Biogenouest

ifb
INSTITUT FRANÇAIS DE BIOINFORMATIQUE

EMBRC FRANCE
CENTRE NATIONAL DE RESSOURCES BIOLOGIQUES MARINES

OCEANOMICS

IDEALG
seaweed for the future

Abims 4

Cluster Initiation

Cycle de formation 2017

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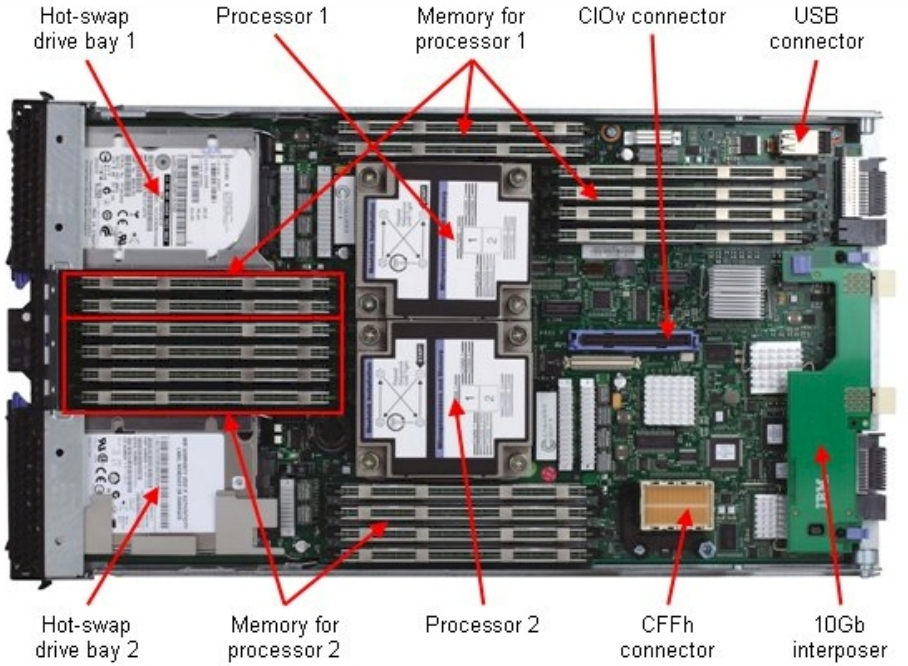
cnrs

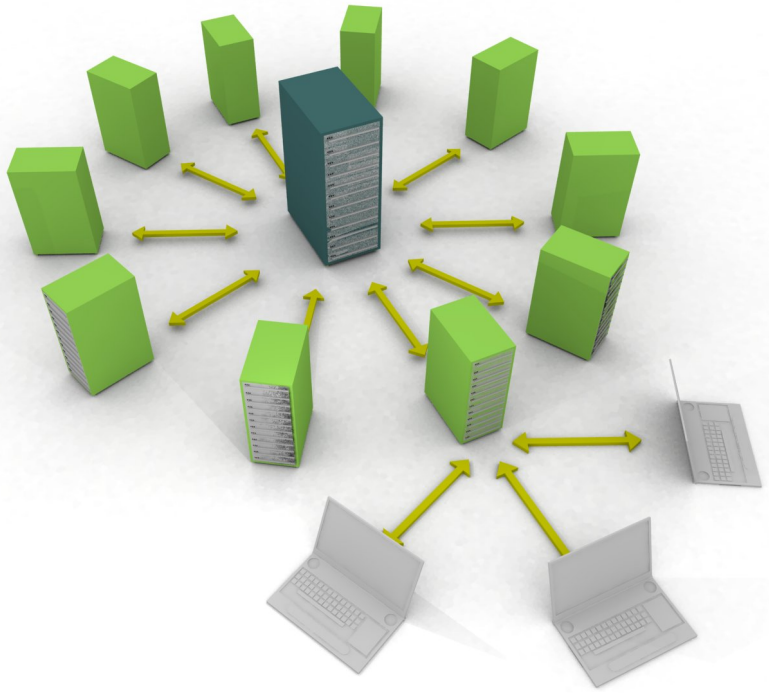
http://abims.sb-roscoff.fr/resources/cluster/howto

Principle

- Aggregation of computers / machines
  - Machine = node
- Distributed computing + shared access
- Transparent managment for users
- Community system → rules!

Hardware


Hot-swap drive bay 1
Processor 1
Memory for processor 1
CIOv connector
USB connector
Hot-swap drive bay 2
Memory for processor 2
Processor 2
CFFh connector
10Gb interposer



DISTRIBUTED COMPUTING

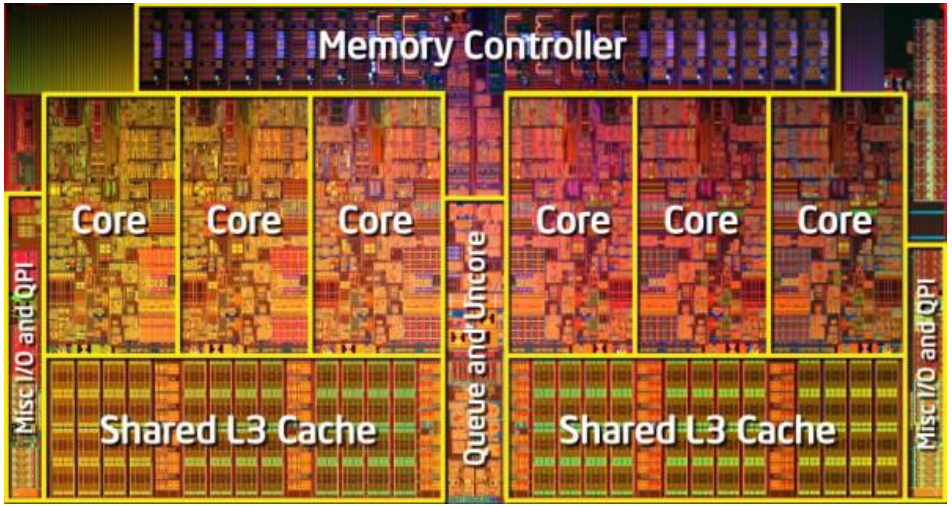
Distributed computing

- Distribution
  - Make a job as atomic as possible
  - Simple and robust
  - Linear gain
- Generate independent tasks
  - Split the data
  - Change parameters

Multithreading

- Thread
  - Tasks running on the same machine but on several CPU or core
  - Shared memory
  - Nonlinear gain

