Job Queuing System SGE

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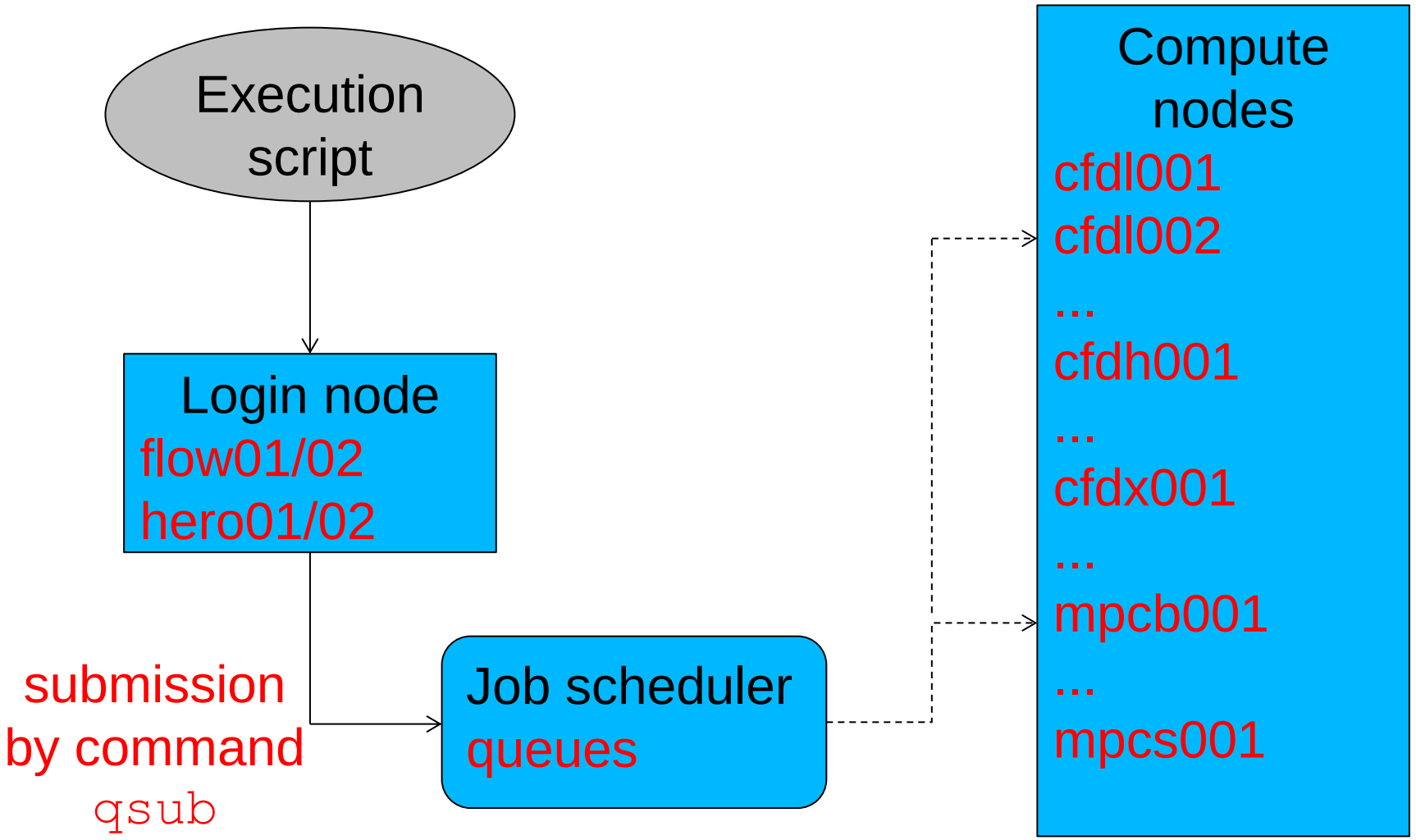
Overview

Introduction to the usage of SGE

1. Introduction
2. Preparations
3. Getting started
   - submitting, monitoring and controlling
4. Special jobs
   - I/O intensive jobs
   - parallel jobs
   - job arrays
5. Additional information
6. Job placement

INTRODUCTION
JOB SCHEDULER

Job scheduler



Tasks of a job scheduler

- acceptance of jobs
  (i.e. job script with requests for computing resources)
- prioritize jobs
  (e.g. to enable a fair share of computational resources between the users)
- places jobs in queue until they can be run
- organize workload on HPC system
  (e.g. avoid overload of nodes, balance workload on nodes)
- sends jobs from queue to execution hosts (computational node)
- manages/monitors running jobs
- logs
  - stdout/stderr of job script
  - details of finished jobs
- terminate jobs if uses more resources than requested

