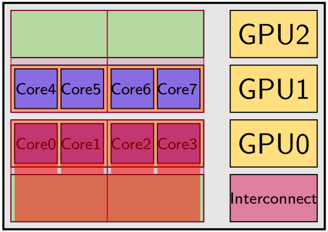


- OMP uses the `OMP_NUM_THREADS` environment variable to set the number of threads

Terminal

```
alice@hpc:$ export OMP_NUM_THREADS=2
alice@hpc:$ ./my_omp_prog.x
```

Shared Memory Jobs

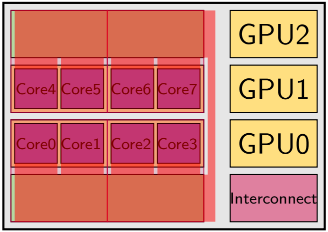


- OMP uses the `OMP_NUM_THREADS` environment variable to set the number of threads

Terminal

```
alice@hpc:$ export OMP_NUM_THREADS=4
alice@hpc:$ ./my_omp_prog.x
```

Shared Memory Jobs



- OMP uses the `OMP_NUM_THREADS` environment variable to set the number of threads

Terminal

```
alice@hpc:$ export OMP_NUM_THREADS=8
alice@hpc:$ ./my_omp_prog.x
```

Exercise 4

1. Read the `shared_mem_job.sh` script and fill in all `FIX_ME`
2. Read the shared-mem outputfile and check the pinning

Exercise 4

RUB

1 Read the `shared_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
# Define number of threads
export OMP_NUM_THREADS=                                  <= FIX_ME
...
```

Exercise 4

1 Read the `shared_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
# Define number of threads
export OMP_NUM_THREADS=4
...
```

Exercise 4

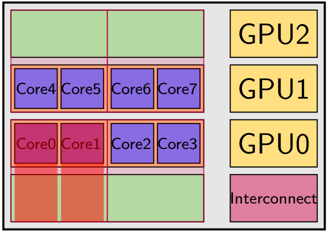
2 Read the shared-mem outputfile and check the pinning

Terminal

```
alice@hpc:$ cat shared_mem-1234.out
Running process  0/1, thread  0/4 on cpu 2/48 on hpc-cpu01
Running process  0/1, thread  1/4 on cpu 0/48 on hpc-cpu01
Running process  0/1, thread  2/4 on cpu 3/48 on hpc-cpu01
Running process  0/1, thread  3/4 on cpu 8/48 on hpc-cpu01
```

Distributed Memory Jobs

- In distributed memory parallelized programs several processes are started without direct access to the other processes memory

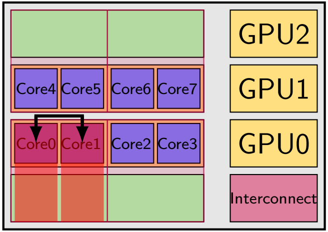


Terminal

```
alice@hpc:$
alice@hpc:$
```

Distributed Memory Jobs

- Exchange of data between processes is usually done via the Message Passing Interface (MPI)

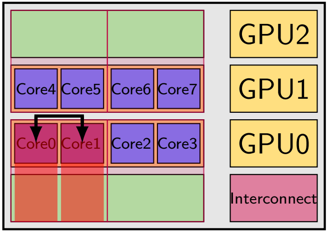


Terminal

```
alice@hpc:$
alice@hpc:$
```

Distributed Memory Jobs

- Most common MPI implementaions are OpenMPI and IntelMPI

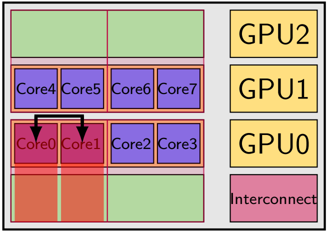


Terminal

```
alice@hpc:$
alice@hpc:$
```

Distributed Memory Jobs

- `mpirun` is a wrapper that manages process spawning and the communication channels between them

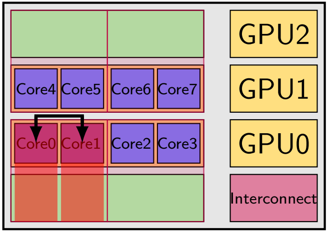


Terminal

```
alice@hpc:$ mpirun -np 2 ./myprog.x                                    #OpenMPI
alice@hpc:$ mpirun -n 2 ./myprog.x                                     #IntelMPI
```

Distributed Memory Jobs

- OpenMPI: `-np <n>` ⇒ number of processes
- IntelMPI: `-n <n>` ⇒ number of processes

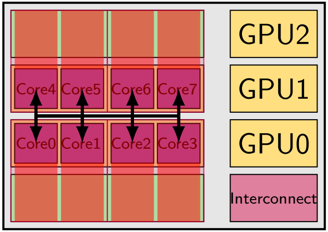


Terminal

```
alice@hpc:$ mpirun -np 2 ./myprog.x                                  #OpenMPI
alice@hpc:$ mpirun -n 2 ./myprog.x                                   #IntelMPI
```

Distributed Memory Jobs

- OpenMPI: `-np <n>` ⇒ number of processes
- IntelMPI: `-n <n>` ⇒ number of processes

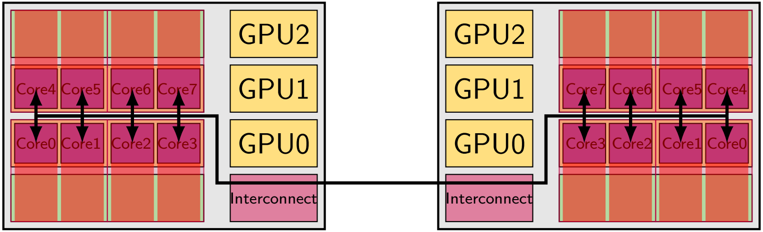


Terminal

```
alice@hpc:$ mpirun -np 8 ./myprog.x                #OpenMPI
alice@hpc:$ mpirun -n 8 ./myprog.x                 #IntelMPI
```

Distributed Memory Jobs

- OpenMPI: `--map-by ppr:<n>:node` ⇒ processes per node
- IntelMPI: `-ppn <n>` ⇒ processes per node

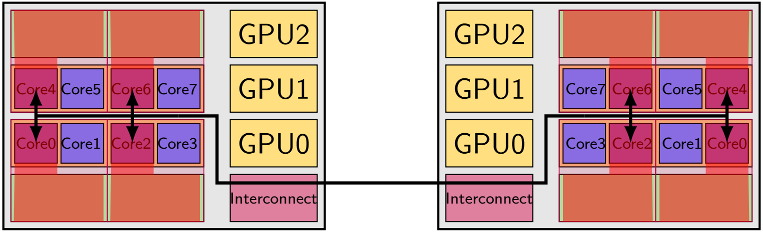


Terminal

```
alice@hpc:$ mpirun -np 16 --map-by ppr:8:node ./myprog.x          #OpenMPI
alice@hpc:$ mpirun -n 16 -ppn 8 ./myprog.x                        #IntelMPI
```

Distributed Memory Jobs

- OpenMPI: `--map-by ppr:<n>:node` ⇒ processes per node
- IntelMPI: `-ppn <n>` ⇒ processes per node



Terminal

```
alice@hpc:$ mpirun -np 8 --map-by ppr:4:node ./myprog.x          #OpenMPI
alice@hpc:$ mpirun -n 8 -ppn 4 ./myprog.x                         #IntelMPI
```

Exercise 5

1 Read the `distributed_mem_job.sh` script and fill in all `FIX_ME`
2 Read the mpi outputfile and check the pinning

Exercise 5

RUB

1 Read the `distributed_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=                                <= FIX_ME
...
# execute program with MPI for distributed memory job
mpirun -np <FIX_ME> --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 5

1 Read the `distributed_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# execute program with MPI for distributed memory job
mpirun -np <FIX_ME> --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 5

1 Read the `distributed_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# execute program with MPI for distributed memory job
mpirun -np 4 --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 5

RUB

1 Read the `distributed_mem_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# execute program with MPI for distributed memory job
mpirun -np 4 --map-by ppr:2:node ${pinnalizer}
```

Exercise 5

2 Read the mpi outputfile and check the pinning

Terminal

```
alice@hpc:$ cat distr_mem-1234.out
Running process  0/4 on cpu  0/48 on hpc-cpu01
Running process  1/4 on cpu  2/48 on hpc-cpu01
Running process  2/4 on cpu  0/48 on hpc-cpu02
Running process  3/4 on cpu  2/48 on hpc-cpu02
```

Exercise 6

1. Read the `hybrid_job.sh` script and fill in all `FIX_ME`
2. Read the hybrid outputfile and check the pinning

Exercise 6

RUB

1 Read the `hybrid_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=                                <= FIX_ME
...
# Define number of threads
export OMP_NUM_THREADS=                         <= FIX_ME
# execute program with MPI for distributed memory job
mpirun -np <FIX_ME> --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 6

1 Read the `hybrid_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# Define number of threads
export OMP_NUM_THREADS=                          <= FIX_ME
# execute program with MPI for distributed memory job
mpirun -np <FIX_ME> --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 6

1 Read the `hybrid_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# Define number of threads
export OMP_NUM_THREADS=2
# execute program with MPI for distributed memory job
mpirun -np <FIX_ME> --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 6

1 Read the `hybrid_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# Define number of threads
export OMP_NUM_THREADS=2
# execute program with MPI for distributed memory job
mpirun -np 4 --map-by ppr:<FIX_ME>:node ${pinnalizer}
```

