



# Shark Cluster Overview

36 Execution Nodes

1 Head Node (shark)

1 Graphical login node (rivershark)

596 Cores = slots

437 TB Storage



```
.''. .;o00o.
0MMMMMMWKxc. 'LOWMMNc
0MMMMMMMMMMMMW0d:.;xWMMMMWl
lWMMMMMMMMMMMMMMMMMMMMMM'
.xWMMMMMMMMMMMMMMMMMMMMMW
.onMMMMMMMMMMMMMMMMMMMo
cXMMMMMMMMMMMMMMMMMMO;. ;xNMMWWMX
cMMMMMMMMMMMMMMMMMMN0o;'.....';lknMMMMWx. ;l
cMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMN0.
dMMMMMMWXK00XWMMMMMMMMMMMMMMMMMMMMMMWk,
xMMmk' .,cdOKNMMMMMMMMMMXd,
dMMN' .....k
.WN.
;;
Welcome to the Shark cluster @ the research network
This cluster is still under development.
Please report problems to M.P.Villierius.
```



# Introduction

## What is a cluster?

- A cluster is a group of computers connected with a tcp/ip-network.
  - The group can work as one large computer or as single computers called nodes.
  - The cluster is controlled by a resource manager Open Grid Scheduler

## There are different type of nodes

- Head node
  - Uses a resource manager to manage all the resources
- Compute node
  - A single blade server
- Login node
  - `Shark.researchlumc.nl` / `rivershark.researchlumc.nl`
- Storage node
  - Isilon storage



## Key Terms

Cluster	= are a groups of PC's coupled together
Blade server	= a compact like workstation (PC)
Chassis	= where we store max. 16 blade servers together
Node	= is a blade server attached to a cluster
Head node	= is the controller/master node of a cluster
Execute node	= is the blade that calculate your jobs
Worker node	= same as execution node
Storage node	= is a special server that will store your data on hard disks
CPU	= Central Processing Unit
Core	= is another name for the CPU
Slot	= in a cluster one CPU is also called a SLOT
Job	= your job that needs to be calculated
Queue	= a waiting line for all jobs (jobs that cannot be processed)
Fair share	= everyone gets CPU power according to what the paid for.
SSH	= Secure Shell, a protocol to connect to a server
OGS	= Open Grid Scheduler/Grid Engine batch-queuing system for distributed resource management.



# Open Grid Scheduler

- OGS is a scheduler which divides the available resources(CPU,mem,etc) into queues
- OGS places the compute tasks (jobs) in a large list.
- OGS searches the right queue for the requested resources in a job and starts that job.
- When the resources are full, the jobs are placed in a waiting list
- Jobs with a higher priority are placed higher in the list
- The priority is based on the priority resource and the fair-share policy



# Where can I place my data?

Directory	Description	Size
<b>/exports/</b>	Mount point for Isilon every department has his own bought isilon export mounted here	715TB
<b>/home/</b>	Home dir, can hold: scripts, R library, compiled code	2TB
<b>/bam-export</b>	Everyone can save BAM files here that can be reached from the UCSC genome browser. External address : <a href="https://barmsijs.lumc.nl/.....">https://barmsijs.lumc.nl/.....</a>	1TB

## Location of important directories

- **/usr/local** *Where programs are located*
- **/usr/local/Genomes** *Where the reference genomes are located*



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# What is your responsibility

- Describe what resources are necessary to ensure success for your jobs (**memory, run time**, disk space, **number of cores**, CPU usage, network)
- Not to overload the systems resources, CPU, mem, disk space, network, run time
- Kill the job if the system is getting overloaded
- Keep track of jobs when you are not sure what resources the job uses

Important Note :  
qdel "JOB\_ID" to kill a job  
qdel -u "your username" to kill all your jobs