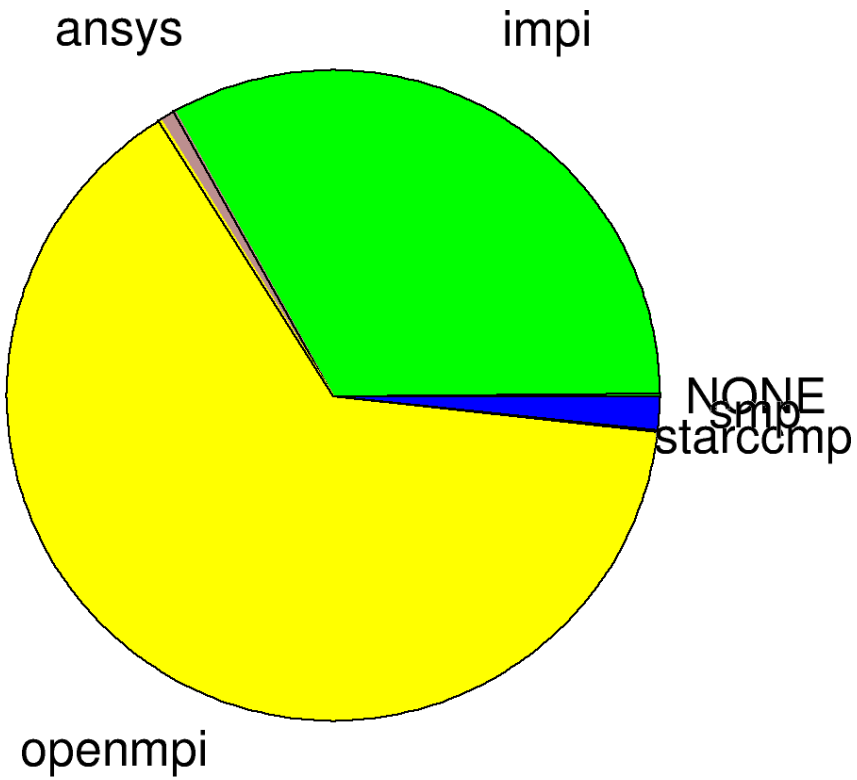
Tasks of a job scheduler

Job scheduler on FLOW/HERO

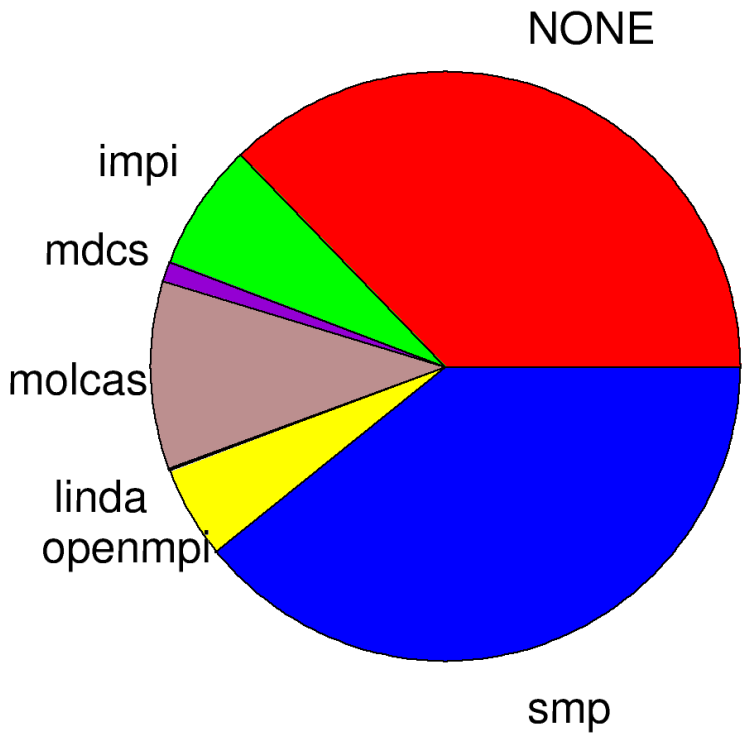
- Sun Grid Engine (SGE)
  (other schedulers: PBS/MOAB, SLURM, LSF)
- here: heterogeneous user community
  - $\mathcal{O}(200)$ active users (~1/3 FLOW, ~2/3 HERO)
  - 34 different working groups (from faculties 2, 5, 6)
  - different users, different needs, e.g.
    - parallel computations
    - multiple serial computations
    - computations with memory requirements

Usage of the cluster (2014)

FLOW



HERO



PREPARATIONS

Preparations before submitting

In case of using *commercial/open-source* program

- check if program already available on login nodes
  - typically programs installed as modules
    → command to show all available modules

    ```
    module av
    ```
  - most programs within modules are runtime optimized (e.g. by selection of the compiler/libraries)
- if many people uses the program
  - please ask for a global installation as module
    - Stefan.Albensoeder@uni-oldenburg.de (FLOW)
    - Stefan.Harfst@uni-oldenburg.de (HERO)

Preparations before submitting

In case of using *own code*

- first make tests on your local machine
  - compile your code
  - perform
    - debugging
    - optimization & profiling
  - perform small test runs
- when tests successful
  - compile your code on login nodes
  - and start with small test cases again

GETTING STARTED

How to submit a job?