Exercise 6

RUB

1 Read the `hybrid_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --nodes=2
...
# Define number of threads
export OMP_NUM_THREADS=2
# execute program with MPI for distributed memory job
mpirun -np 4 --map-by ppr:2:node ${pinnalizer}
```

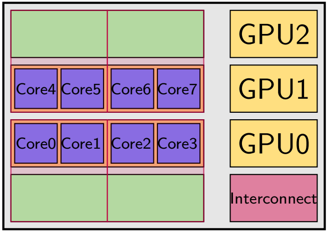
Exercise 6

2 Read the hybrid outputfile and check the pinning

Terminal

```
alice@hpc:$ cat hybr_mem-1234.out
Running process  0/4, thread  1/2 on cpu  1/48 on hpc-cpu01
Running process  0/4, thread  0/2 on cpu  0/48 on hpc-cpu01
Running process  1/4, thread  0/2 on cpu  3/48 on hpc-cpu01
Running process  1/4, thread  1/2 on cpu  2/48 on hpc-cpu01
Running process  2/4, thread  1/2 on cpu  1/48 on hpc-cpu02
Running process  2/4, thread  0/2 on cpu  0/48 on hpc-cpu02
Running process  3/4, thread  0/2 on cpu  3/48 on hpc-cpu02
Running process  3/4, thread  1/2 on cpu  2/48 on hpc-cpu02
```

(NVIDIA–) GPU Accelerated Jobs

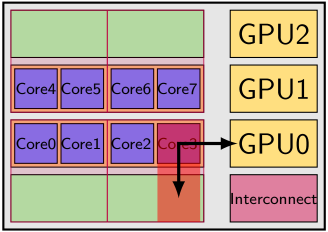


- The GPU acceleration is part of the CUDA program.

Terminal

```
alice@hpc:$
```

(NVIDIA–) GPU Accelerated Jobs

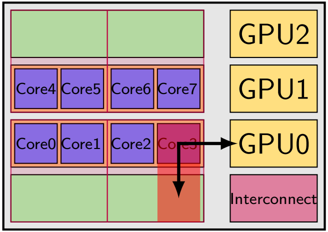


- The GPU acceleration is part of the CUDA program.
- GPUs need a CPU-Host for data transfer, I/O, . . .

Terminal

```
alice@hpc:$ ./my_CUDA_prog.x
```

(NVIDIA–) GPU Accelerated Jobs

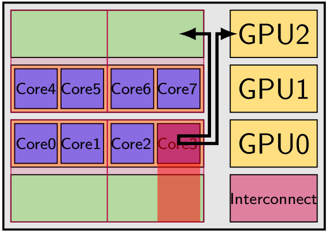


- The `CUDA_VISIBLE_DEVICES` environment variable selects the GPUs
- GPUs can be closer to one of the CPUs making them better suited for host tasks. Check with `nvidia-smi`

Terminal

```
alice@hpc:$ export CUDA_VISIBLE_DEVICES=0
alice@hpc:$ ./my_CUDA_prog.x
```

(NVIDIA–) GPU Accelerated Jobs



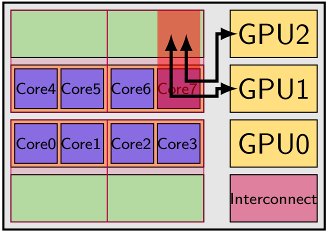
- The `CUDA_VISIBLE_DEVICES` environment variable selects the GPUs
- GPUs can be closer to one of the CPUs making them better suited for host tasks. Check with `nvidia-smi`

Terminal

```
alice@hpc:$ export CUDA_VISIBLE_DEVICES=2
alice@hpc:$ ./my_CUDA_prog.x
```

(NVIDIA–) GPU Accelerated Jobs

RUB



- The `CUDA_VISIBLE_DEVICES` environment variable selects the GPUs
- GPUs can be closer to one of the CPUs making them better suited for host tasks. Check with `nvidia-smi`

Terminal

```
alice@hpc:$ export CUDA_VISIBLE_DEVICES=1,2
alice@hpc:$ ./my_CUDA_prog.x
```

Exercise 7

1. Read the `cuda_job.sh` script and fill in all `FIX_ME`
2. Read the cuda outputfile and check the pinning and GPU

Exercise 7

RUB

1 Read the `cuda_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --partition=                              <= FIX_ME
...
# CUDA_VISIBLE_DEVICES is also set by SLURM,
# depending on the allocated gpus
export CUDA_VISIBLE_DEVICES=                      <= FIX_ME
...
```

Exercise 7

RUB

1 Read the `cuda_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --partition=gpu
...
# CUDA_VISIBLE_DEVICES is also set by SLURM,
# depending on the allocated gpus
export CUDA_VISIBLE_DEVICES=                       <= FIX_ME
...
```

Exercise 7

1 Read the `cuda_job.sh` script and fill in all `FIX_ME`

Terminal

```
...
#SBATCH --partition=gpu
...
# CUDA_VISIBLE_DEVICES is also set by SLURM,
# depending on the allocated gpus
export CUDA_VISIBLE_DEVICES=0
...
```

Exercise 7

2 Read the cuda outputfile and check the pinning and GPU

Terminal

```
alice@hpc:$ cat cuda-1234.out
...
|-----------------------------------------+-...-+
| GPU  Name                  Persistence-M | ... |
| Fan  Temp   Perf           Pwr:Usage/Cap | ... |
|                                          | ... |
|=========================================+=...=|
|   0  Tesla V100-PCIE-16GB           Off | ... |
| N/A   33C    P0             25W /  250W | ... |
|                                          | ... |
+-----------------------------------------+-...-+
...
```

Exercise 7

2 Read the cuda outputfile and check the pinning and GPU

Terminal

```
...
+-----------------------------------------------...------------+
| Processes:                                    ...            |
|  GPU   GI   CI        PID   Type   Process name ... GPU Memory |
|        ID   ID                                  ... Usage      |
|===============================================...============|
|  No running processes found                     ...            |
+-----------------------------------------------...------------+
...
```

Exercise 7

2 Read the cuda outputfile and check the pinning and GPU

Terminal

```
...
        GPU0     CPU Affinity     NUMA Affinity    GPU NUMA ID
GPU0     X       0-31,64-95       0                N/A
...
```

Exercise 7

2 Read the cuda outputfile and check the pinning and GPU

Terminal