  - Ex: Tophat, CLC, Blast,…

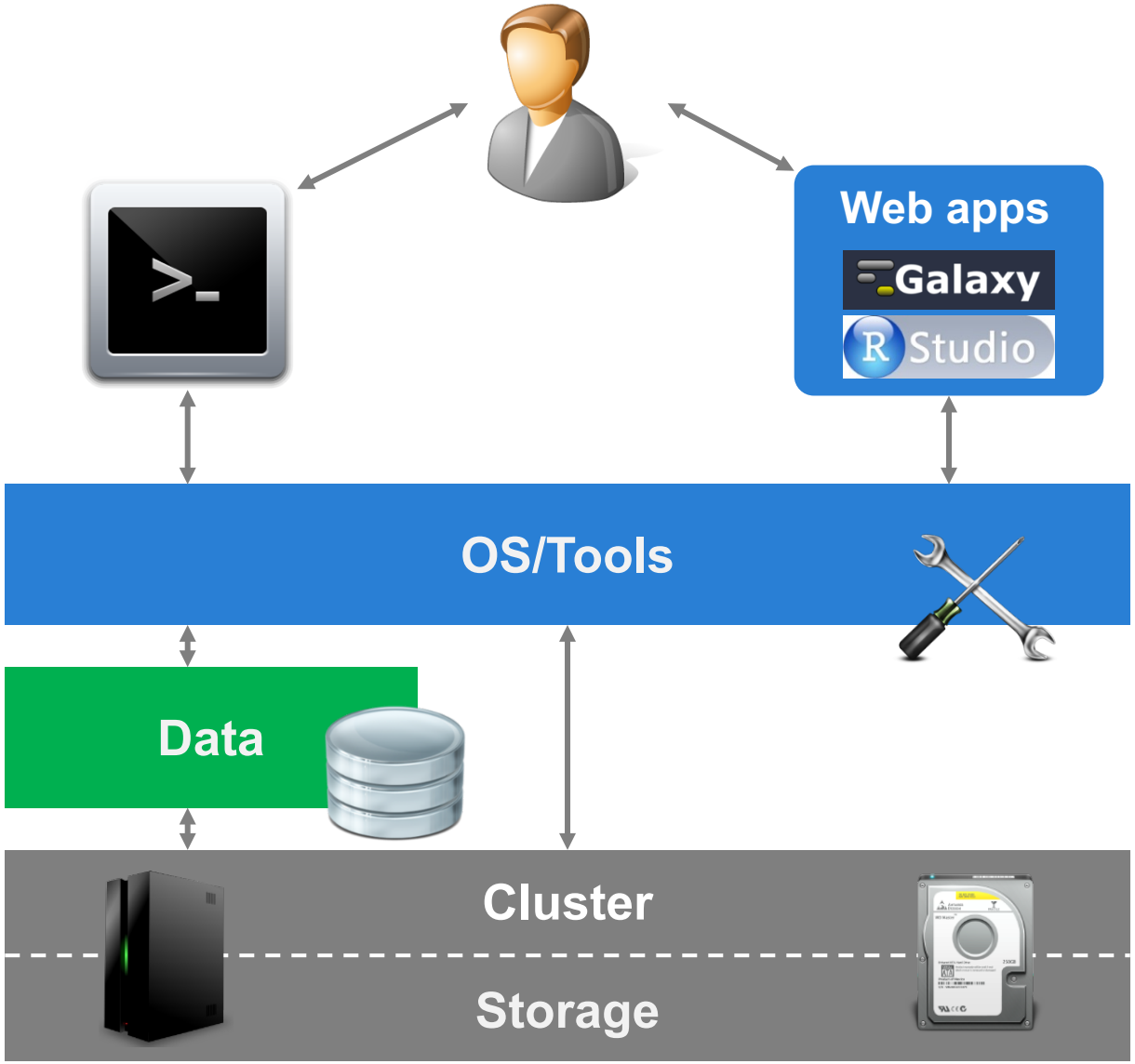


Parallel computing

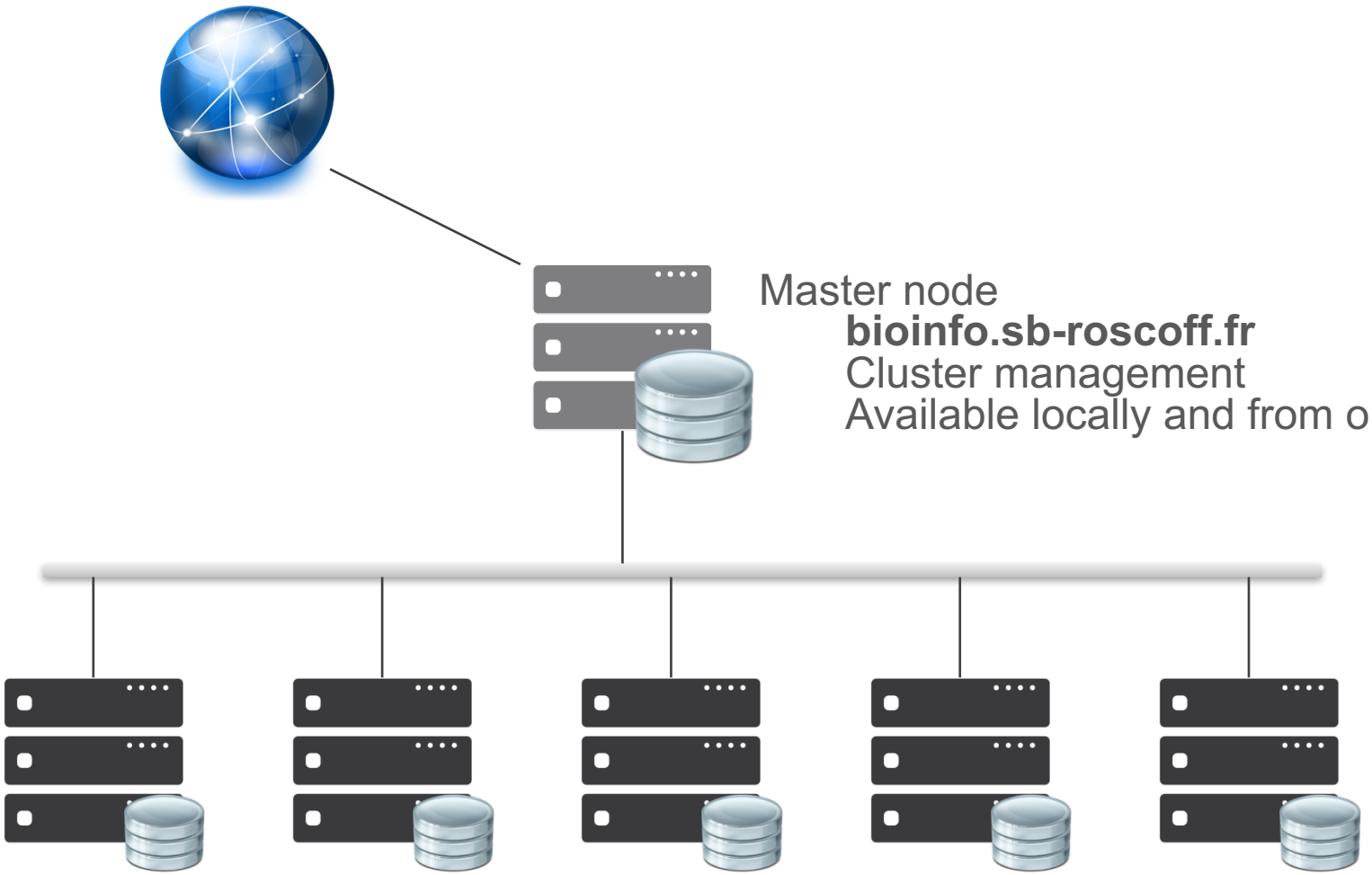
- MPI (Message Parsing Interface)
  - Tasks are running on different machines
  - Communication between tasks over the network
  - Variable gain. Nonlinear in general

  - Ex: PhyML-MPI, ClustalW-MPI

Environment



Cluster


Master node
bioinfo.sb-roscoff.fr
Cluster management
Available locally and from outside

Cluster

DIFFERENTS TYPES OF NODE

Group	Node	Type	Function	Processor	RAM
@@bigcpu	n40-n55	Dell blade M630	Multithreaded treatements	Intel 32 x 2.4 GHz	128 Go
	n60-n75	Dell blade M605	Reserved for some applications	AMD 8 x 2.4 GHz	32 Go
@@bignode	n76-n79	Dell R815	Multithreaded treatements Memory usage	AMD 48 x 2.2 GHz	256 Go
@@bigcpu	n80-n95	Dell C6220	Multithreaded treatements	Intel 32 x 2.2 GHz	128 Go
@@bigmem	n99	Dell R910	Memory usage	Intel 40 x 2.0 GHz	1 To