- SGE is resource driven
  → you need to know the *real needs* of your program
  - memory consumption
  - run time (wall clock time)
  - disk space
  - in case of parallel programs
    - number of slots (on FLOW/HERO equal to number of cores)
    - used implementation of MPI, or
      (*Message Passing Interface*)
    - *Shared Memory* based parallelization
      (*OpenMP, PThread*)
- Requirements will be guaranteed/reserved by SGE
  → *too high resource requirements can block other jobs!*
- SGE accepts only scripts for submission

How to submit a job?

Simple example script `submitMyProgram.sge`

```
#!/bin/bash
#------------- Shell to start with -----------------------
#$ -S /bin/bash
#---- Run job in directory where job was submitted from ----
#$ -cwd
#------------- Name of the job ----------------------------
#$ -N myTest
#------------- Maximum wall clock time of the job ---------
#$ -l h_rt=24:00:00
#------------- Maximum memory usage per slot --------------
#$ -l h_vmem=1800M
#------------- Maximum of used disk space -----------------
#$ -l h_fsize=100G
#------------- Merge stdout/stderr ------------------------
#$ -j y

./myProgramCommand
```

→ submit job by `qsub submitMyProgram.sge`

How to submit a job?

Alternative way to submit script

`submitMyProgramAlt.sge`

```
#!/bin/bash

./myProgramCommand
```

→ submit job by

```
qsub -S /bin/bash -cwd -N myTest \
 -l h_rt=24:00:00,h_vmem=1800M \
 -l h_fsize=100G -j y \
 submitMyProgramAlt.sge
```

Note: *Specifications in command line will overwrite specifications in script*

What happens when submitting?

During execution of `qsub`

- SGE makes a copy your script
  → changes in script after submission will not considered!
- if jobs was accepted, SGE returns a job ID
  → the ID can be used to make changes to the job

After execution of `qsub` (in background)

- Computation of the priority of the job
  (function of number of jobs per user, number of requested slots, requested wall clock time....)
- find the right queue w.r.t. the job requirements
- find free resources w.r.t. the queue and execute script

More regarding queues later…

How to monitor a job?

Checking status of submitted job

- monitor job status using `qstat` (show all own jobs)

```
abcd1234@flow01:~ > qstat
job-ID  prior   name    user      state submit/start at
queue                         slots ja-task-ID
-----------------------------------------------------------------------------
1234567 0.50500 myTest  abcd1234  qw    09/29/2014 16:05:35
                              1
```

- somewhat later:

```
abcd1234@flow01:~ > qstat
job-ID  prior   name    user      state submit/start at
queue                         slots ja-task-ID
-----------------------------------------------------------------------------
1234567 0.50500 myTest  abcd1234  r     09/29/2014 16:06:32
cfd_lom_shrt.q@cfdl003        1
```

- when job is running stdout/stderr is written to file `${jobName}.o${jobID}, ${jobName}.e${jobID}`
  → here: `myTest.o1234567`

How to monitor a job?

More details of submitted job

- use `qstat -j <JobID>`

```
abcd1234@flow01:~ > qstat -j 1234567 | head -n 30
==============================================================
job_number:                 1234567
exec_file:                  job_scripts/1234567
submission_time:            Mon Sep 29 16:05:35 2014
...
sge_o_shell:                /bin/bash
sge_o_workdir:              /user/fw/abcd1234/test
sge_o_host:                 flow01
...
reserve:                    y
hard resource_list:         h_rt=86400,h_vmem=1800M,h_fsize=100G
...
job_name:                   myTest
…
parallel environment:       NONE
usage    1:                 cpu=00:01:24, mem=953.12500 GBs, io=6.75942,
vmem=1.203G, maxvmem=1.303G
...
```

How to monitor a job?

Get information about an ended job (within the last month)

- use `qacct -j <JobID>` (can take time)

```
abcd1234@flow01:~ > qacct -j 1234567
qname        cfd_lom_shrt.q
hostname     cfdl003.cm.cluster
...
qsub_time    Tue Sep 29 16:05:35 2014
start_time   Tue Sep 29 16:06:32 2014
end_time     Tue Sep 29 17:06:32 2014
...
failed       0
exit_status  0
ru_wallclock 3600
ru_utime     3123.184
ru_stime     98.746
...
cpu          6461.930
mem          2266.224
io           0.014
iow          0.000
maxvmem      1.303G
arid         undefined
```

How to control a job?