```
...
Running process  0/1 on cpu 79/128 on hpc-gpu01 with 1 X Tesla V100-PCIE-16GB
```

Software Versions

User Requirements Differ

Alice:
I need the newest GNU-compiler.

User Requirements Differ

<u>Alice:</u>
I need the newest GNU-compiler.

<u>Bob:</u>
My CUDA code does not work with GNU-compilers of version $> 10.x$.

User Requirements Differ

Alice:
I need the newest GNU-compiler.

Carol:
My OpenMPI needs to be tuned to work with Intel-compilers.

Bob:
My CUDA code does not work with GNU-compilers of version $> 10.x$.

User Requirements Differ

Alice:
I need the newest

Dave:
But my OpenMPI needs to be tuned to work with GNU-compilers.

Carol:
My OpenMPI needs to be tuned to work with Intel-compilers.

Bob:
My CUDA code does not work with GNU-compilers of version $> 10.x$.

User Requirements Differ

Alice:
I need the

Dave:
But my OpenMP
needs to be tuned
to work with GNU
compilers.

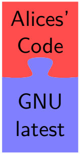
Carol:
My OpenMPI needs to be tuned to work with Intel-compilers.

Eve:
I need this one specific combination of compiler/mpi/fftw/BLAS/Lapack-/Scalapack/. But I need everything for two different compilers to see which is faster.

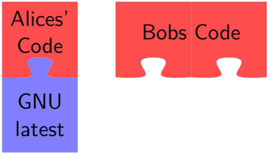
not work with GNU-compilers of version $> 10.x$.

A Modular Approach

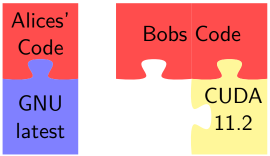
A Modular Approach



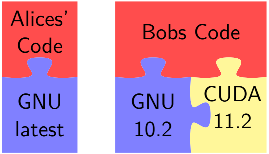
A Modular Approach



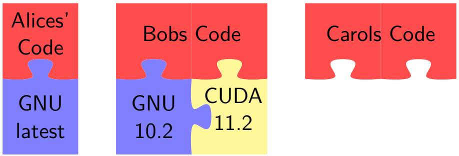
A Modular Approach



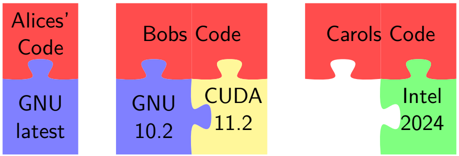
A Modular Approach



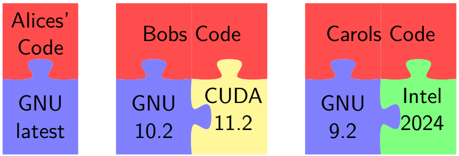
A Modular Approach



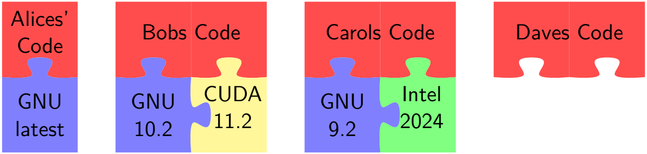
A Modular Approach



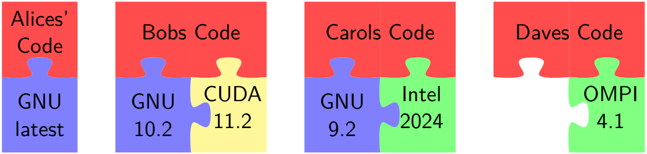
A Modular Approach



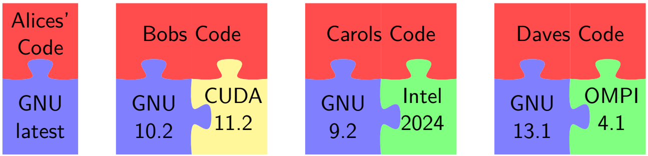
A Modular Approach



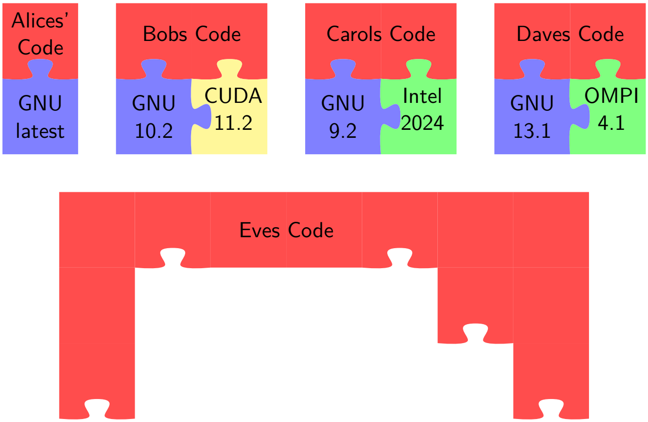
A Modular Approach



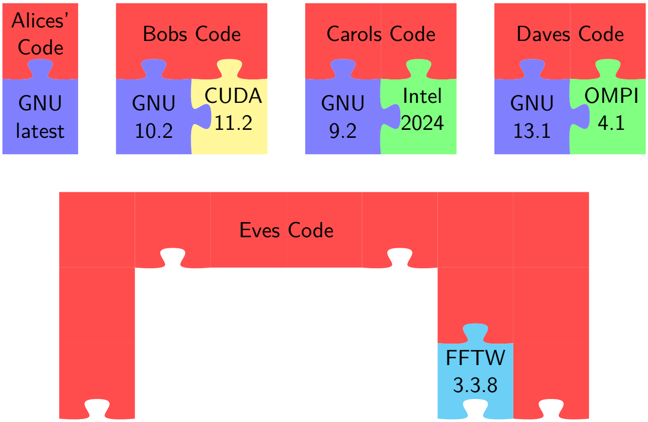
A Modular Approach



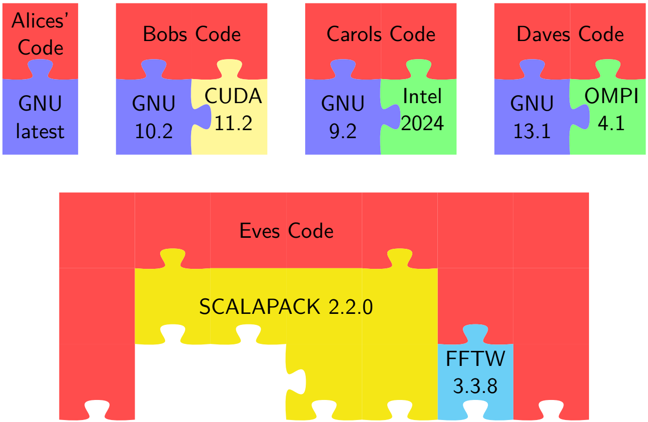
A Modular Approach



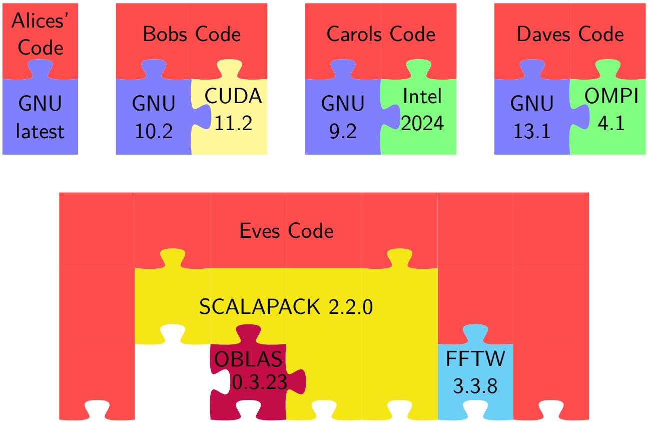
A Modular Approach



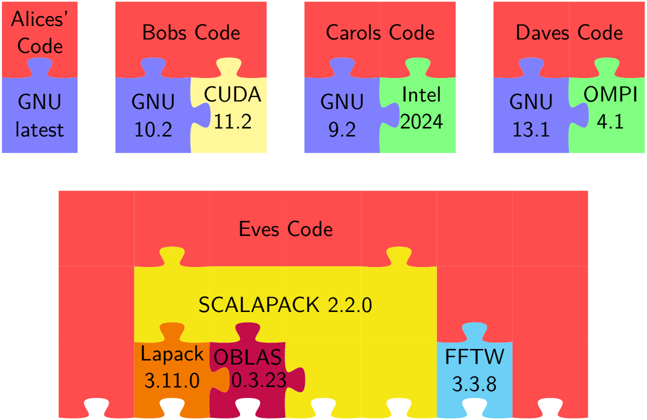
A Modular Approach



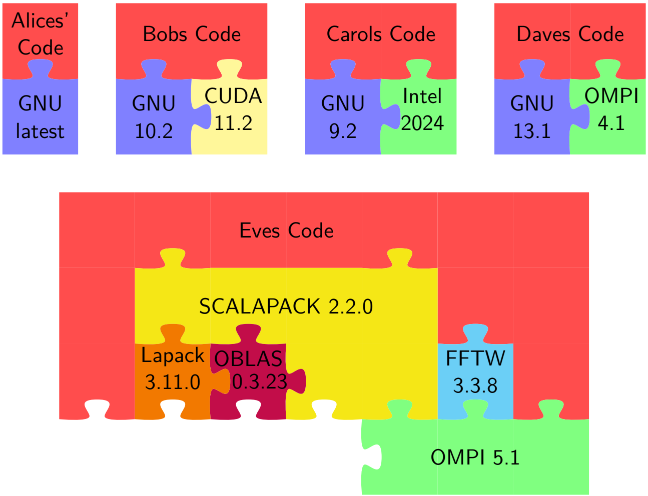
A Modular Approach



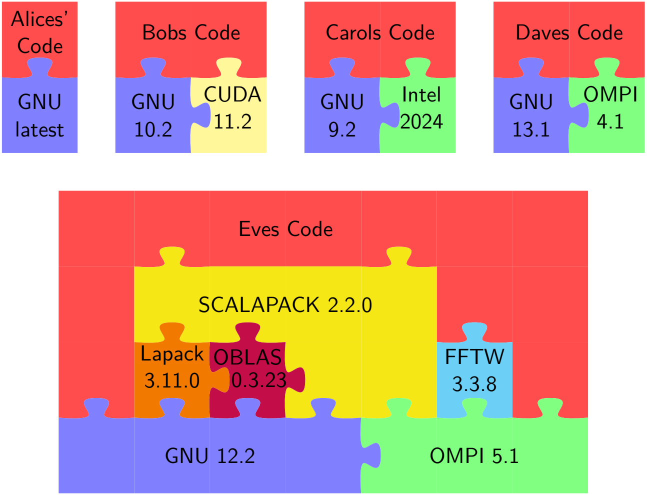
A Modular Approach



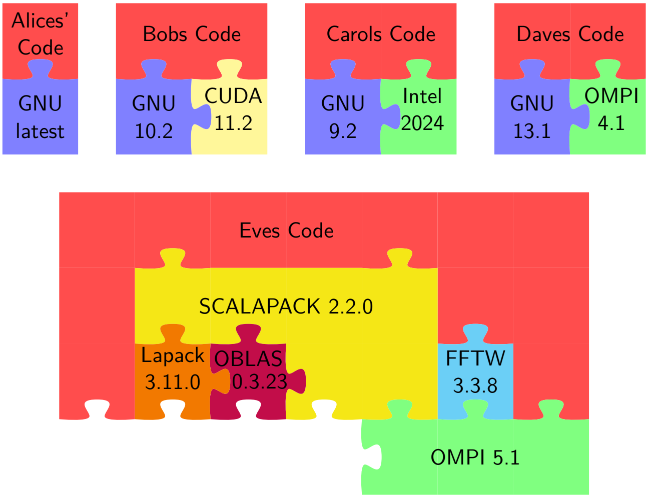
A Modular Approach



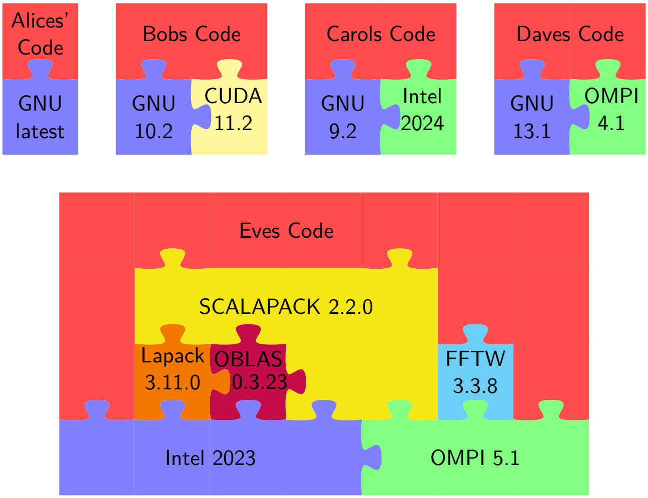
A Modular Approach



A Modular Approach



A Modular Approach



Environment modules allow users to temporarily change default executable/library path.

Terminal