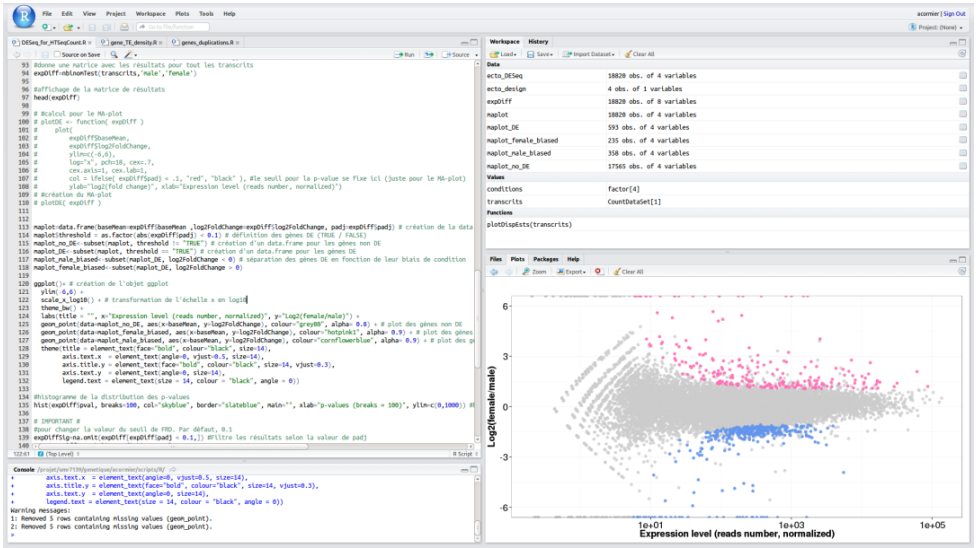

Environment

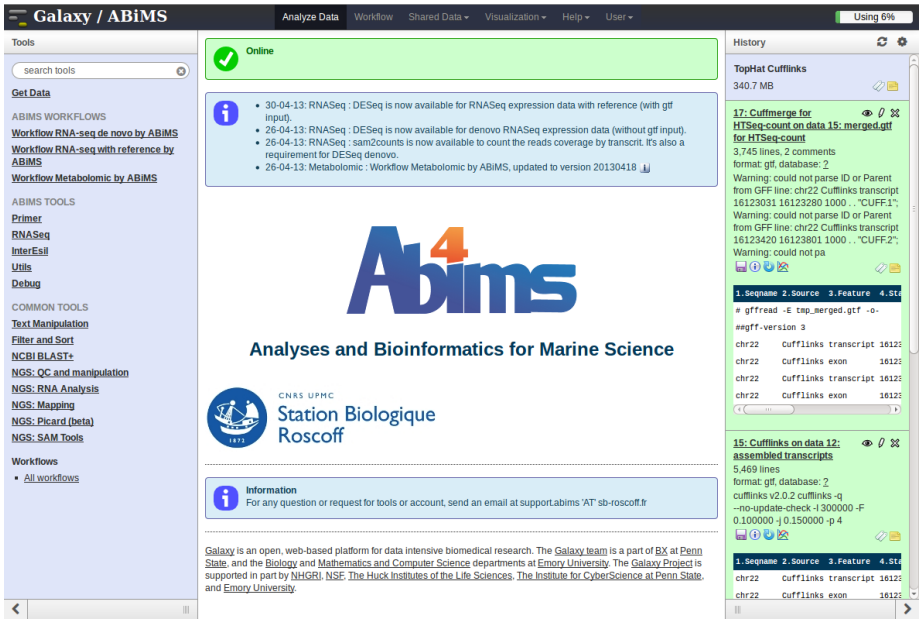
- Command-line
  - Knowledge in Unix / Bash
  - Integrated in computer resources and storage

```
acormier@n0:/tmp
drwx------   2 root            root           16384 avr 15  2009 lost+found
srwxr-xr-x   1 caron           sib                0 oct 30  2012 mapping-caron
srwxr-xr-x   1 corre           sib                0 avr 18 14:08 mapping-corre
srwxr-xr-x   1 ewcorre         lbm                0 jun 25 15:37 mapping-ewcorre
srwxr-xr-x   1 jkervellec      sib                0 fév 22 13:52 mapping-jkervellec
srwxr-xr-x   1 jmaroumougom    sib                0 nov  3  2011 mapping-jmaroumougom
srwxr-xr-x   1 ndebs           lbm                0 jun 28 15:11 mapping-ndebs
srwxr-xr-x   1 root            root               0 avr 17  2009 mapping-root
srwxr-xr-x   1             5000 root               0 avr 28  2009 mapping-toto
drwx------   2 llegrand        inra            4096 jui  5 10:28 mozilla-media-cache
drwxr-xr-x 258 hfcollector     application    20480 jui  6 04:48 ODV_hfcollector
drwx------   3 nhenry          eppo            4096 jui  2 13:43 openmpi-sessions-nhenry@n0.sb-roscoff.fr_0
drwx------   2 acormier        genetique       4096 mai  3 20:57 orbit-acormier
drwx------   2 cock            genetique       4096 avr  7 13:18 orbit-cock
drwx------   2 corre           sib             4096 jun 24 09:58 orbit-corre
drwx------   2 ewcorre         lbm             4096 jui  3 13:50 orbit-ewcorre
drwx------   2 gdm             gdm             4096 avr  5 18:30 orbit-gdm
drwx------   2 hfcollector     application     4096 jui  4 10:16 orbit-hfcollector
drwx------   2 lecorguille     sib             4096 jun 20 02:48 orbit-lecorguille
drwx------   2 llegrand        inra            4096 jui  5 10:35 orbit-llegrand
drwx------   2 mhoebeke        sib             4096 jun 25 13:30 orbit-mhoebeke
drwx------   2 ndebs           lbm             4096 jun 28 16:17 orbit-ndebs
drwx------   2 stage02         stage           4096 mai 13 10:40 orbit-stage02
drwx------   2 wcarre          sib             4096 jun 20 09:53 orbit-wcarre
srwxr-xr-x   1 ewcorre         lbm                0 nov 10  2011 OSL_PIPE_6108_SingleOfficeIPC_eebd8121e860c31ca9a23ed86a44ce
drwxr-xr-x   4 root            root            4096 sep 30  2009 perl5
drwxr-xr-x   2 acormier        genetique       4096 jun 25 15:58 perl_formation
drwxr-xr-x   2 mhoebeke        sib             4096 jun 25 11:45 phyloclusters
srwxr-xr-x   1 root            root               0 avr 11  2012 sfcbLocalSocket
drwxr-xr-x   5 root            root            4096 fév 20  2010 sge
-r--------   1 root            root            3066 mai 23  2011 shadow
-rw-r--r--   1 root            root           10978 jui  5 23:00 stat_sge.txt
drwxr-xr-x   3 root            root            4096 jun 26  2012 toto
[acormier@n0 tmp]$
```

Web applications

- Web interface
  - Galaxy
  - R-studio: dedicated to R





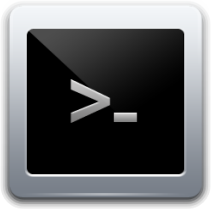
http://r.sb-roscoff.fr/

http://galaxy.sb-roscoff.fr/

CONNEXION AND STORAGE

Prerequisite

- Account
  → http://abims.sb-roscoff.fr/account
  → support.abims@sb-roscoff.fr
- Email
- X11 terminal
  - Windows: Putty or MobaXterm (X11)
  - Mac OS : XQuartz (X11)
  - Linux: integrated
- Text editor
  - Vim, nano, gedit, emacs…
- SFTP client



Connection

```
$ ssh -Y acormier@bioinfo.sb-roscoff.fr # -Y → for graphic (X11) flux redirection
```

Connection

```
$ ssh -Y acormier@bioinfo.sb-roscoff.fr # -Y → for graphic (X11) flux redirection

Last login: Wed May 17 13:39:19 2017 from 192.168.4.180
```

```
                .      ___   4   .     .   ___
               / \    |   )      |\   /|(
              /___\   |--|   |   | \/ | `-.
             /     \  |   ) |   |    |    )
            /       \|__/  |   |    |___/

     Analysis and Bioinformatics for Marine Science

   http://abims.sb-roscoff.fr - support.abims@sb-roscoff.fr
```

```
Please have a look at the training material:
http://abims.sb-roscoff.fr/sites/abims.sb-roscoff.fr/files/formation_2016/formation_cluster_v5.1.pdf

IMPORTANT:
   - nz:       Never launch job on this server -> Use a qlogin
   - /home:    Never launch job from this space
   - /projet:  Use your /projet folder for its performance, its volumetry
               and its independence from the /home space
   - /scratch: For your huge temporary files, please use /scratch
               but note that files older than 30 days are automatically deleted

CITATION: Please cite the plateform ABiMS in the Acknowledgement of your future publication

WARNING: 27/03/2017 - We are facing some issues with the disk server NZ.
We will inform you as soon as we get further information.
Meanwhile, we can expect some random interruptions. Sorry for that!
```

WORKING DIRECTORIES

Data

- Personal data

- Shared data:
  - By team / group
  - By UMR
  - For a community
  - Public data

- Databank
  - Genbank, Uniprot, InterPro banks, etc.
  - Format : Blast, FASTA, EMBL, etc.
  - Private & Public

Workspace

projet → nz

home → brazil

db → banko

Galaxy → cfs10

Workspace

projet

→ per person
→ by team
→ by subject

home

→ only for connexion (Environment variable)

db

→ Databank (Blast, Genbank, Interpro…)

Galaxy

→ ftp
→ files

Workspace

projet

Partial backup

home

Partial backup

db

No backup

Galaxy

No backup

Workspace

scratch → nz

20 To

Space for all the primary analysis - generated huge amount of temporary/useless files

- **Mutualised storage** between all users
- Data are **not backed up**
- All files older than **30 days** are automatically **deleted**

Working directory: ~~home~~

When I'm connecting, I arrive in my:

home

```
$ pwd #print working directory

  /home/umr8227/ga/acormier
```

Not for storage / computing

Working directory: scratch

I have to work in:

scratch

For all analysis

```
$ cdscratch
$ pwd

  /projet/umr8227/ga/acormier
```

- Structuration:
  → by user

- Shared between all nodes
- Available from outside

Working directory: scratch – structure

- No particular structuration

- Don’t forget this:
  - **All files older than 30 days are automatically deleted** (based on the last modification date)

Working directory: projet

I have to save my results in:

projet

To store raw data, final results and scripts

```
$ cdprojet #alias for fast moving in my project directory
$ pwd

  /projet/umr8227/ga/acormier
```

- Structuration:
  - → by team: /projet/umr8227/ga/acormier
  - → by subject: /projet/abims/ectocarpus
- Shared between all nodes
- Available from outside

Working directory: projet – structure

Each project needs to have particular folders:

Working directory: projet – structure

Each project needs to have particular folders:

Backup system: by inclusion.

Only these folder are saved:

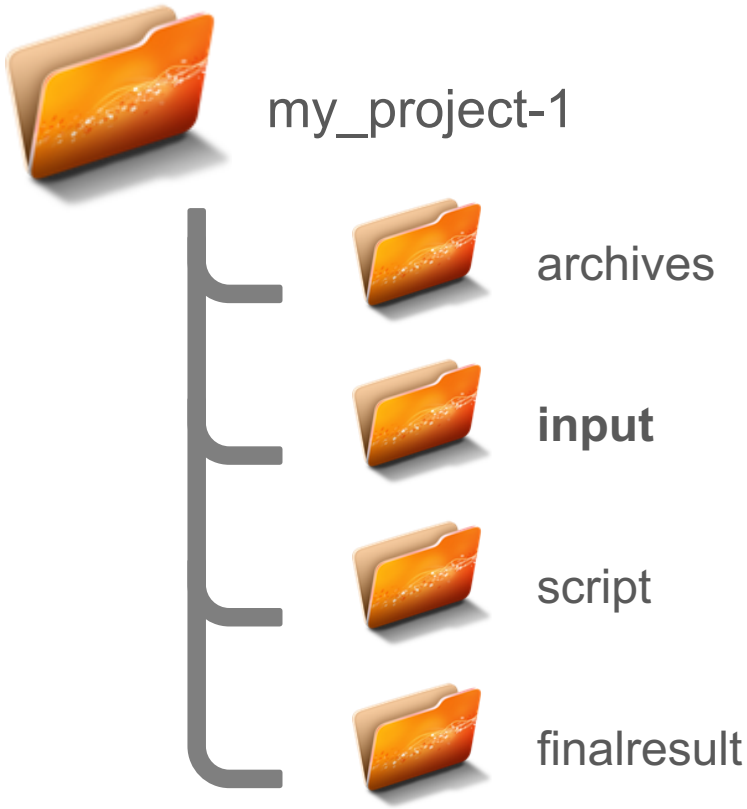
- **finalresult**
- **script**
- **archives**

Pay attention to typo! Case sensitive

Working directory: projet – structure

Original data sources.
Rarely used, only for archiving.
E.g. Raw data from sequencing (Sanger, DNA-seq, RNA-seq, etc)

Working directory: projet – structure



Data used as input file for analysis
E.g. Cleanded data from sequencing, fasta files, etc

Working directory: projet – structure

Qsub files
R scripts and workspace
Python/perl/C/Ruby/… scripts

Working directory: projet – structure

my_project-1

archives

input

script

finalresult

Results of analysis that need to be conserved.