- delete job
  - use `qdel <jobID>`
  - `qdel '*'` deletes all own jobs
- alter resource requirements
  - modify resources with `qalter`
  - e.g.
    ```
    qalter -l h_vmem=2G,h_fsize=100G,h_rt=24:00:00
    1234567
    ```
  - Note: `qalter` overwrites resource list, hence all resource keywords need to be specified
  - most resources can only be changed before a job runs!

Summary of useful SGE commands

- `qsub` – submit your job to the scheduler
- `qstat` – monitor status of queued jobs
- `qacct` – retrieve details for finished jobs
- `qdel` – delete jobs
- `qalter` – alter jobs
- `qhold` – hold jobs
- `qrls` – release jobs from hold state
- `qhost` – show host usage
- `qrsh/qlogin` – request interactive sessions
- `qconf` – examine SGE configuration (for experts)
- `qmon` – graphical interface to SGE

SGE

I/O INTENSIVE JOBS (ONLY HERO)

I/O intensive jobs

- programs which
  - reads or writes data several times
  - needs highly temporary storage
- avoid /work or /users directory for I/O
  (avoid I/O over slow network)
- fast local scratch disk only available on HERO
  → unique path to local scratch in `$TMPDIR`
- on FLOW scratch directory `$TMPDIR` exists,
  but should not be used!

I/O intensive jobs (only HERO) - Example

```
#!/bin/bash

#$ -S /bin/bash
#$ -N myIOJob
#$ -l h_rt=24:00:00
#$ -l h_vmem=1200M
#$ -l h_fsize=100G
#$ -j y

# go to local scratch directory (only usable on HERO)
cd $TMPDIR

# copy input data from submission dir to local scratch
cp $SGE_O_WORKDIR/inputData .

# run program in scratch dir
myProgramCmd inputData outputData

# copy results back to submission directory
cp outputData $SGE_O_WORKDIR
```

SGE

PARALLEL JOBS

Parallel jobs

- for parallel jobs a parallel environment has to be defined
  - the parallel environment has to fit to the used parallelization
  - available environments

Name	Description
smp	Shared memory parallelization (e.g. OpenMP, PThread) → can run only on one node (maximal 12 slots on HERO, 16 slots on FLOW)
impi	Intel MPI
openmpi	OpenMPI
starccmp	PE for StarCCM+
ansys	PE for ANSYS
mcds	PE for Matlab
molcas	PE for Molcas

- additionally the number of slots (cores) has to be defined

Parallel jobs – Intel MPI Example

```
#!/bin/bash

#$ -S /bin/bash
#$ -cwd
#$ -N myMPIJob
#$ -l h_rt=24:00:00
#$ -l h_vmem=1200M
#$ -l h_fsize=100G
#$ -j y

#------------- run with 36 processes ---------------------
#$ -pe impi 36

# need to load the Intel MPI module
# which was used for compilation
module load impi/5.0.0.028/64/intel

# start MPI program in parallel (use not mpiexec!)
mpirun -np $NSLOTS ./myMPIProgram
```

Parallel jobs – OpenMPI Example

```
#!/bin/bash

#$ -S /bin/bash
#$ -cwd
#$ -N myMPIJob
#$ -l h_rt=24:00:00
#$ -l h_vmem=1200M
#$ -l h_fsize=100G
#$ -j y

#------------- run with 36 processes --------------
#$ -pe openmpi 36

# need to load the OpenMPI module, e.g. for gcc compiled progs
module load openmpi/1.8.4/gcc

# start MPI program in parallel (use not mpiexec!)
# for HERO add: --mca btl ^openib,ofud
# (to avoid message 'librdmacm: Fatal: no RDMA devices found')
mpirun -machinefile $TMPDIR/machines \
       -np $NSLOTS ./myMPIProgram
```

Parallel jobs – OpenMP Example

```
#!/bin/bash

#$ -S /bin/bash
#$ -cwd
#$ -N myOpenMPJob
#$ -l h_rt=24:00:00
#$ -l h_vmem=1200M
#$ -l h_fsize=100G
#$ -j y

#------------- run with 12 processes ---------------------
#$ -pe smp 12

# set number of used threads module load
export OMP_NUM_THREADS=$NSLOTS

# start OpenMP program
./myOPenMPProgram
```

Parallel jobs

Additional files from parallel environment

- `${jobName}.po${jobID}`, `${jobName}.pe${jobID}`
- contain information about allocated hosts, MPI setup,...