```
alice@hpc:$ which gcc
/usr/bin/gcc
```

Environment modules allow users to temporarily change default executable/library path.

`module load <modulename>` loads a module and changes executable/library path.

Terminal

```
alice@hpc:$ which gcc
/usr/bin/gcc
alice@hpc:$ module load gnu9/9.4.0
alice@hpc:$ which gcc
/opt/ohpc/pub/compiler/gcc/9.4.0/bin/gcc
```

Linux Environment Modules

Environment modules allow users to temporarily change default executable/library path.

`module unload <modulename>` removes a loaded module.

Terminal

```
alice@hpc:$ which gcc
/usr/bin/gcc
alice@hpc:$ module load gnu9/9.4.0
alice@hpc:$ which gcc
/opt/ohpc/pub/compiler/gcc/9.4.0/bin/gcc
alice@hpc:$ module unload gnu9/9.4.0
alice@hpc:$ which gcc
/usr/bin/gcc
```

Linux Environment Modules

RUB

Environment modules allow users to temporarily change default executable/library path.
`module list` shows the currently loaded modules.

Terminal

```
alice@hpc:$ module list

Currently Loaded Modules:
1) autotools 2) gnu9/9.4.0
```

Linux Environment Modules

Environment modules allow users to temporarily change default executable/library path.

`module purge` unloads all modules.

Terminal

```
alice@hpc:$ module list

Currently Loaded Modules:
1) autotools 2) gnu9/9.4.0
alice@hpc:$ module purge
```

Linux Environment Modules

Environment modules allow users to temporarily change default executable/library path.

`module purge` unloads all modules.

Terminal

```
alice@hpc:$ module list

Currently Loaded Modules:
1) autotools 2) gnu9/9.4.0
alice@hpc:$ module purge
alice@hpc:$ module list
No modules loaded
```

Linux Environment Modules

Environment modules allow users to temporarily change default executable/library path.
`module avail` shows the available modules.

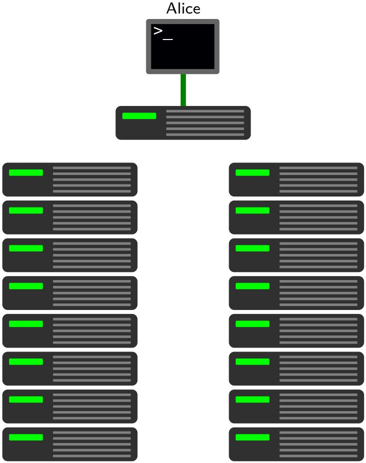
Terminal

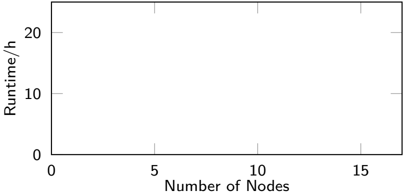
```
alice@hpc:$ module avail