Working directory: projet – structure

Results of analysis that need to be conserved.

~/.bashrc

```
alias mkp='mkdir archive input script tmp finalresult finalresult/document; \
ln -s finalresult output; ln -s finalresult/document'
```

Storage limitation

Regularly, check the volume of my project to prevent saturation. The storage is not by user, but by team…

```
$ df -h . #report filesystem disk space usage
  Sys. de fich.          Tail. Occ. Disp. %Occ. Monté sur
  cfs1:/projet/umr8227/ga  1,4T  651G  658G  50% /projet/umr8227/ga

$ cdscratch
$ du -sh * #size of each file/folder -> who is the biggest?

  68G    assembly
  341G   pagit
  3,8G   remapping
  12K     cache_tmp
  17M     chr_similarity
  1008M   galaxy_dataset
  669M    metrics
  2.1M    Tes

$ du -sh assembly/*

  11G     assembly/transcriptome_V1
  9.8G    assembly/transcriptome_V2
  48G     assembly/trinity
```

Management of my project directory

Compress your data!

```
$ ll -h

  -rw-rw-r--+ 1 acormier    ga  26G mars  8 08:16 140220_SND393_B_L006_GPO-12_R1.fastq
  -rw-rw-r--+ 1 acormier    ga  26G mars  8 08:16 140220_SND393_B_L006_GPO-12_R2.fastq

$ gzip 140220_SND393_B_L006_GPO-12_R1.fastq
$ gzip 140220_SND393_B_L006_GPO-12_R2.fastq

$ ll -h

  -rw-rw-r--+ 1 acormier    ga 7,7G mars  7 12:25 140220_SND393_B_L006_GPO-12_R1.fastq.gz
  -rw-rw-r--+ 1 acormier    ga 7,9G mars  7 12:29 140220_SND393_B_L006_GPO-12_R2.fastq.gz
```

Some softwares are capable to use directly compressed data (TopHat2, Trimmomatic,…)

Management of my project directory

It is therefore imperative to remove unnecessary data

```
$ ll

  drwxr-xr-x 3 acormier ga     4096 mai 29 21:30 remapping
  drwxr-xr-x 2 acormier ga     4096 mai 30 18:32 pagit
  -rw-r--r-- 1 acormier ga   134761 Nov 29 10:02 autosomes_contigs.gff3
  -rw-r--r-- 1 acormier ga 35214029 Nov 29 09:40 autosomes.gff3
  -rw-r--r-- 1 acormier ga    20802 Nov 28  2012 FeV4_24112012.gff3

$ rm autosomes.gff3 FeV4_24112012.gff3 #rm = remove

  rm: remove regular file `autosomes.gff3'? y
  rm: remove regular file `FeV4_24112012.gff3'? y

$ rm -r pagit/ # -r for a folder

  rm: remove directory `pagit/'? y #n to cancel

$ ll

  drwxr-xr-x 3 acormier ga     4096 mai 29 21:30 remapping
  -rw-r--r-- 1 acormier ga   134761 Nov 29 10:02 autosomes_contigs.gff3
```

Management of my project directory

Conclusion:

- Work in the scratch directory
- Save your data on the project directory for:
  - **performance - storage – safety**
- Respect the structuration of my project directory
- Check the available space in my project directory
- **Regularly delete unnecessary data!**

RESSOURCES

Tools

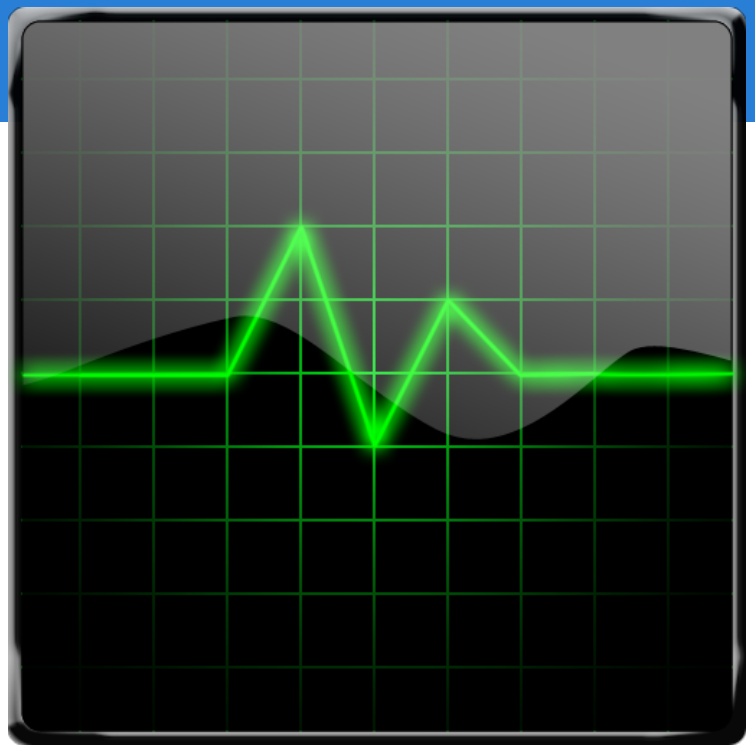
- Applications (x700)
  - /usr/local/genome2/
    - Localisation of all software available on the cluster
    - Soon: a list of all tools
  - /usr/local/genome2/script/
    - Scripts developed by people of the SBR
    - Just send an email to support.abims@sb-roscoff.fr if you want to share your scripts

- The software components are shared:
  - One installation in a unique place
  - Request to add or update: support.abims@sb-roscoff.fr

Genomes databank

- /db/
  - Public databank:
    - NCBI
    - GenBank
    - UniProt
    - InterPro
    - Etc
  - SBR databank
    - Start with the prefix “sbr_”
    - Description of these databank is currently in progress

BioMAJ



How to use the cluster?

SUN GRID ENGINE - SGE

Job management system

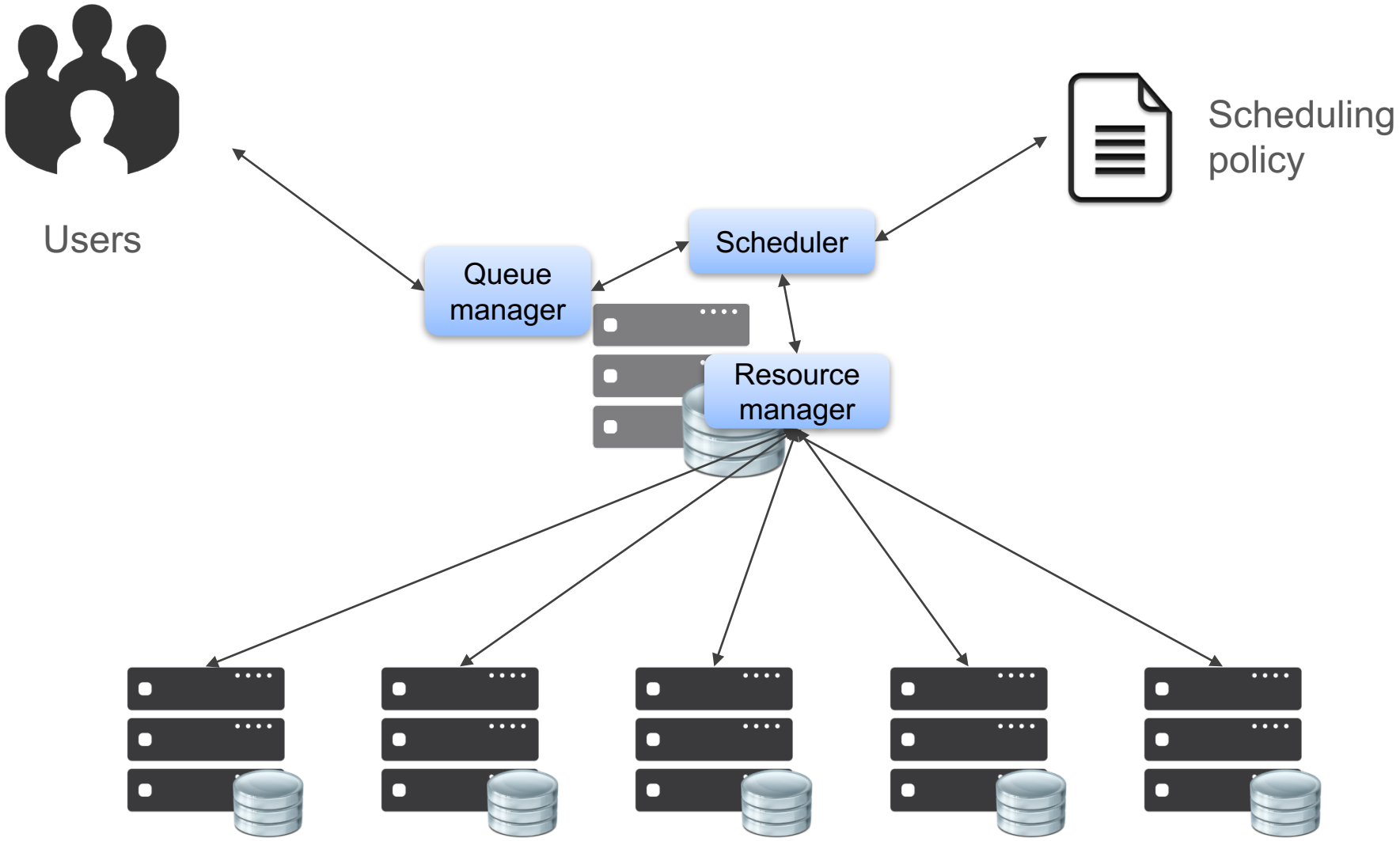
- Sun Grid Engine (SGE)
  - Scheduler in charge of the jobs management
  - User interface for submitting and controlling jobs

- Task scheduling
  - Resources allocation
  - Nodes load
  - Priority
- Management policy and resource sharing
  - CPU / Memory
  - Execution time
- Reporting and errors
  - History
  - Usage statistics

Concepts

- Job
  - Task unit
  - There are several types of jobs:
    - Batch (script)
    - Interactive
  - Serial vs parallel
    - Serial: only need 1 processor
    - Parallel: require more than 1 processor
- Slots
  - Number of jobs allowed on one node
- Queue
  - Type of resources (node groupe, execution time…)
- Priority
  - **Fair Share :** calculated on 1 week → sliding window

Job management system



Queues

	Time out	Available resources	Purpose
short.q	12 hours	High priority - 50 % of all CPU (- n99)	Regular jobs
long.q	10 days	Standard priority - 50 % of all CPU (- n99)	Long jobs
infinite.q	no limit	Low priority - 25 % of all CPU (- n99)	Really really long jobs
bigmem.q			For treatements requiring a lot of RAM
qlogin.q	2 days		For connections in qlogin mode
clc.q		n76	For **CLC** use (please contact **support.abims@sb-roscoff.fr**).