Monitoring of parallel jobs

- use `qstat -g t` to get information about the master/slave nodes
- alternatively you can use the script `qjobs`

Checking of free resources (mostly for FLOW users)

- `qfreenodes` shows you number of free nodes

Parallel jobs

PE memory issue (especially on HERO)

- jobs distributed over several nodes
- master process sets up/maintains ssh-connection to slaves
- per additional host ≈ 90Mb (`ssh` and `qrsh`)
- accumulate for master only (other nodes need less)
  → common problem: MASTER might run out of resources if jobs distributed over many nodes!

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JOB ARRAYS

Job arrays

- Job array start same script several times
- Each running job gets an own task ID (environment variable `SGE_TASK_ID` during execution)
- Useful for parameter studies

Name	Description
`SGE_TASK_FIRST`	First task ID of job array.
`SGE_TASK_ID`	Task ID of job within a job array.
`SGE_TASK_LAST`	Last task ID of job array.
`SGE_TASK_STEPSIZE`	Step size within the task ID of job arrays.

Job arrays - Example

```
#!/bin/bash

#$ -S /bin/bash
#$ -cwd
#$ -N myJobArray
#$ -l h_rt=24:00:00
#$ -l h_vmem=1200M
#$ -l h_fsize=100Gb
#$ -j y

#------------- Task ID from 1-100, step size 2 ------------
#$ -t 1-100:2
#------------- Maximum 3 running task at same time --------
#$ -tc 3

# fetch line SGE_TASK_ID from paraList.dat
# as command line parameter
./myProgramCmd $(sed -n ${SGE_TASK_ID}'p' paraList.dat)
```

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RESOURCE REQUIREMENTS OVERVIEW

Resource requirements

Several resource requirement can be specified

Option	Description	FLOW	HERO
`-l h_rt=05:30:00`	Set the wall clock limit of the job (default: 15min for interactive shell, 24h for job scripts, maximum: 48h for interactive jobs)	x	x
`-l h_vmem=1850M`	Maximum memory usage of a job per slot (default 1200M)	x	x
`-l h_fsize=200G`	Maximum number of disk blocks that a job writes to disk (default 10G)	x	x
`-l exclusive=true`	Enable exclusive use of nodes (default false)		x
`-l excl_flow=false`	Disable exclusive use of nodes (usually set automatically: default true if PE is active, otherwise false)	x	

Note: With option `-l` the so called complexes can be specified

(list of all complexes by `qconf -sc`)

Further options

Option	Description
`-N jobName`	Set job name
`-j y`	Merge stdout and stderr of job script output
`-S /bin/bash`	Selects the shell in which the job starts.
`-cwd`	Starts the job in the directory of the job submission.
`-e errorFile`	Redefine the name of the stdout file.
`-o stdoutFile`	Redefine the name of the stdout file.
`-hold_jid jobIDList`	Enable holding of job until other jobs has been finished.
`-R y`	Turning on the resource reservation.
`-M myemail@adress`	Email address.
`-m b|e|a|s|n,...`	Send mail at begin, end, abort, suspending of a job or not

Further options see

- HPC-Wiki
- by using `man qsub`

SGE

ENVIRONMENT VARIABLES

Environment variables

During execution SGE sets environment variable which can be used in the job script

Name	Description
JOB_ID	Job ID of current jobs
JOB_NAME	Name of the job (e.g. defined by SGE option -N).
JOB_SCRIPT	Name of the submitted job script.
PE_HOSTFILE	Host file of the parallel environment.
NHOSTS	Number of used hosts.
NSLOTS	Number of used slots.
SGE_O_HOST	Submitting host.
SGE_STDERR_PATH	Output file name of stderr.
SGE_STDERR_PATH	Output file name of stdout.
SGE_O_WORKDIR	Submission directory.
TMPDIR	Path to local temporary scratch directory.

SGE

SUBMISSION PROCESS

What happens when submitting?

During execution of `qsub`

- SGE makes a copy your script
  → changes in script after submission will not considered!
- if jobs was accepted, SGE returns a job ID
  → the ID can be used to make changes to the job

After execution of `qsub` (in background)

- Computation of the priority of the job
  (function of number of jobs per user, number of requested slots, requested wall clock time....)
- find the right queue w.r.t. the job requirements
- find free resources within the right queue

What are queues?