----- /opt/ohpc/pub/modulefiles -----
EasyBuild/4.6.2         nvhpc/22.11
autotools               os
cmake/3.24.2            pmix/4.2.1
gnu12/12.2.0            prun/2.2
gnu9/9.4.0              singularity/3.7.1
...
```

Performance Scaling

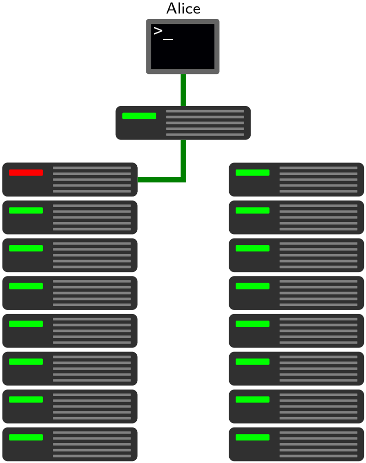
Performance Scaling

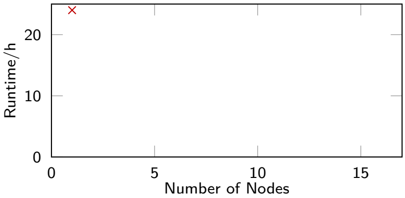




Alice is conducting Research on an HPC cluster.

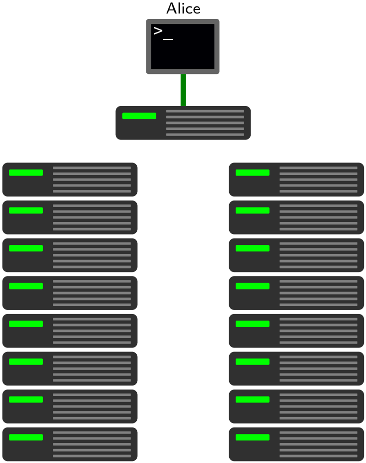
Performance Scaling

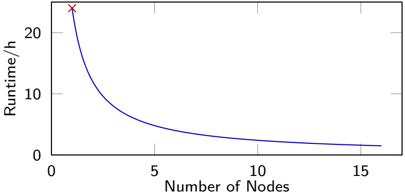




Alice runs a job on one node and measures a runtime of 24 h.

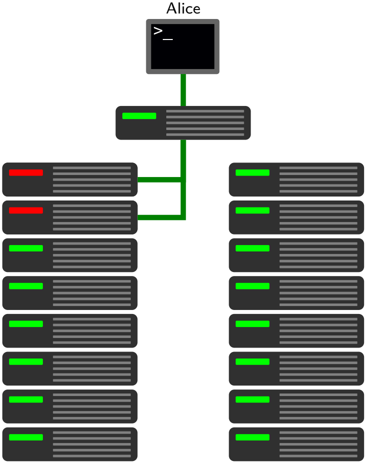
Performance Scaling

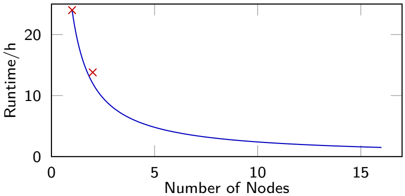




Alice guesses that the runtine scales as $t_N = \frac{t_1}{N}$.

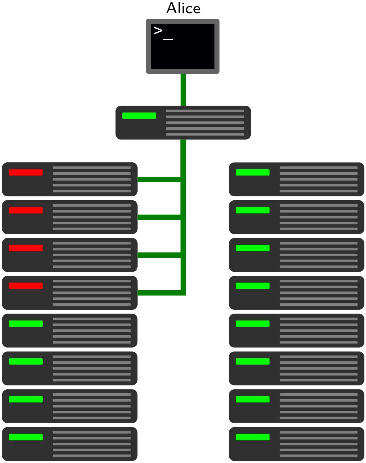
Performance Scaling

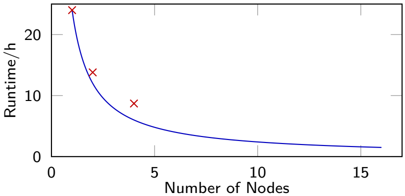




Alice doubles the number of nodes to cut the runtime in half.

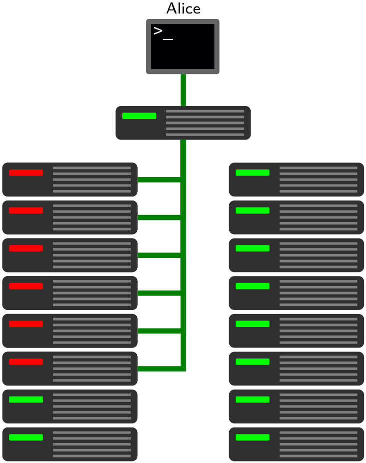
Performance Scaling

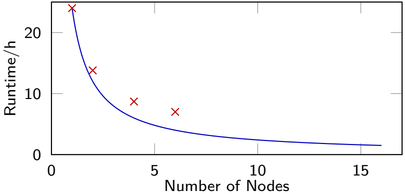




Alice measures a few different node numbers.

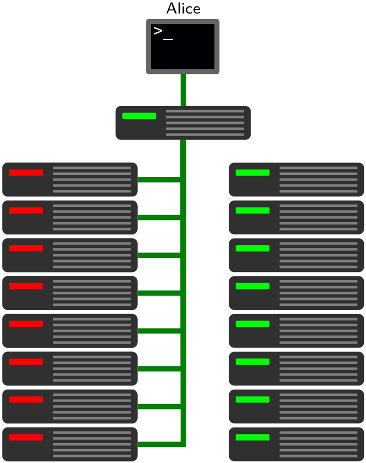
Performance Scaling

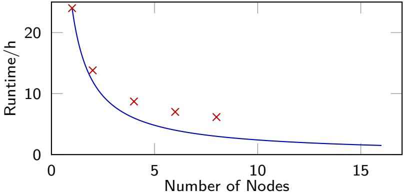




Alice measures a few different node numbers.

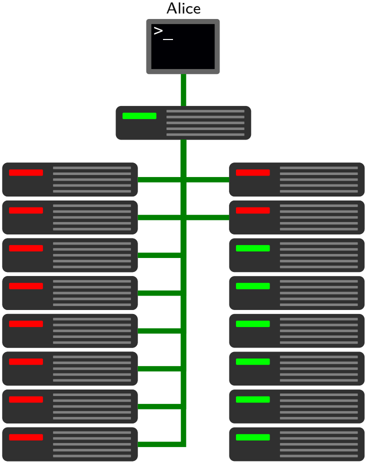
Performance Scaling

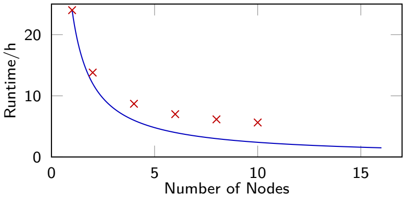




Alice measures a few different node numbers.

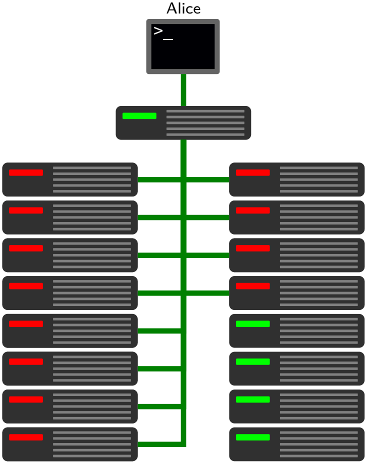
Performance Scaling

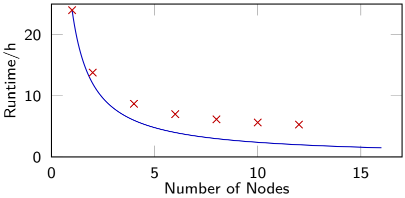




Alice measures a few different node numbers.

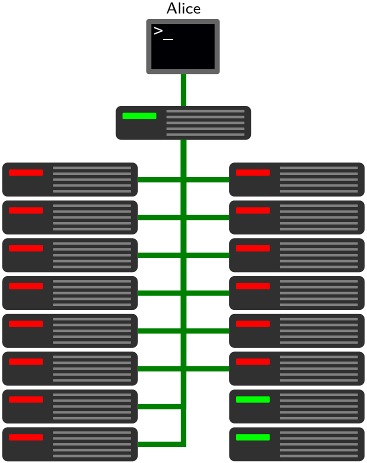
Performance Scaling

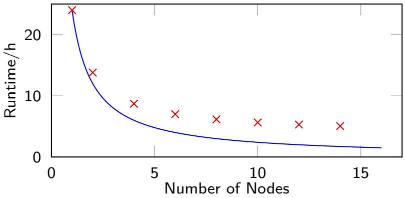




Alice measures a few different node numbers.

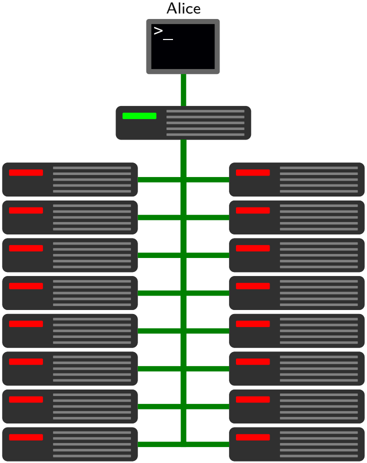
Performance Scaling

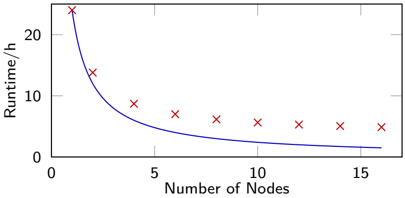




Alice measures a few different node numbers.

Performance Scaling





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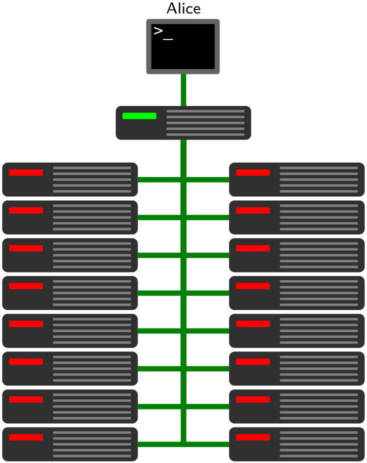
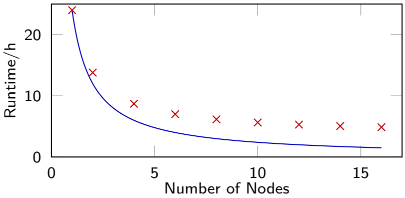
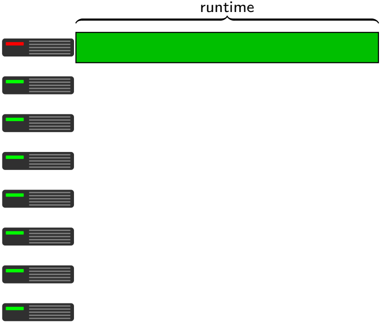
Performance Scaling

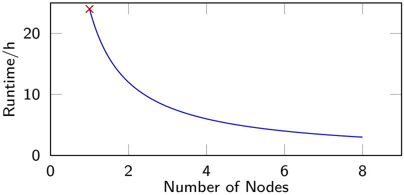




Alice finds a significant discrepancy between her idea of scaling and the measurement.

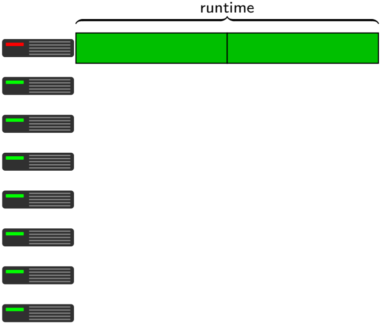
Performance Scaling: Ideal Scaling (Alice's Guess)

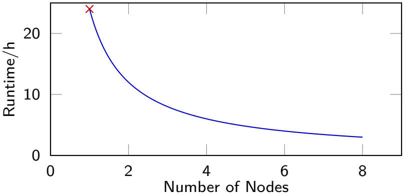




Alice runs a job on one node and measures a runtime of 24 h.

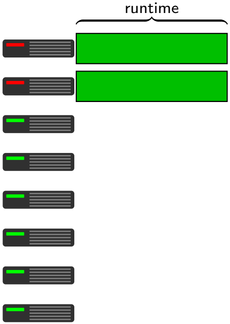
Performance Scaling: Ideal Scaling (Alice's Guess)

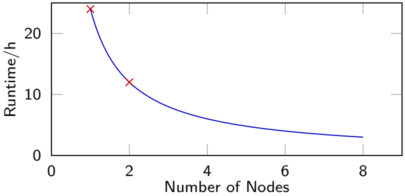




Alice splits the work into two equal parts.

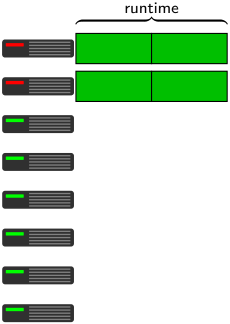
Performance Scaling: Ideal Scaling (Alice's Guess)

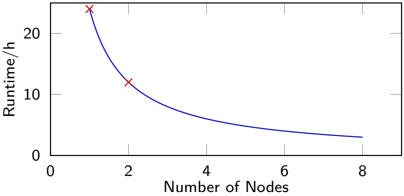




Computing both parts in parallel splits the runtime in two.

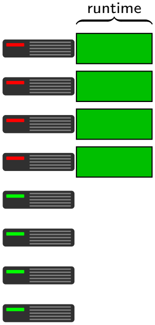
Performance Scaling: Ideal Scaling (Alice's Guess)

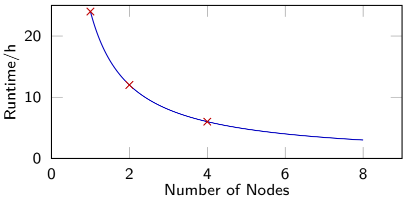




Alice splits each part in two equal parts again.

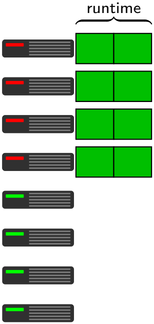
Performance Scaling: Ideal Scaling (Alice's Guess)

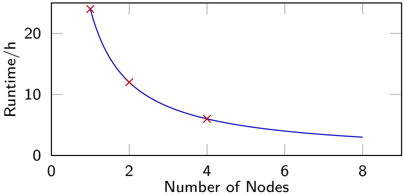




Computing all parts in parallel splits the runtime in two again.

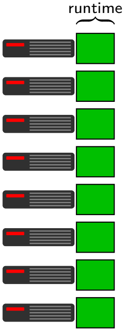
Performance Scaling: Ideal Scaling (Alice's Guess)