Max load: 1,25

→ **By default, no queue!**

Nodes groups

DIFFERENTS TYPES OF NODE

Group	Node	Type	Function	Processor	RAM
@@bigcpu	n40-n55	Dell blade M630	Multithreaded treatements	Intel 32 x 2.4 GHz	128 Go
	n60-n75	Dell blade M605	Reserved for some applications	AMD 8 x 2.4 GHz	32 Go
@@bignode	n76-n79	Dell R815	Multithreaded treatements Memory usage	AMD 48 x 2.2 GHz	256 Go
@@bigcpu	n80-n95	Dell C6220	Multithreaded treatements	Intel 32 x 2.2 GHz	128 Go
@@bigmem	n99	Dell R910	Memory usage	Intel 40 x 2.0 GHz	1 To

Queues

```
$ qstat -g c #displays the available queues

CLUSTER QUEUE                   CQLOAD   USED    RES  AVAIL  TOTAL aoACDS   cdsuE
--------------------------------------------------------------------------------
short.q                           0.32    140      0    184    324        0       0
long.q                            0.32     93      0    231    324        0       0
infinite.q                        0.32      0      0     66     66        0       0
bigmem.q                          0.60     20      0     20     40        0       0
qlogin.q                          0.30      7      0     23     30        0       0
clc.q                             0.28     10      0     38     48        0       0
formation.q                       0.61      3      0     57     60        0       0
galaxy.q                          0.72      0      0    140    140        0       0
galaxy1.q                         0.33      0      0     72     72        0       0
```

The queues freely available:

- short.q
- long.q
- infinite.q
- qlogin.q → for interactive jobs

On request:

- bigmem.q : for jobs that require a lot of RAM
- clc.q : for CLC Assembly Cell

Monitoring

```
$ qhost #liste of all nodes
```

HOSTNAME	ARCH	NCPU	LOAD	MEMTOT	MEMUSE	SWAPTO	SWAPUS
n0	lx24-amd64	8	0.10	7.8G	841.7M	4.0G	81.6M
n60	lx24-amd64	8	0.03	31.5G	2.3G	1.0G	656.0K
n61	lx24-amd64	8	0.03	31.5G	350.3M	1.0G	180.0K
n62	lx24-amd64	8	1.32	31.5G	208.5M	1.0G	80.5M
n63	lx24-amd64	8	0.03	31.5G	1.8G	1.0G	72.2M
n64	lx24-amd64	8	1.00	31.5G	335.0M	1.0G	82.4M
n76	lx24-amd64	48	13.59	252.0G	22.4G	2.0G	28.5M
n77	lx24-amd64	48	11.12	252.0G	21.3G	2.0G	240.0K
n78	lx24-amd64	48	5.02	252.0G	22.4G	2.0G	58.8M
n79	lx24-amd64	48	37.07	252.0G	24.6G	2.0G	0.0
n80	lx24-amd64	32	22.14	126.0G	2.9G	1024.0M	11.0M
n81	lx24-amd64	32	32.02	126.0G	2.8G	1024.0M	0.0
n82	lx24-amd64	32	32.03	126.0G	2.8G	1024.0M	0.0
n83	lx24-amd64	32	32.02	126.0G	2.8G	1024.0M	0.0
n84	lx24-amd64	32	32.02	126.0G	3.1G	1024.0M	0.0
n99	lx24-amd64	40	24.00	1009.7G	238.6G	4.0G	107.6M

Allows to check load level on each node:

- Load level on the cluster

Monitoring

```
$ qhost                 # available nodes and some indicators

$ qhost -j     # list of jobs on each node

$ qhost -q     # list of queues/slots on each node

$ man qhost    # help!
```

Jobs

```
$ qstat #shows all jobs

job-ID  prior   name       user         state submit/start at     queue       slots ja-task-ID
-----------------------------------------------------------------------------------------------
1236477 0.50000 QLOGIN     wcarre       r     04/30/2012 15:10:26 long.q@n77      1
1236479 0.50000 QLOGIN     wcarre       r     04/30/2012 15:11:12 long.q@n77      1
1268627 1.00000 QLOGIN     balzano      r     05/03/2012 09:39:24 long.q@n74      1
1302170 0.06667 alpha0.sh  mrescan      r     05/06/2012 12:05:48 long.q@n64      1
1302173 0.06667 alpha3.sh  mrescan      r     05/06/2012 12:06:18 long.q@n72      1
1302174 0.06667 alpha4.sh  mrescan      r     05/06/2012 12:06:33 long.q@n70      1
1302175 0.06667 alpha5.sh  mrescan      r     05/06/2012 12:06:43 long.q@n63      1
1302261 0.06667 alpha6.sh  mrescan      r     05/06/2012 12:07:03 infinite.q@n60 1
1314908 0.21765 evol.sh    ablanckaert  qw    05/07/2012 10:04:39                 20
2216309 0.00045 sge_blastn gfarrant     qw    05/23/2013 14:43:03                 1 69-2379:1
```

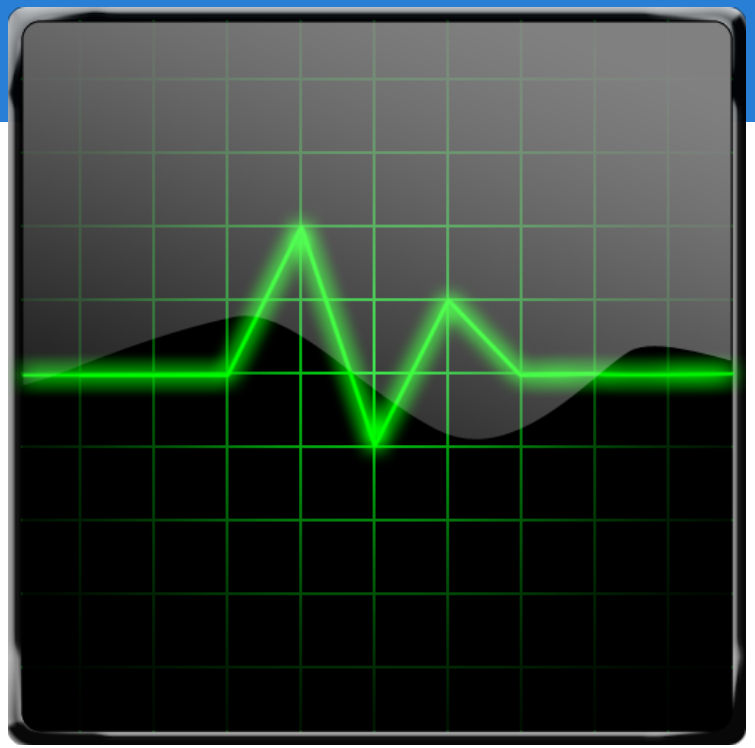
- Prior: priority level
  - Higher when close to 1.0000
- State
  - r: running
  - qw: pending
  - Eqw: in error
- Slots: cores used
- Ja-task-ID: job array

Jobs type

- Interactive mode: qlogin
  - Short job and/or development
  - Prerequisite: none
  - Note: disconnect you at the end of the session

- Batch mode: qsub
  - Heavy jobs
  - Prerequisite: text editor
  - One script per job

nz (master node) never should be used for computing!