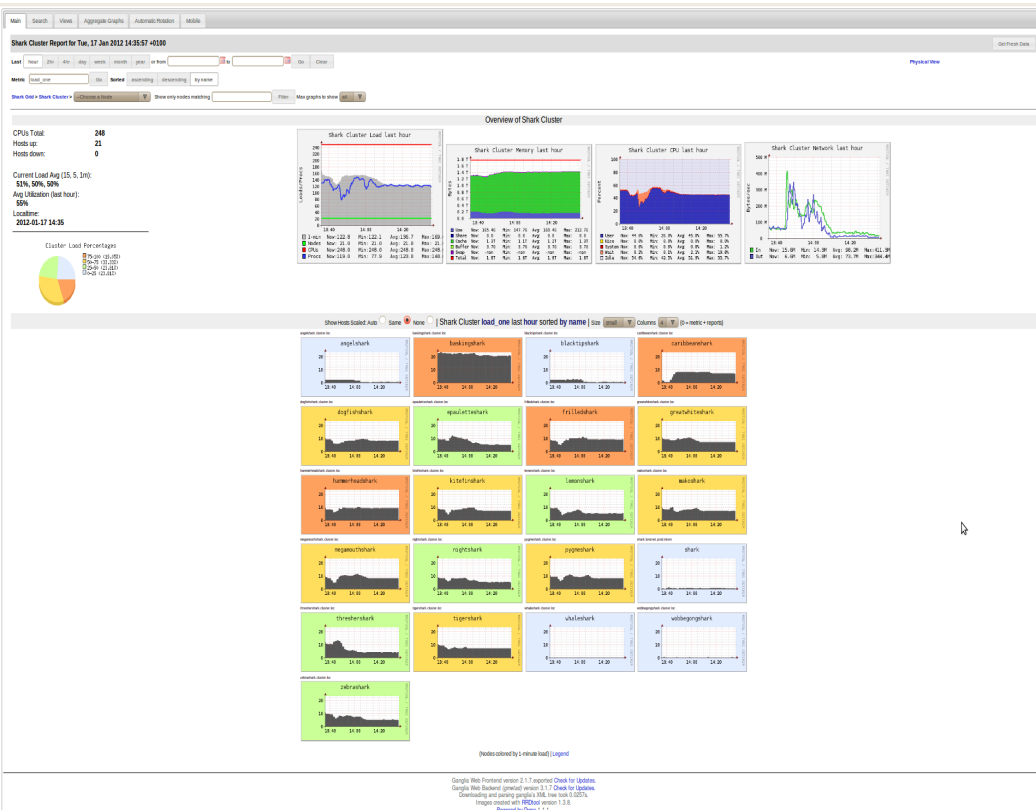




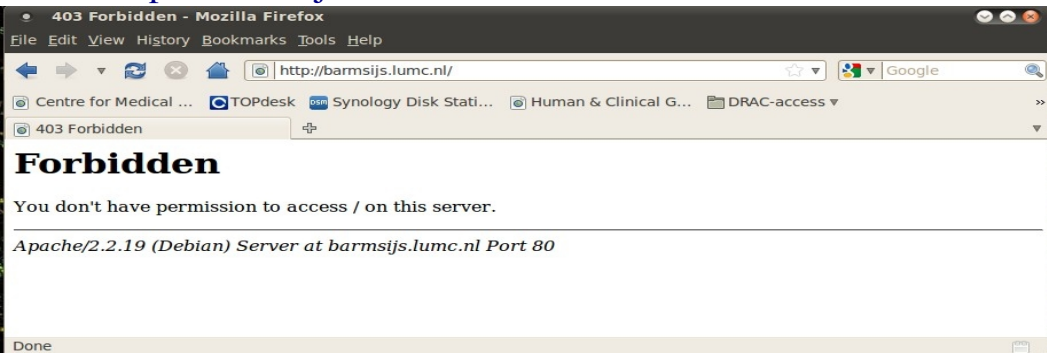
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<http://shark.lumcnet.prod.intern/ganglia/>