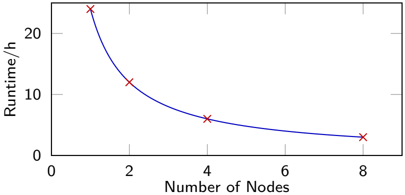




Alice splits each part in two equal parts again.

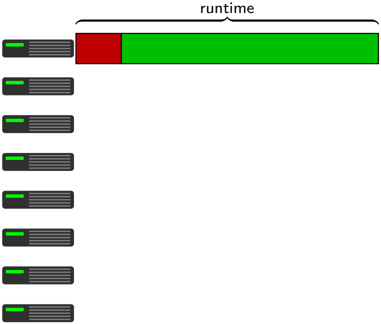
Performance Scaling: Ideal Scaling (Alice's Guess)

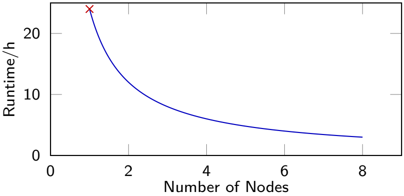




Computing all parts in parallel splits the runtime in two again.

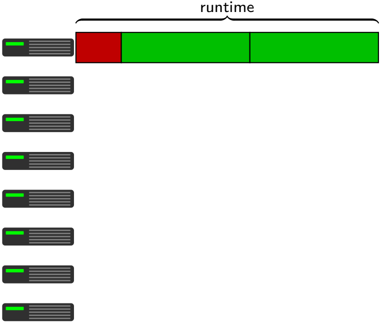
Performance Scaling: Amdahl's Law

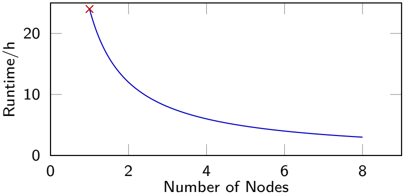




Alice' code contains some unparallelizable (serial) part (red).

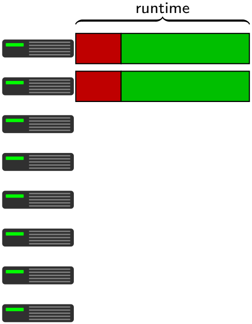
Performance Scaling: Amdahl's Law

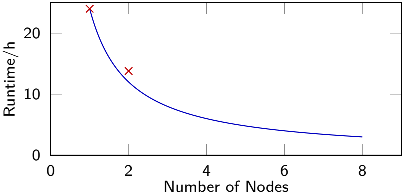




Alice splits the parallelizable work into two equal parts.

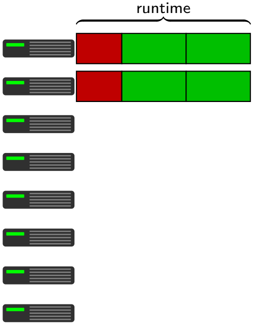
Performance Scaling: Amdahl's Law

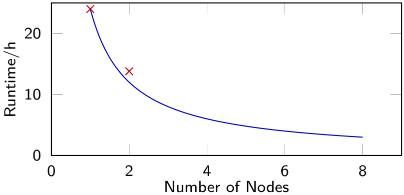




The serial part stays constant.

Performance Scaling: Amdahl's Law





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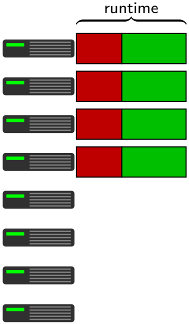

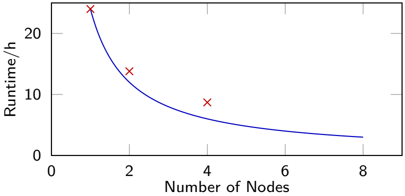

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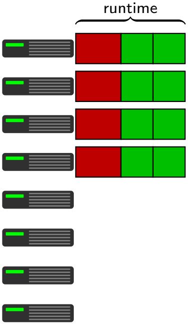

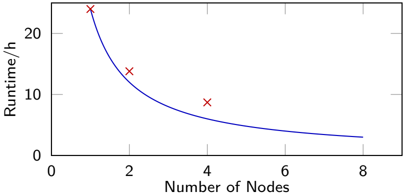

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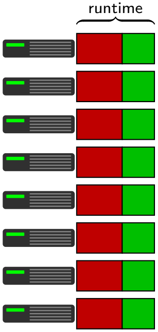

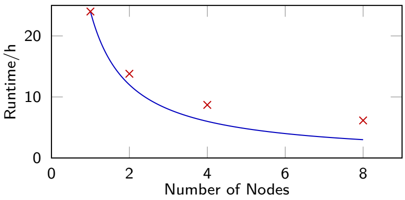

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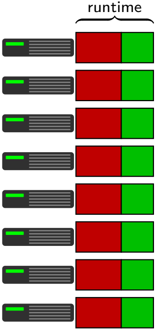
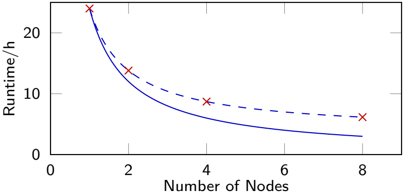
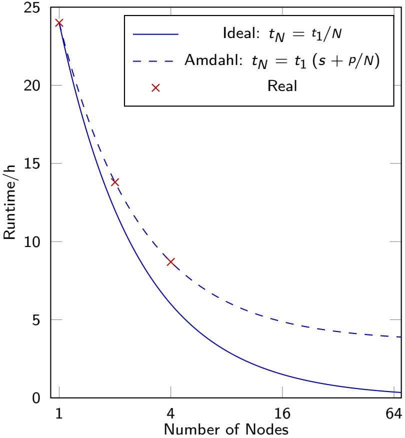




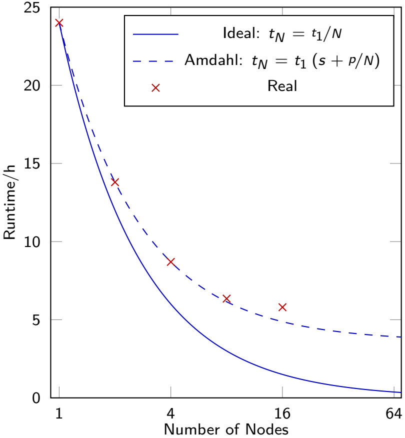
A partial parallel code scales as: $t_N = t_1 \left(s + \frac{p}{N}\right)$.

Performance Scaling: Real Scaling



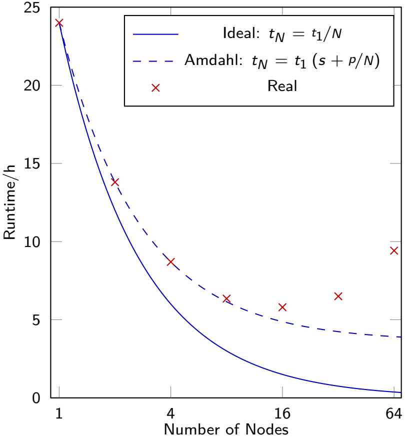
- For small node numbers many HPC codes follow an Amdahl like behavior.

Performance Scaling: Real Scaling



- For small node numbers many HPC codes follow an Amdahl like behavior.
- At some point the real behavior will deviate from Amdahl's law and stagnate.

Performance Scaling: Real Scaling



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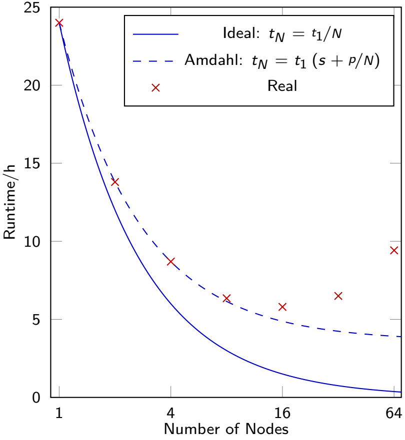

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  - Workload cannot be split into smaller sections.

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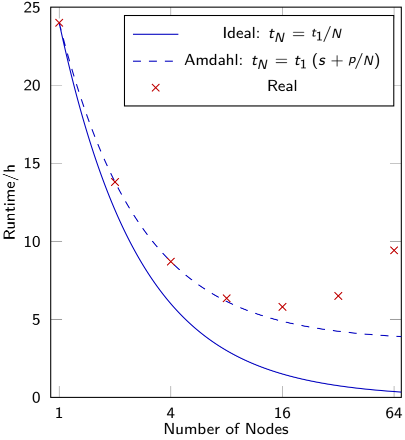


- For small node numbers many HPC codes follow an Amdahl like behavior.
- At some point the real behavior will deviate from Amdahl's law and stagnate.
- In many cases the runtime can worsen with higher node numbers because:
  - Workload cannot be split into smaller sections.
  - Network latency and bandwidth limitations.

Code of Conduct

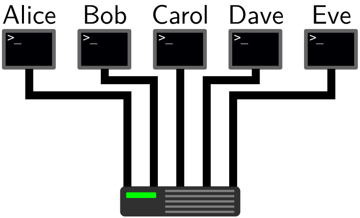
RUB

Rules

1. Participating on an HPC system requires constant care and mutual respect.
2. A person using an HPC system shall act in such a way as not to hinder or inconvenience any other person more than is unavoidable in the circumstances.

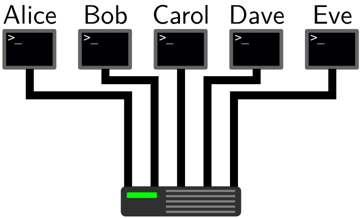
[1] Based on: Deutsche Straßenverkehrs-Ordnung(StVO) § 1 Grundregeln

Example: Copying Data from/to HPC Cluster



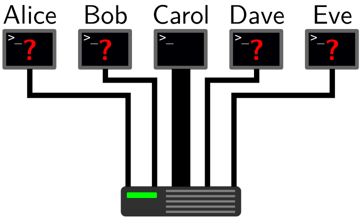
- Multiple users are connected to the login node.

Example: Copying Data from/to HPC Cluster



- Multiple users are connected to the login node.
- Carol wants to copy huge amounts of data to/from the cluster.