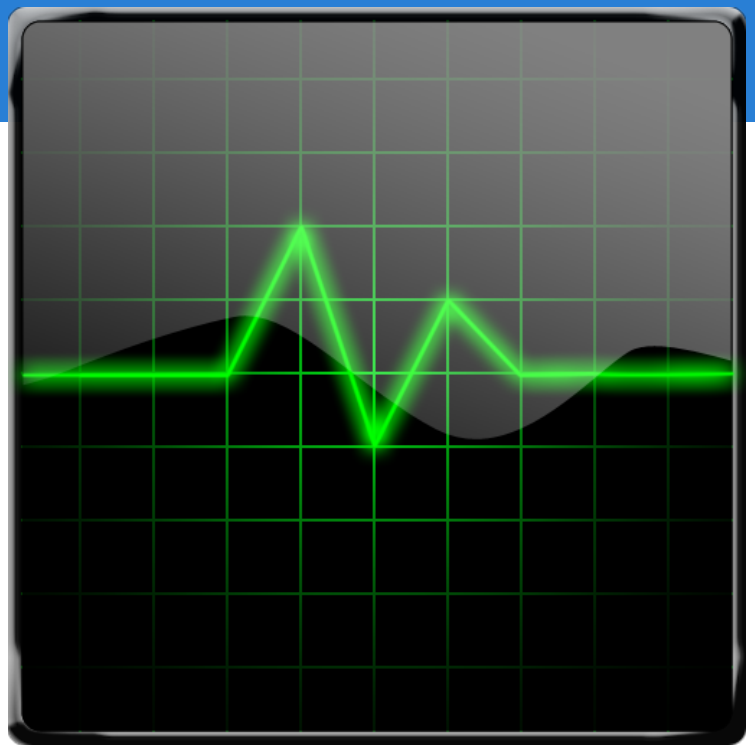
qlogin

SUN GRID ENGINE - SGE

qlogin: Interactive mode

- Connexion on:
  - A queue: qlogin -q qlogin.q
  - A node : qlogin -q qlogin.q@n72
  - A group : qlogin -q qlogin.q@@blade

```
$ qlogin -q qlogin.q

  Your job 2217414 ("QLOGIN") has been submitted
  waiting for interactive job to be scheduled ...
  Your interactive job 2217414 has been successfully scheduled.
  Establishing /opt/sge/qlogin.sh session to host n78 ...
  Last login: Mon Apr 15 10:22:01 2013 from n0.sb-roscoff.fr

@n78$ cdprojet
.
<my test>
.
@n78$ exit

  Connection to n78 closed.
  /opt/sge/qlogin.sh exited with exit code 0

$
```



qsub

SUN GRID ENGINE - SGE

qsub: Batch mode

- Progress:
  - Script edition
  - Choose the right queue
  - Submitting → Execution → Results

- Edition
  - In command line: vi, vim, nano…
  - In graphic mode: gedit, kate…

How to?

1. Prepare script of executable commands

2. Submit to batch system

3. Use the job ID for job control (query status, cancel, ...)

4. Check the job status (no execution error)

1. Prepare script of executable commands

The minimum

script.qsub

Header

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
```

cmd lines

```
echo "Hello world!" > output.txt
```

Essential for qsub:

- The header:
  - Shell path
  - -S : path to shell (for SGE)
  - -V : load the environment variables (~/.bashrc → /etc/bashrc)
  - -cwd : work in the current working directory
- The command line(s)

1. Prepare script of executable commands

Other practical settings

script.qsub

Header

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -o blastn.out
#$ -e blastn.err
```

cmd lines

```
blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

- The header:
  - -o stdout filename
  - -e stderr filename

1. Prepare script of executable commands

Other practical settings

script.qsub

Header

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -M foo.bar@sb-roscoff.fr
#$ -m bea
```

cmd lines

```
blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

- The header:
  - -m b|e|a|s|n|...: send mail at beginning|end|...of the job
  - -M: E-mail address for notification

1. Prepare script of executable commands

Other practical settings

script.qsub

Header

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -l mem_free=50G
```

cmd lines

```
blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

- The header:
  - -l mem_free=XXG

2. Submit to batch system

```
$ qsub -q short.q script.qsub
  Your job 2217418 ("script.qsub") has been submitted
```

-q : select a queue

script.qsub

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -q short.q

blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

```
$ qsub script.qsub
  Your job 2217418 ("blast.qsub") has been submitted
```

2. Submit to batch system

```
$ qsub script.qsub
  Your job 2217418 ("script.qsub") has been submitted
```

script.qsub

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -q short.q

blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

script.sh

```
#!/bin/bash

blastp -db nr -query query_1.fa -out blastout_1.txt
blastp -db nr -query query_2.fa -out blastout_1.txt
```

```
$ qsub -S /bin/bash -V -cwd -q short.q script.sh
  Your job 2217418 ("script.sh") has been submitted
```

2. Submit to batch system

- The choice of the queue is subject to several criteria …
  - Job duration:
    - < 12 hours → short.q
    - < 10 days → long.q
    - > 10 days → infinite.q
  - RAM
    - < 4 Go / CPU → @@bigcpu
    - > 4 Go / CPU → @@bignode
    - > 25 Go / CPU → bigmem.q
  - Tools:
    - CLC Assembly Cell → clc.q

```
$ qsub -q short.q script.qsub
$ qsub -q short.q@@bigcpu script.qsub
$ qsub -q lonq.q@@bignode script.qsub
$ qsub -q bigmem.q script.qsub
$ qsub -q clc.q script.qsub
```

OR

script.qsub

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -q short.q@@bigcpu

blastall -p blastp -d nr -i query_1.fa …
blastall -p blastp -d nr -i query_2.fa …
```

2. Submit to batch system

- Multithreading

script.qsub

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -q short.q@@bigcpu
#$ -pe thread 8

bowtie2 -1 r1.fastq -2 r2.fastq -x ref -S align.sam --threads 8
```

BEWARE: You must set the same value in both SGE (#$) and software settings

If not, you will use some ressources you haven't reserved.
The risk is to overload the node.

2. Submit to batch system

- Multithreading
  - TopHat: -p / --num-threads
  - Bowtie2: -p / --threads
  - Trinity: --CPU
  - CLC Assembly Cell: --cpus

Multithreading is not possible with all software

RTFM

2. Submit to batch system

```
Job 1236477 (tophat.sh) Started
 User       = acormier
 Queue      = long.q
 Host       = n77
 Start Time = 05/25/2013 13:30:39
```

2. Submit to batch system

- ... But also rules, because you are not alone on the cluster!
  - **Work in the scratch directory**
  - Choose the more adapted queue (by default, used long.q)
  - Disconnect you from your qlogin

3. Use the job ID for job control (status,...)

```
$ qstat #shows all jobs

job-ID  prior   name       user         state submit/start at     queue       slots ja-task-ID
-----------------------------------------------------------------------------------------------
1236477 0.50000 QLOGIN     wcarre       r     04/30/2012 15:10:26 long.q@n77      1
1236479 0.50000 QLOGIN     wcarre       r     04/30/2012 15:11:12 long.q@n77      1
1268627 1.00000 QLOGIN     balzano      r     05/03/2012 09:39:24 long.q@n74      1
1302174 0.06667 alpha4.sh  mrescan      r     05/06/2012 12:06:33 long.q@n70      1
1302175 0.06667 alpha5.sh  mrescan      r     05/06/2012 12:06:43 long.q@n63      1
1302261 0.06667 alpha6.sh  mrescan      r     05/06/2012 12:07:03 infinite.q@n60 1
1314908 0.21765 evol.sh    ablanckaert  qw    05/07/2012 10:04:39                 20
2216309 0.00045 sge_blastn gfarrant     qw    05/23/2013 14:43:03                 1 69-2379:1
```

- Prior: priority level
- State
  - r: running
  - qw: pending
  - Eqw: in error
- Slots: cores used

```
$ \qstat #shows my jobs

job-ID  prior   name       user         state submit/start at     queue       slots ja-task-ID
-----------------------------------------------------------------------------------------------
1236477 1.00000 tophat.sh  acormier       r     05/25/2013 15:10:26 long.q@n77      8
```

3. Use the job ID for job control (status,...)

`qstat`	shows all jobs (running, pending, error)
`qstat -s r`	shows only running jobs
`qstat -s p`	shows only pending jobs
`\qstat`	shows only **my** jobs
`qstat -g c`	list available queues
`qstat -j <job id>`	informations about the job
`man qstat`	help

3. Use the job ID for job control (status,...)

```
$ qdel 2217417 #deletion by the job-ID

  acormier has registered the job 2217417 for deletion

$ qdel –f 2217418

  acormier has registered the job 2217418 for deletion

$ qdel –u acormier #deletion by user name

  acormier has registered the job 2217419 for deletion
  acormier has registered the job 2217420 for deletion
  acormier has registered the job 2217421 for deletion
  acormier has registered the job 2217422 for deletion
```

```
Job 2217424 (clc_mapping_info.sh)
was killed by acormier@n0.sb-
roscoff.fr
```

```
Job 2217424 (clc_mapping_info.sh) Aborted
 Exit Status       = 137
 Signal            = KILL
 User              = acormier
 Queue             = clc.q@n76
 Host              = n76.sb-roscoff.fr
 Start Time        = 05/30/2013 21:24:06
 End Time          = 05/30/2013 21:24:08
 CPU               = 00:00:01
 Max vmem          = 75.023M
failed assumedly after job because:
job 2217424.1 died through signal KILL (9)
```

4. Check the job status (no execution error)

- Logs