<https://barmsijs.lumc.nl/>



<https://humgenprojects.lumc.nl/trac/shark/>

<https://git.lumc.nl/shark/SHARK/wikis/home>



# How to connect to Shark from LUMC

- You need to use your RESEARCHLUMC username and password to connect to the Shark cluster
- Linux / MAC use SSH protocol
  - Command in terminal : `ssh researchlumcusername@145.88.65.151`
- Windows
  - use putty, cygwin or mobaxterm
  - host : `shark.researchlumc.nl`
  - port : 22
- Login from outside the LUMC
  - Use the SSH jump server : ip = 145.88.35.10





## SSH schema

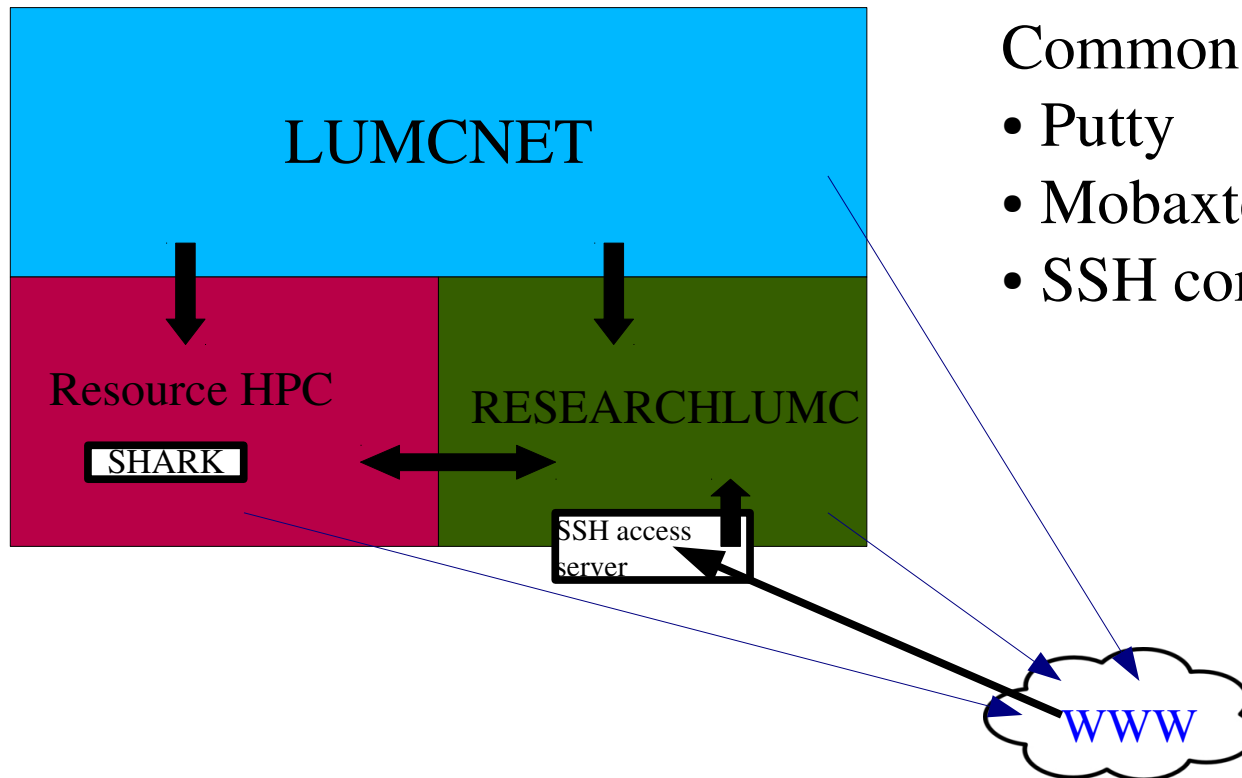
- SSH Default SSH port : 22
- SFTP
- SCP
- SSHFS

### SSH server properties

- 3 times wrong user name / session : ip banned
- 3 times wrong password / session : ip banned

### Common SSH programs

- Putty
- Mobaxterm
- SSH command





# Getting started

Important Note : default memory of every job is set to  
3GB / slot

qlogin.q and notebook.q maximum  
run time 12 hrs.