Example: Copying Data from/to HPC Cluster



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- Carol hugs all the bandwidth.

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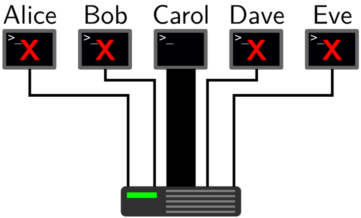


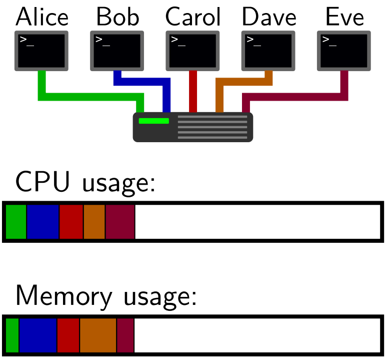
- Multiple users are connected to the login node.
- Carol wants to copy huge amounts of data to/from the cluster.
- Carol hugs all the bandwidth.
- The connection for everyone else gets unusable.

Example: Copying Data from/to HPC Cluster

Copying Data from/to HPC Cluster

1. Utilize a bandwidthlimit (e.g. `rsync -bwlimit=<rate>`)
2. Multiple parallel copy processes are not faster than one process.
3. Copying multiple small files is more demanding than few big ones. Use `tar` to pack files together.

Example: Exhausting Login Node Resources



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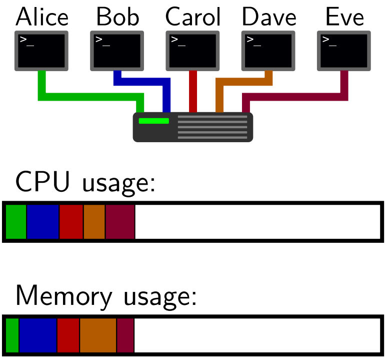

- Multiple users are connected to the login node.
- The CPU is idling and memory is free. Everyone has enough resources for their work.

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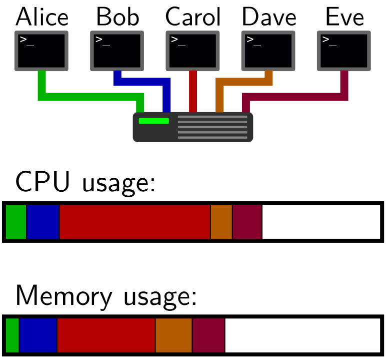

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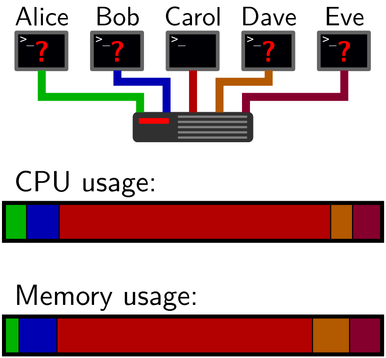

- Multiple users are connected to the login node.
- The CPU is idling and memory is free. Everyone has enough resources for their work.
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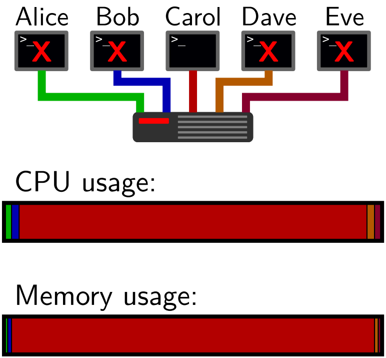

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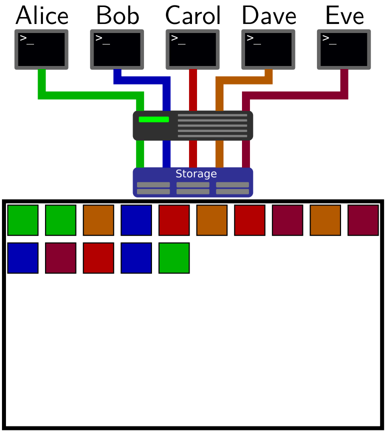
Example: Exhausting Login Node Resources

Exhausting Login Node Resources

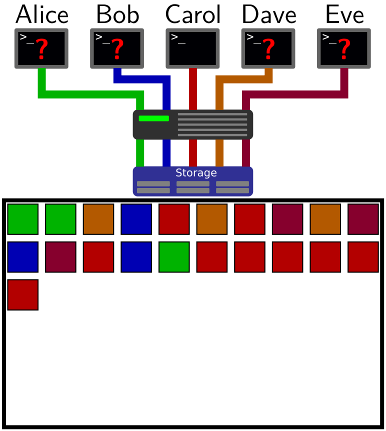
1. The login node is only suited for small analysis/compilation tasks.
2. If lots of resources are required for analysis/compilation/... request a compute node.
3. Intense processes on the login node will be killed.
4. Repeated offenders might be banned from using HPC Clusters.

Example: Stress Shared File System



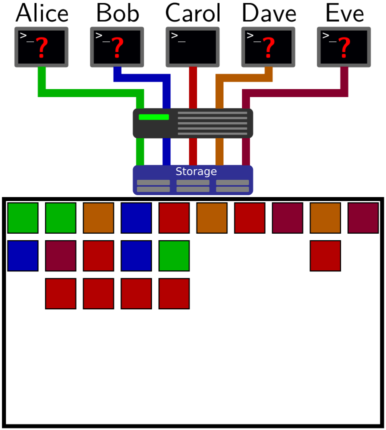
- Multiple users utilize the global storage system.

Example: Stress Shared File System



- Multiple users utilize the global storage system.
- Carol's computations quickly writes/deletes/opens/closes a lot of files on the global files system.

Example: Stress Shared File System



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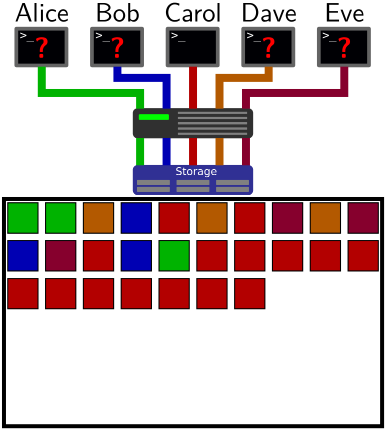

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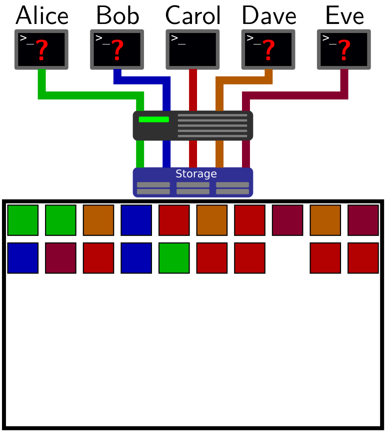

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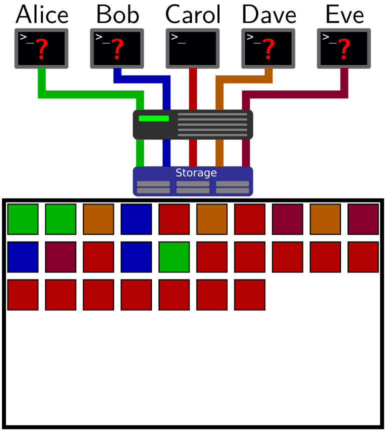

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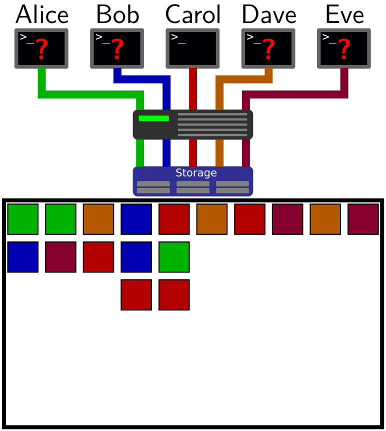

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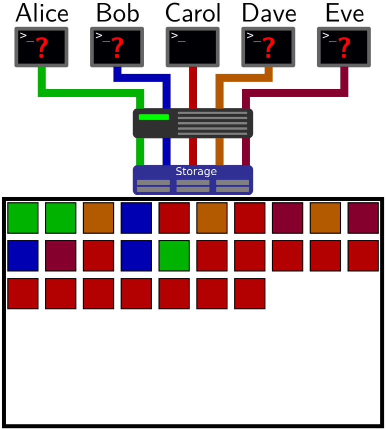

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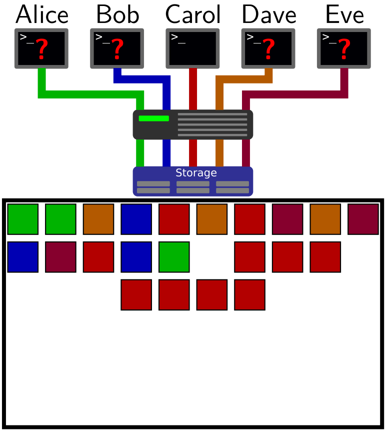

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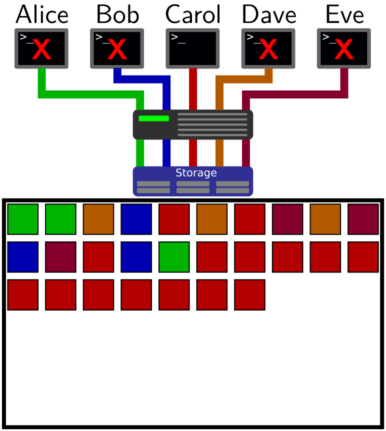


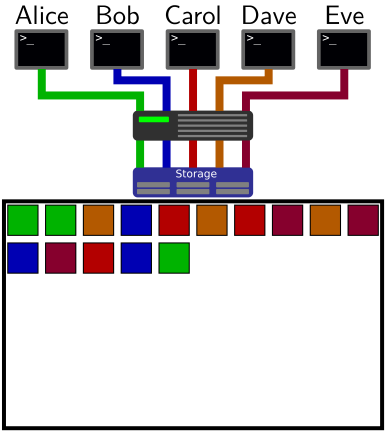
- Multiple users utilize the global storage system.
- Carol's computations quickly writes/deletes/opens/closes a lot of files on the global files system.