```
Job 1236477 (tophat.qsub) Complete
 User             = acormier
 Queue            = long.q@n77
 Host             = n77
 Start Time       = 05/25/2013 13:30:39
 End Time         = 05/25/2013 17:39:00
 User Time        = 04:01:31
 System Time      = 00:06:02
 Wallclock Time   = 04:08:21
 CPU              = 04:07:33
 Max vmem         = 10.976G
 Exit Status      = 0
```

<my_script>**.e**<job-ID> : error file and/or progress bar

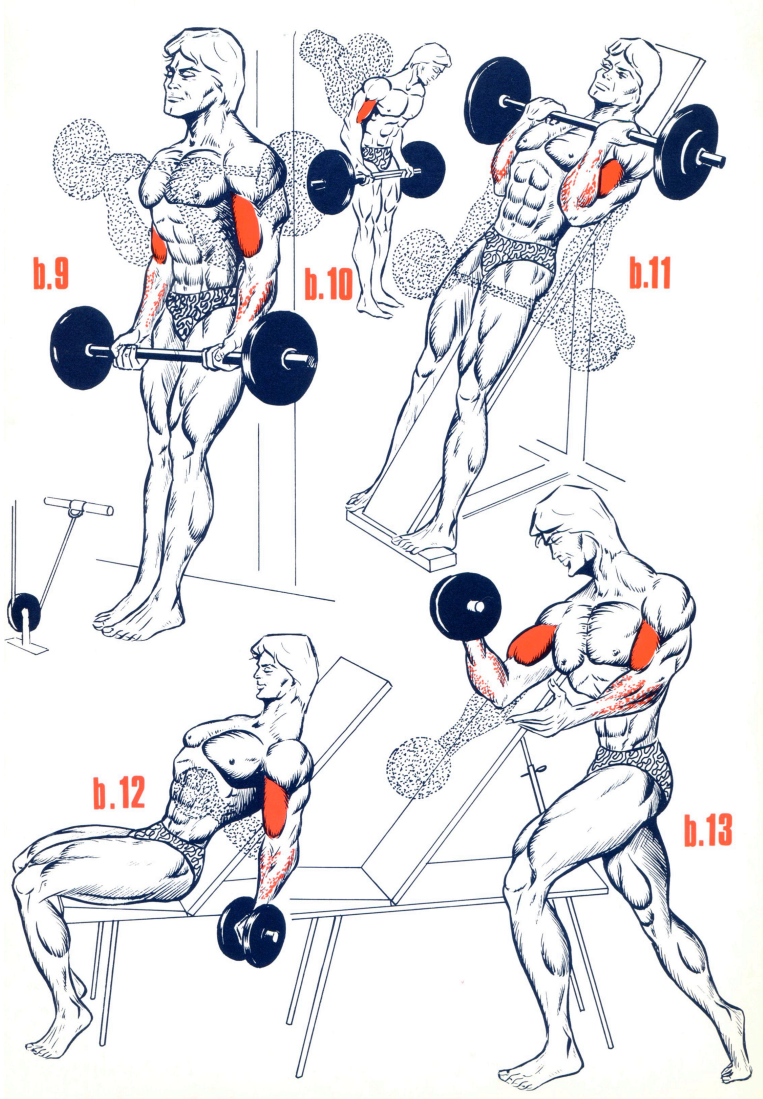
<my_script>**.o**<job-ID> : results, except if the program provides an option to output file.

And in mutlithreading mode:

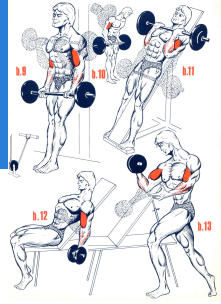
<my_script>**.pe**<job-ID>

<my_script>**.po**<job-ID>

EXERCICE / EXAMPLES



Exercises/Examples



Search for sequence similarities using *blastn* on the fasta file *insulin.fas* again the database *nt*

Parameters:

-query insulin.fas

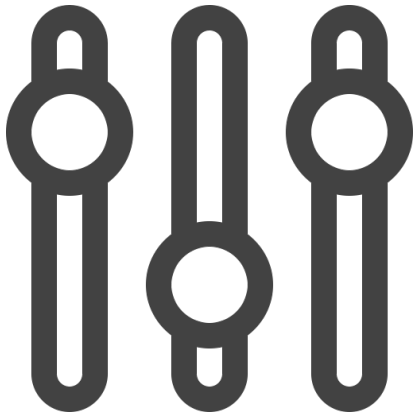
-outfmt 6

-evalue 1e-6

-max_target_seqs 5

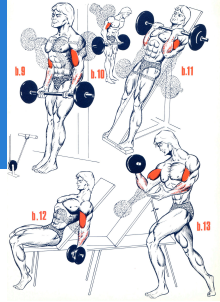
-db /db/blast/all/nt

-out insulin_nt.blastn.tab



Tips: keep in mind that your project directory is structured (input, script…)

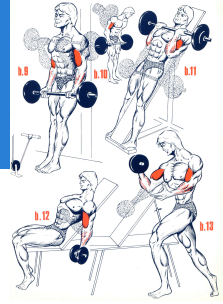
Exercises/Examples



Using:

1. qlogin
2. qsub: Simple script
3. qsub: Multithread script
4. qsub: Job-array

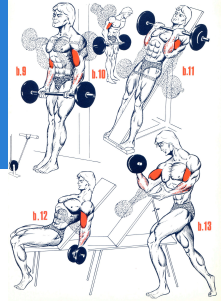
1. qlogin



1. Open a connection using `qlogin` on a node

```
$ qlogin -q qlogin.q

  Your job 2217414 ("QLOGIN") has been submitted
  waiting for interactive job to be scheduled ...
  Your interactive job 2217414 has been successfully scheduled.
  Establishing /opt/sge/qlogin.sh session to host n78 ...
  Last login: Mon Apr 15 10:22:01 2013 from n0.sb-roscoff.fr

@n78$ cdprojet
@n78$ cd tp-cluster/tmp
@n78$ blastn -help
@n78$ blastn -query ...
```

2. qsub: simple script



1. Edit a text file using `gedit` or `vim`

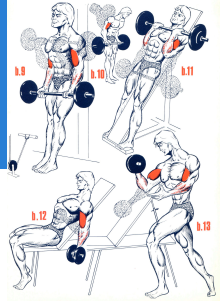
```
$ gedit script/blastn.qsub
```

```
$ vim script/blastn.qsub
```

2. Add settings for SGE

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -M foo.bar@sb-roscoff.fr
#$ -m bea
```

2. qsub: simple script



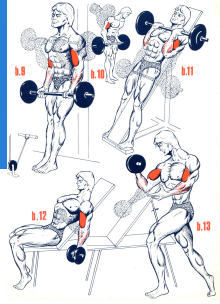
3. Append with the command line

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -M foo.bar@sb-roscoff.fr
#$ -m bea

INPUT="../input/insulin.fas"
OUTPUT="insulin.blast"
DATABASE="/db/blast/all/nt"

blastn -query $INPUT -db $DATABASE -out $OUTPUT -outfmt 6 -evalue 1e-6 -max_target_seqs 5
```

4. Launch a qsub request in the terminal

```
$ qsub -q short.q blastn.qsub

Your job 744348 ("blastn.qsub") has been submitted
```

2. qsub: simple script



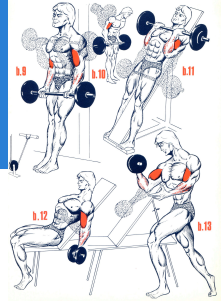
5. Monitor your job (quickly)

- Results in a other terminal
- Cluster state
- Jobs running

```
$ \qstat
744348 1.00000 blastn.qsu fbar      qw    05/13/2016 08:58:06                                    1
$ \qstat
744348 1.00000 blastn.qsu fbar      r     05/13/2016 08:58:06 short.q@n78.sb-roscoff.fr          1
```

```
$ ll

  -rw-r--r-- 1 fbar grp       474 mai 31 09:53 blastn.qsub
  -rw-r--r-- 1 fbar grp         0 mai 31 09:53 blastn.qsub.e744348
  -rw-r--r-- 1 fbar grp      1538 mai 31 09:53 blastn.qsub.o744348
```

3. qsub: Multithread script



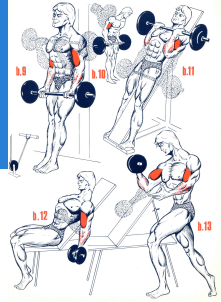
2. Add settings for SGE
3. for `blastn`

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -M foo.bar@sb-roscoff.fr
#$ -m bea
#$ -pe thread 2
#$ -q short.q

INPUT="../input/insulin.fas"
OUTPUT="insulin.blast"
DATABASE="/db/blast/all/nt"

blastn -query $INPUT -db $DATABASE -out $OUTPUT -outfmt 6 -evalue 1e-6 -max_target_seqs 5
-num_threads 2
```

4. Launch

```
$ qsub blastn.qsub

Your job 744349 ("blastn.qsub") has been submitted
```

2. qsub: simple script



5. Monitor your job (quickly)

```
$ \qstat
744349 1.00000 blastn.qsu fbar      qw    05/13/2016 08:58:06                                    2
$ \qstat
744349 1.00000 blastn.qsu fbar      r     05/13/2016 08:58:06 short.q@n78.sb-roscoff.fr          2
```

3. qsub: MPI script

- Using software version developed for MPI

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -pe mpi 10
#$ -q long.q

mpirun -np 10 phyml-mpi -i alignment.phy -d aa -m LG -b 1000 -c 4 -a e
```

```
$ qsub qsub.phyml-mpi.sh
```

Job-array

- Job-array: the idea is to split a job in a large number of sub-job
  - Very high load on the cluster
  - Problem with slot reservation
  - To prevent this problem:

Job-array should be run only on short.q!

4. qsub: Job-array

<u>Problem:</u> a large number of jobs to run and they are largely identical in terms of the command to run.

For example, you may have 1000 data sets, and you want to run a single program on each of them.

<u>Naive solution:</u> generate 1000 shell scripts, and submit them to the cluster.

<u>Best solution:</u> on SGE systems – array jobs. The advantages are:

→ You only have to write one shell script

One Script to rule them all, One Script to find them,
One Script to bring them all and in the darkness bind them

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

1. Create the structure

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q




ustacks -f $INPUT -o . -m 2
```

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

2. Get the nth INPUT / the SGE_TASK_IDth

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q



INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")



ustacks -f $INPUT -o . -m 2
```

- NR = Number of Row
- $( ) means launch the command and get back the result

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

3. Set the SGE_TASK_ID range

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q
#$ -t 1:42


INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")


ustacks -f $INPUT -o . -m 2
```