Queues respect different resource limits, e.g. short, low memory queue on FLOW:

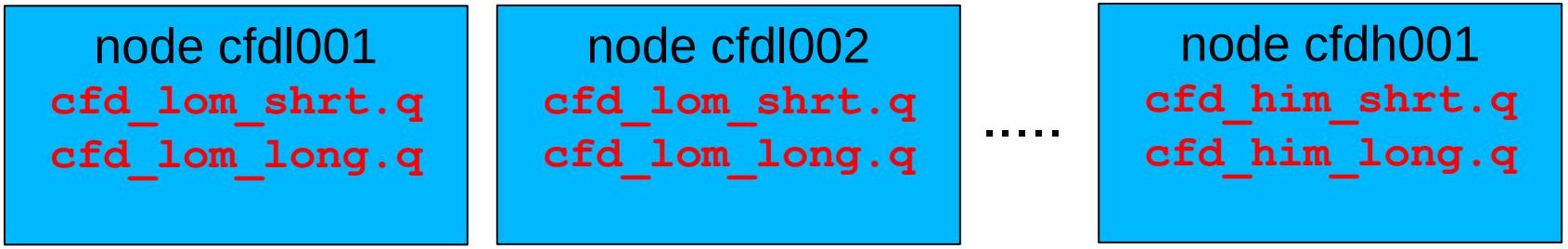
```
abcd1234@flow02:~ > qconf -sq cfd_lom_shrt.q
qname                 cfd_lom_shrt.q
seq_no                2000
hostlist              @cfdl
...
pe_list               ansys_westmere impi_westmere ....
...
complex_values        h_vmem=22G,h_fsize=10000G,cluster=flow
...
h_rt                  192:0:0
h_vmem                1850M
...
```

- resource allocation statements determine fitting queue
- search order by sequence number of queue

What are queues?

Execution hosts feature several queue instances

- queue instances jointly consume memory and slots on host
- consider e.g. standard nodes on FLOW:



- resource allocation statements determine fitting queue(s)

How does SGE places jobs on execution host?

General

- SGE try to make a load balancing between nodes
  → on the free cluster 2 serial jobs will be placed on two different nodes
- e.g. 2 serial jobs on HERO

node mpcs001	node mpcs002	node mpcs003
free slots: 12	free slots: 12	free slots: 12
free h_vmem: 23G	free h_vmem: 23G	free h_vmem: 23G

job 1	job 2
slots=1	slots=1
h_vmem=1G	h_vmem=1G

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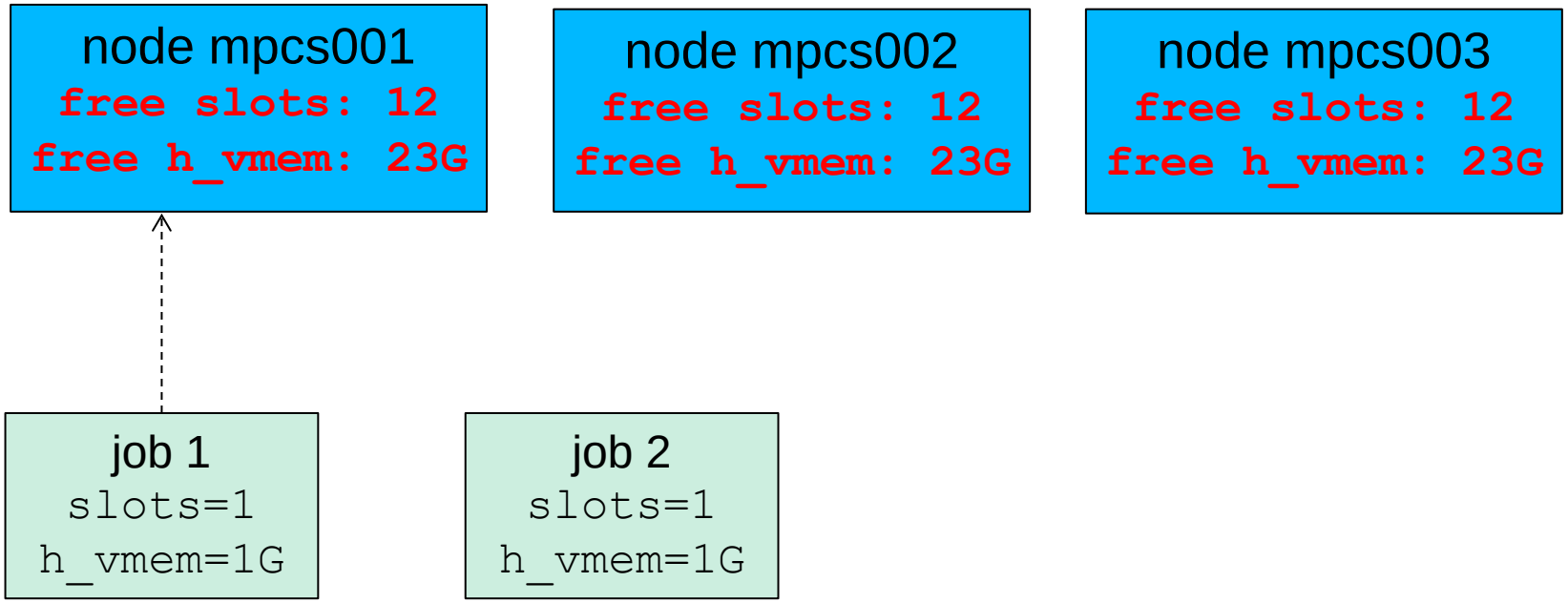