- Many quick global operations are poison for shared file systems, rendering it useless for everyone.

Example: Stress Shared File System

Stress Shared File System

1. Utilize local file systems for temporary data.
2. Write/read to/from the shared file system in few big chunks.

Example: Fill the Filesystem



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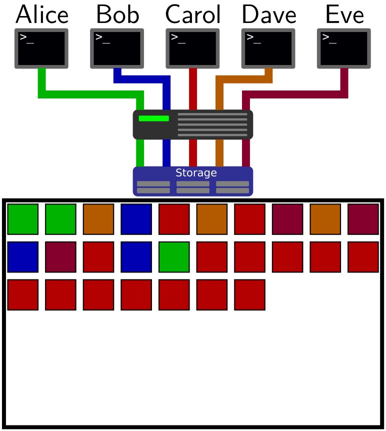

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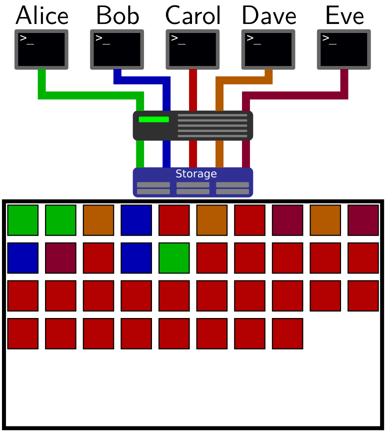

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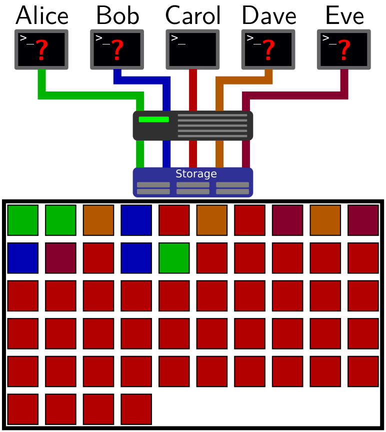

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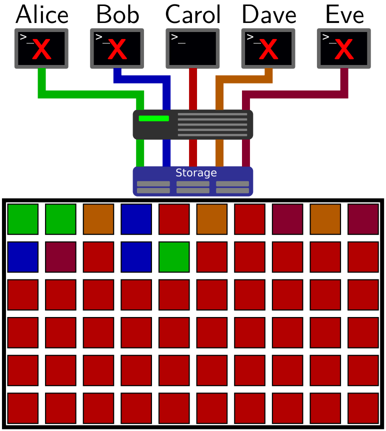


- Multiple users utilize the global storage system.
- Carol's computations dump a lot of data onto the global files system.
- There is no longer enough storage left for everyone to use.

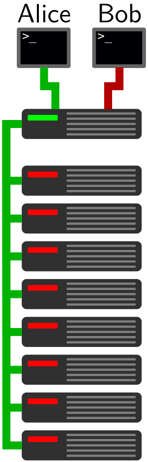
Example: Fill the Filesystem

RUB

Fill the Filesystem

1. The Filesystem utilizes quotas, preventing users from storing more data than a certain share.
2. Regularly tidy up your data to keep the storage free for further computations.

Example: Work on Already Used Nodes



- All nodes are allocated for jobs.

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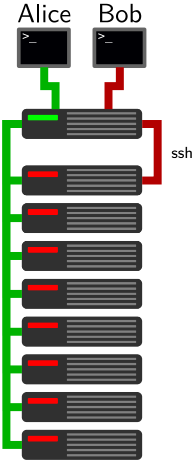

- All nodes are allocated for jobs.
- Bob does not want to wait for his slot, ignores the resource manager and connects to a node directly.

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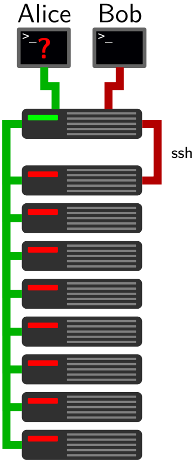


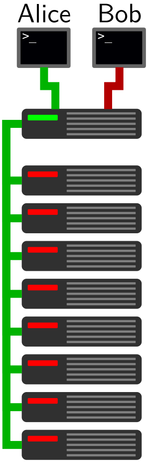
- All nodes are allocated for jobs.
- Bob does not want to wait for his slot, ignores the resource manager and connects to a node directly.
- Alice wonders why her calculation slows down.

Example: Work on Already Used Nodes

Work on Already Used Nodes

1. Resource allocation should always be done via SLURM.
2. The HPC-Clusters are setup such that ssh connections to nodes are denied unless the user also owns the job running on that node.

Example: Hugging Compute Nodes



- Alice is not computing anything, but she reserved all nodes for an extended period of time just in case.

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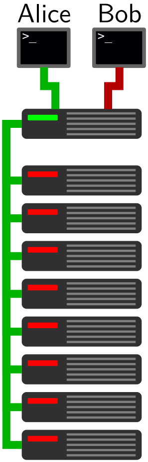

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- Bob has urgent research, but cannot get free nodes.

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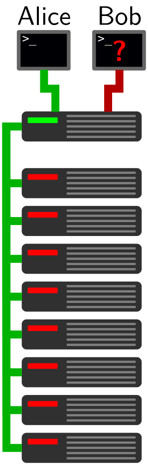

- Alice is not computing anything, but she reserved all nodes for an extended period of time just in case.
- Bob has urgent research, but cannot get free nodes.
- Alice is wasting valuable resources.

Example: Hugging Compute Nodes

RUB

Hugging Compute Nodes

1. Jobs have a maximum time to prevent node-hugging.
2. Node-hugging is punished by the SLURM accountant by lowering the users priority for scheduling new jobs.

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- Keep your private key private! Use TFA for secure access!
- HPC resources are shared. Be considered of others!
- Assist the scheduler with accurate runtime estimates!
- The accounting will ensure that everybody gets their share of computing time!
- More resources will not necessarily speedup your computation!

Happy Computing!