- -t 1:1000
- -t 250:500

4. qsub: Job-array

```
$ \qstat

  job-ID  prior   name       user         state submit/start at     queue       slots ja-task-ID
  -----------------------------------------------------------------------------------------------
  2216309 0.00045 blastn.qsu foobar       r     05/23/2013 14:19:56 short.q@n78     1        64
  2216309 0.00045 blastn.qsu foobar       r     05/23/2013 14:22:12 short.q@n43     1        65
  2216309 0.00045 blastn.qsu foobar       r     05/23/2013 14:25:03 short.q@n41     1        66
  2216309 0.00045 blastn.qsu foobar       r     05/23/2013 14:35:05 short.q@n78     1        67
  2216309 0.00045 blastn.qsu foobar       r     05/23/2013 14:40:02 short.q@n77     1        68
  2216309 0.00045 blastn.qsu foobar       qw    05/23/2013 14:43:03                 1 69-2379:1
```

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q
#$ -t 1:42


INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")


ustacks -f $INPUT -o . -m 2
```

- -t 1:1000
- -t 250:500

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

4. [optional] manage the stdout and stderr

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q
#$ -t 1:42


INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")


ustacks -f $INPUT -o . -m 2 > $INPUT.ustacks.stdout 2> $INPUT.ustacks.stderr
```

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

5. [optional] save a link table

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q
#$ -t 1:42


INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")

echo -e $(date '+%y%m%d-%H:%M')"\t"$SGE_TASK_ID"\t"$INPUT >> qsub_array_files.tab

ustacks -f $INPUT -o . -m 2 > $INPUT.ustacks.stdout 2> $INPUT.ustacks.stderr
```

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

5. [optional] limit the number of running jobs

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q
#$ -t 1:42
#$ -tc 5
#$ -sync no

INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")

echo -e $(date '+%y%m%d-%H:%M')"\t"$SGE_TASK_ID"\t"$INPUT >> qsub_array_files.tab

ustacks -f $INPUT -o . -m 2 > $INPUT.ustacks.stdout 2> $INPUT.ustacks.stderr
```

4. qsub: Job-array

```
$ ls *.fq

488_albifrons_bret.fq       493_albifrons_bret.fq       577_praehirsuta_bret.fq
584_praehirsuta_bret.fq     594_hybride_norm.fq         703_praehirsuta_norm.fq
714_albifrons_norm.fq       724_praehirsuta_norm.fq     490_albifrons_bret.fq
570_praehirsuta_bret.fq     580_praehirsuta_bret.fq     587_hybride_norm.fq
595_hybride_norm.fq         707_praehirsuta_norm.fq     719_albifrons_norm.fq
```

5. [optional] Super Saiyan transformation

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q

#$ -tc 5
#$ -sync no

INPUT=$(ls *.fq | awk "NR==$SGE_TASK_ID")

echo -e $(date '+%y%m%d-%H:%M')"\t"$SGE_TASK_ID"\t"$INPUT >> qsub_array_files.tab

ustacks -f $INPUT -o . -m 2 > $INPUT.ustacks.stdout 2> $INPUT.ustacks.stderr

#qsub -t 1-$(ls *.fq | wc -l) ustacks_array.qsub
```

```
$ qsub -t 1-$(ls *.fq | wc -l) ustacks_array.qsub
```

4. qsub: Job-array: Atomicblastplus.py

Standard blast: weak performances with big dataset against huge databases (nr, nt,…)

Solution: splitting your set of sequences in order to create a job-array:

- A way to parallelized blast

```
$ atomicblastplus -p blastn -i input.fasta -o myproject/tmp/blast/input_vs_nr -d
/db/blast/all/nt -e 1e-4 -n 100 --verbose

!!! This is Atomic Blast !!!

PROGRAM:
blastn: 2.2.28+
Package: blast 2.2.28, build Mar 12 2013 16:52:31

QUERY: insulin.fasta
DB: /db/blast/all/nt
OUTDIR: test

INFO: The query was splitted into 1 subfiles

INFO: SGE qsub script was written to test/qsub.insulin.atomic_blastn_vs_nt.sh

INFO: Running job-array on SGE...

CMD: qsub -q short.q -t 1-1 -tc 100 -sync yes -N at_blastn_insulin.atomic_blastn_vs_nt
test/qsub.insulin.atomic_blastn_vs_nt.sh
```

```
$ atomicblastplus -p blastn -i input.fasta -o myproject/tmp/blast/input_vs_nr -d
/db/blast/all/nt -e 1e-4 -n 10 --dont_wait --verbose
```

ADVANCED PRACTICE

Advanced parcticed

- Pass arguments to a qsub script

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q

ustacks -f $1 -o . -m $m -M $M > $1.ustacks.stdout 2> $1.ustacks.stderr
```

```
$ qsub -v m=10,M=5 ustacks.qsub 488_albifrons_bret.fq
```

Advanced parcticed

- For loop

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q

ustacks -f $1 -o . -m $m -M $M > $1.ustacks.stdout 2> $1.ustacks.stderr
```

```
$ for i in $(ls *.fq); do qsub -v m=10,M=5 ustacks.qsub $i; done
```

Advanced parcticed

- For loop loop

```
#!/bin/bash
#$ -S /bin/bash
#$ -V
#$ -cwd
#$ -short.q

ustacks -f $1 -o . -m $m -M 5 > $1.ustacks.stdout 2> $1.ustacks.stderr
```

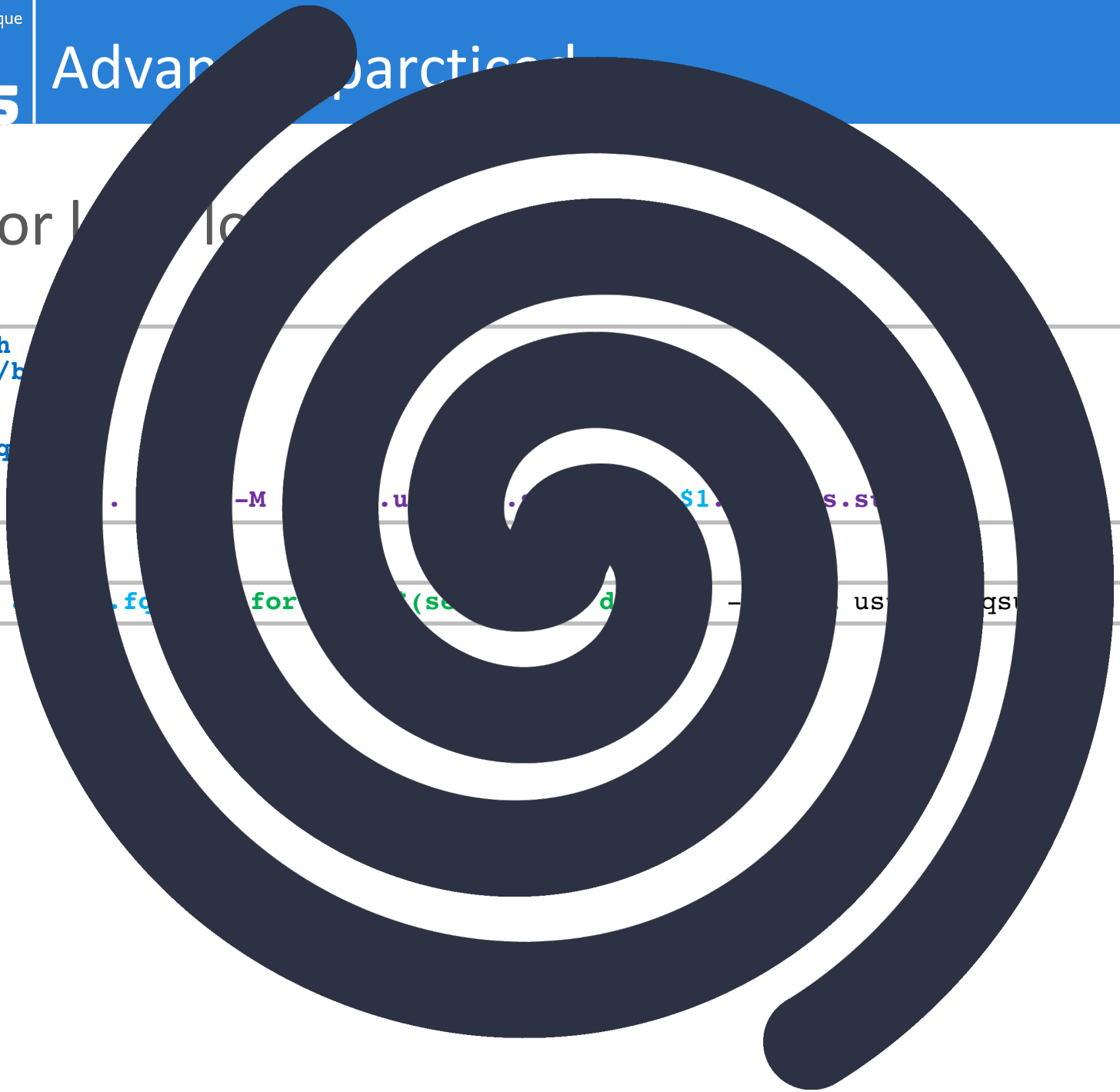
```
$ for i in $(ls *.fq); do for m in $(seq 1 10); do qsub -v m=$m ustacks.qsub $i; done; done
```

Advan parctic l

- For l lo

```
#!/bin/bash
#$ -S /bin/b
#$ -V
#$ -cwd
#$ -short.q

ustacks -f  .  -M  .u  .  $1.  s.s
```

```
$ for i in  .fq  for  (se  d  -  us  qs  done; done
```




The End