## QUEUES

username@shark:~\$ **qstat -g c**

CLUSTER QUEUE	CQLOAD	USED	RES	AVAIL	TOTAL	aoACDS	cdsuE
all.q	0.26	195	0	368	563	0	0
notebook.q	0.63	1	0	8	9	0	0
qlogin.q	0.20	12	0	8	20	0	0

## Parallel environments

username@shark:~\$ **qconf -spl**

Name	allocation rule
BWA	pe_slots
make	pe_slots
mpich2	round_robin



# Interactive use of SGE

```
username@shark:~$ qlogin
```

```
Your job 822125 ("QLOGIN") has been submitted
```

```
waiting for interactive job to be scheduled ...
```

```
Your interactive job 822125 has been successfully scheduled.
```

```
Establishing /usr/local/Scripts/qlogin_wrapper session to host angelshark.researchlumc.nl ...
```

```
username@angelshark:~$ qstat
```

Job-ID	prior	name	user	state	submit/start at	queue	slots	ja-task-ID
822125	0.50075	QLOGIN	username	r	06/04/2014 13:17:25	qlogin.q@angelshark.researchlumc.nl	1	

```
username@shark:~$ qlogin -pe BWA 4 -q all.q
```

```
Your job 110997 ("QLOGIN") has been submitted
```

```
waiting for interactive job to be scheduled ...
```

```
Your interactive job 110997 has been successfully scheduled.
```

```
Establishing built in session to host angelshark.researchlumc.nl ...
```

```
vill@angelshark:~$
```

```
username@angelshark:~$ qstat
```

job-ID	prior	name	user	state	submit/start at	queue	slots	ja-task-ID
110997	0.53227	QLOGIN	vill	r	08/03/2011 03:13:59	all.q@angelshark.researchlumc.nl	4	

Important Note : default memory of every job is set to  
3GB / slot



## Qsub your job

**Only a script can be submitted with qsub !!!!!!!**

Syntax qsub command:

**qsub [ options ] [ scriptfile | -- [ script args ] ]**

Binary files can not be submitted directly to SGE.

Example submit "date" command to SGE (with script):

**#!/bin/bash**

**/bin/date**

Submit this script with:

**\$ qsub sge-date**

SGE will then run the program, and place two files in your home directory:

**sge-date.e    sge-date.o**

The most common options:

- |                    |  |
|--------------------|--|
| -N [name]          | -- The name of the job   |
| -l h_rt=hr:min:sec | -- Maximum walltime for this job   |
| -l h_vmem          | -- Maximum memory your job can use   |
| -r [y,n]           | -- Should this job be re-runnable (default y)  |
| -pe [type] [num]   | -- Request [num] amount of [type] nodes.   |
| -cwd               | -- Place the output files (.e,.o) in the current working directory.<br>The default is to place them in the users home directory. |
| -S [shell path]    | -- Specify the shell to use when running the job script  |

Important Note : default memory of every job is set to 3GB / slot  
-l h\_vmem=3G



# Qsub your job

Qsub options can be placed inside your script.

```
vill@shark:/home/vill/shark/trunk# cat run_my_first_job.sh
```

```
#!/bin/bash
```

```
#$ -S /bin/bash
```

```
#$ -q all.q <= use with care
```

```
#$ -N my_first_job
```

```
#$ -pe BWA 4 <==== the number 4 is only if you need 4 CPU's
```

```
#$ -l h_vmem=4g <== maximum memory that can be used.
```

```
#$ -cwd
```

```
#$ -j Y
```

```
#$ -V
```

```
#$ -m be
```

```
#$ -M email@address.lumc
```

```
echo Start time : `date`
```

```
/bin/hostname
```

```
echo End time : `date`
```

```
username@shark:~/shark/trunk$ qsub run_my_first_job.sh
```