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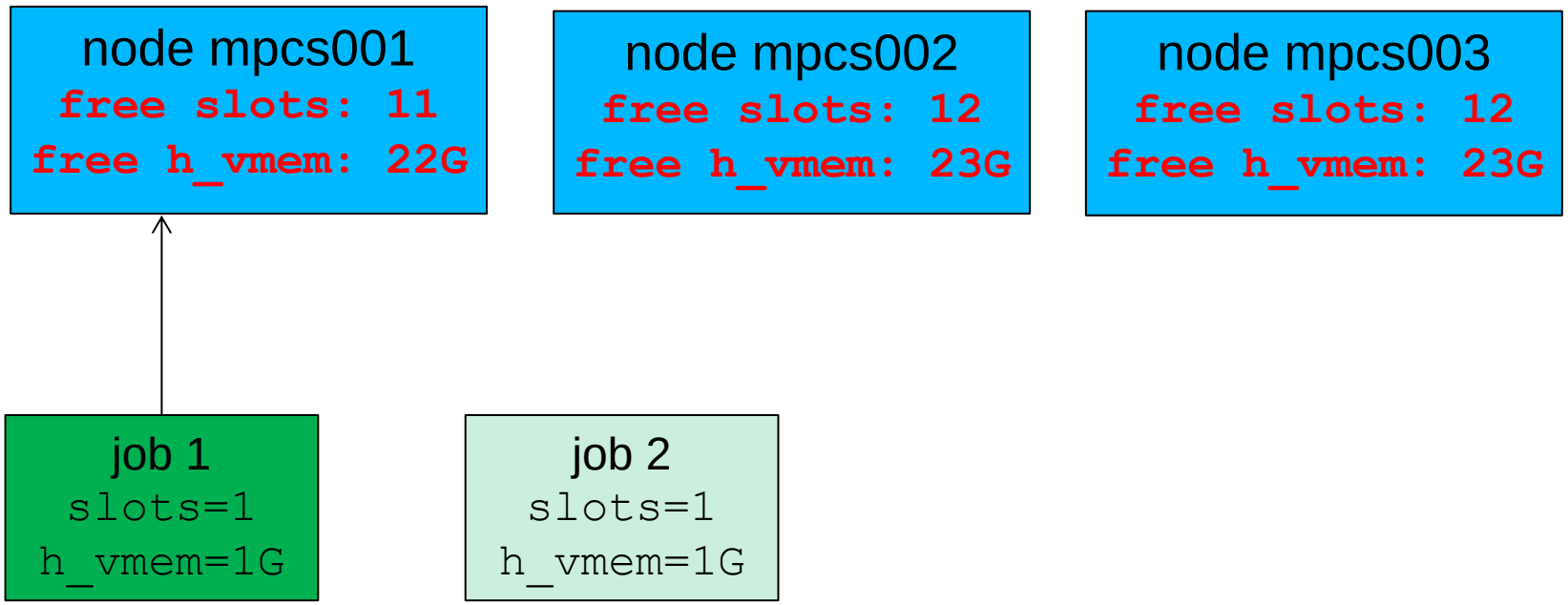

