

File Systems on Marc2

/home	Network file system, accessible from all nodes, backed up regularly. Slow (compared to /scratch), writing lots of IO or massively parallel IO to /home should be avoided.
/scratch	Network file system, accessible from all nodes, no backup. Faster than /home, should be used for jobs that generate high amounts of IO.
/local	Local file systems on the compute node. Only accessible for processes on the same node. May be used for temporary files. Please remove your files or your job script from /local at the end of your program or when you finished your calculation.

Parameter limits

Marc2

h_rt	Mandatory, max. 10 days (864000s), no default.
h_vmem	RAM per core, max. for 64 cores on single node: 4000M, default 1000M.
-pe	Mandatory for multicore, recommended: use smp* for multithreaded jobs (max. 64 cores) and orte* for multiprocess jobs.

qstat

Displaying queued jobs

-u <user>	Displays queued jobs for <user>.
-u "*"	Display all queued jobs.
-j <jobID>	Display detailed info for a job.
-j <jobID>	Explain why this job is in error state.
-explain E	

qalter

Changing script parameters

qalter [options] <jobID>	Use to change or add any qsub parameters like -pe or -l h_rt. If a job is not allowed to start due to wrong parameters, it will run after setting them with qalter.
qalter -w v <jobID>	Display queueing information for this job. Should display "verification: found suitable queue(s)," otherwise it is likely that the job's qsub parameters contain errors.

Other useful commands

qdel <jobID>1	Delete a queued or running job.
qmod -cj <jobID>	Clear error state of a job.
qmod -cj "*"	Clear error state for all of your jobs.
dos2unix <file>	Convert a text file from DOS/Windows to UNIX formatting.

Module

Setting program environments

Syntax	module <command> <modulename>
avail	Display all available modules.
list	Display all loaded modules.
load <module>	Load a module.
unload <module>	Unload a module.
switch <module1> <module2>	Unload module1, load module2.
purge	Unload all currently loaded modules.
. /etc/profile.d/modules.sh	Needed to use the module commands in job scripts.

Possible job states in qstat

q	Queued
w	Waiting
h	On hold
r	Running
d	Deleted
e	Error

qsub

Submitting job scripts

Syntax	qsub [options] jobscript [script options]
-cwd	Use current directory as working directory for a job.
-o <path>	Name and path to the output file.
-e <path>	Name and path to the error file.
-j	Merge output and error streams into one file.
-l <resource=value>	resource-reservation, e.g. h_rt=<max runtime>, h_vmem=<max memory>.
-pe <pe> <n_cores>	Choose the parallel environment <pe> and <n_cores> to be used, e.g. -pe orte* 16 for OpenMPI jobs with 16 cores. Omit this parameter for single core jobs.
-q <queue>	Specify the queue for job execution. Choose from debug, regular or long with different runtime limits (cf. Parameter limits, h_rt).
-V	Export calling environment to job.
-N <name>	Set job name.
-t n[-m[:s]]	Submit a task array with either amount of tasks n, index range n-m or range and step size n-m:s (ex. -t 2-10:2 → 2,4,6,8,10).

Contact, Further Information

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Detailed Information

Marc2

URL: <http://marc2-doc.hrz.uni-marburg.de/trac>