Your **job 220282** ("my\_first\_job") has been submitted

```
vill@shark:~/shark/trunk$ qstat
```

job-ID	prior	name	user	state	submit/start at	queue	slots	ja-task-ID
220282	0.60500	my_first_j	vill	r	09/07/2011 09:26:55	all.q@kitefinshark.cluster.loc	4	

Important Note : default memory of every job is set to 3GB  
-l h\_vmem=4G



vill@shark:~/shark/trunk\$ **qacct -j 220282**

```
=====
qname      all.q
hostname   kitefinshark.cluster.loc
group      NexGenSeq
owner      vill
project     NONE
department defaultdepartment
jobname     my_first_job
jobnumber   220282
taskid      undefined
account     sge
priority    20
qsub_time  Wed Sep  7 09:26:53 2011
start_time Wed Sep  7 09:26:54 2011
end_time   Wed Sep  7 09:27:15 2011
granted_pe  BWA
slots       4
failed      0
exit_status 0
ru_wallclock 21
ru_etime    0.040
ru_stime    0.010
ru_maxrss   1500
ru_ixrss    0
ru_ismrss   0
ru_idrss    0
ru_isrss    0
ru_minflt   2332
ru_majflt   0
ru_nswap    0
ru_inblock  16
ru_oublock  192
ru_msgsnd   0
ru_msgrcv   0
ru_nsignals 0
ru_nvcsw    148
ru_nivcsw    5
cpu        0.050
mem        0.000
io         0.000
iow        0.000
maxvmem    30.523M  <= note the maximum memory that has been used
arid        undefined
```

Important Note : default memory of every job is set to 3GB

Job has been submitted with 4GB times 4 slots = 16GB can be submitted with 15MB

-l h\_vmem=15m





## Configure a task dependency

```
#qsub test1.sh
```

```
#qsub -hold_jid (jobID for test1.sh) test2.sh
```

test2.sh will wait for test1.sh to complete

Run 3<sup>rd</sup> job that depends on test2.sh

```
#qsub -hold_jid (jobID for test2.sh) test3.sh
```



# What can I run where ?

- HEAD Node
  - Small non memory/cpu intensive jobs
  - vi, vim, nano
  - scp, sftp
  - Compile small programs
- Graphical Login Node
  - Firefox, fslview, gedit, etc
- Execution Nodes
  - Large jobs
  - R(run only on here!)
  - Pipelines
  - Matlab

Do not run Qlogin and go to lunch while this slot is doing nothing.



# Environment Modules

- The Environment Modules package provides for the dynamic modification of a user's environment via modulefiles.

```
# module list
```

```
Currently Loaded Modulefiles:
```

```
1) OpenGridScheduler 2) History 3) R/3.0.2
```

```
#module avail
```

```
----- /usr/local/Modules/versions -----
```

```
3.2.10
```

```
----- /usr/local/Modules/3.2.10/modulefiles-----
```

dot	java/Oracle-JRE-1.7	module-info	OpenGridScheduler	R/2.15.3	smrtanalysis
History	java/Oracle-JRE-1.8	modules	python/python-3.4.1	R/3.0.2	use.own
java/openjdk-7	module-git	null	qiime	R/3.1.1	

```
#module load R/3.0.2
```

```
#module unload R/3.0.2
```

```
#module switch R/3.1.1
```



# Summary

- **qsub** submit a job to the batch scheduler
- **qlogin** submit an interactive login session to Grid Engine
- **qstat** examine the job queue
- **qdel** delete a job from the queue
- **qacct** report and account for Grid Engine usage
- **unique-user-slots**
- /home Home dir do not store DATA here
- /data/... for storage of your data
- /usr/local/Genomes/ dir where ref. Files are located
- /bam-export dir for temp. bam files and share files.
- Do not abuse QLOGIN use qsub or qmake
- <http://barmsijs.lumc.nl/>