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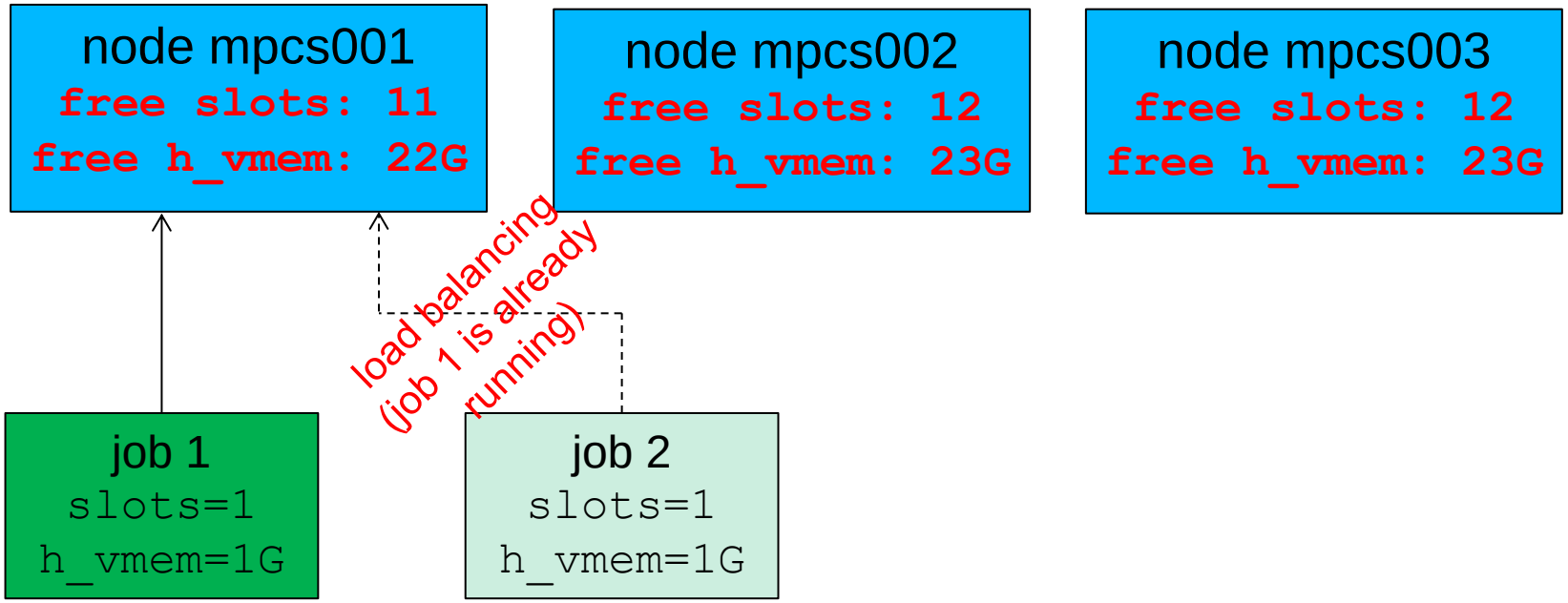

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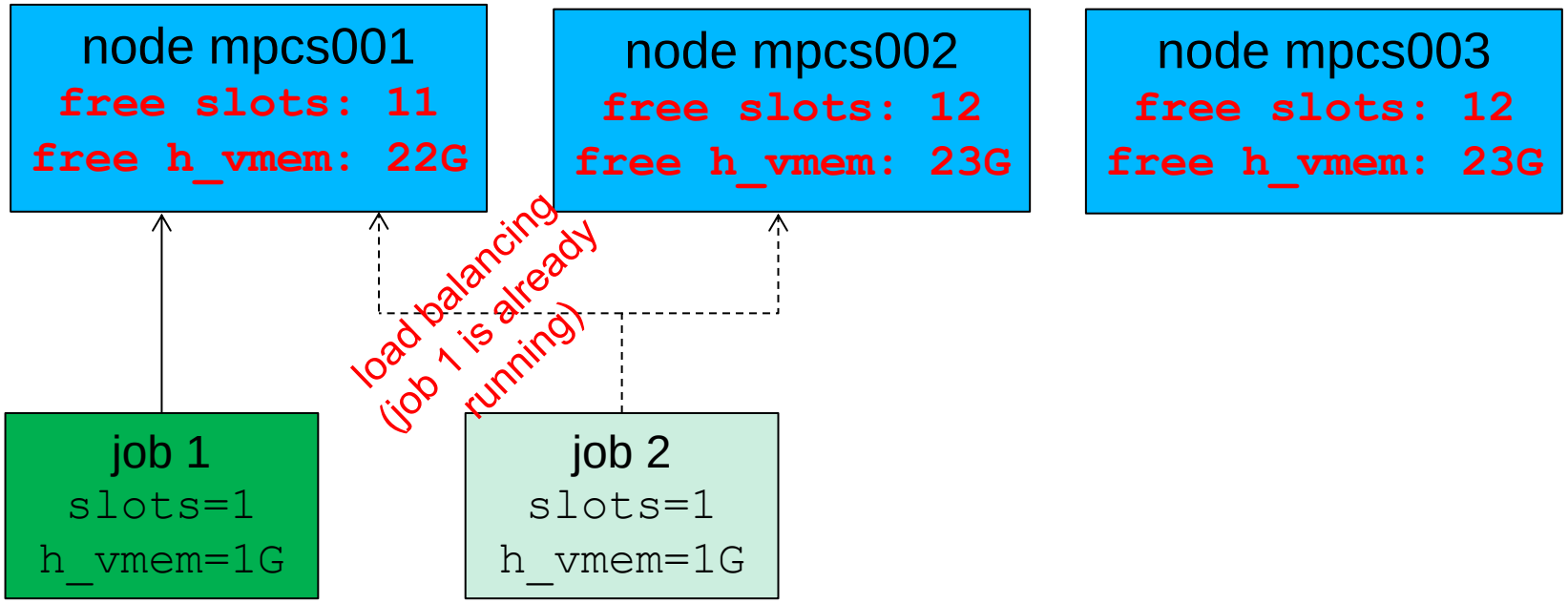

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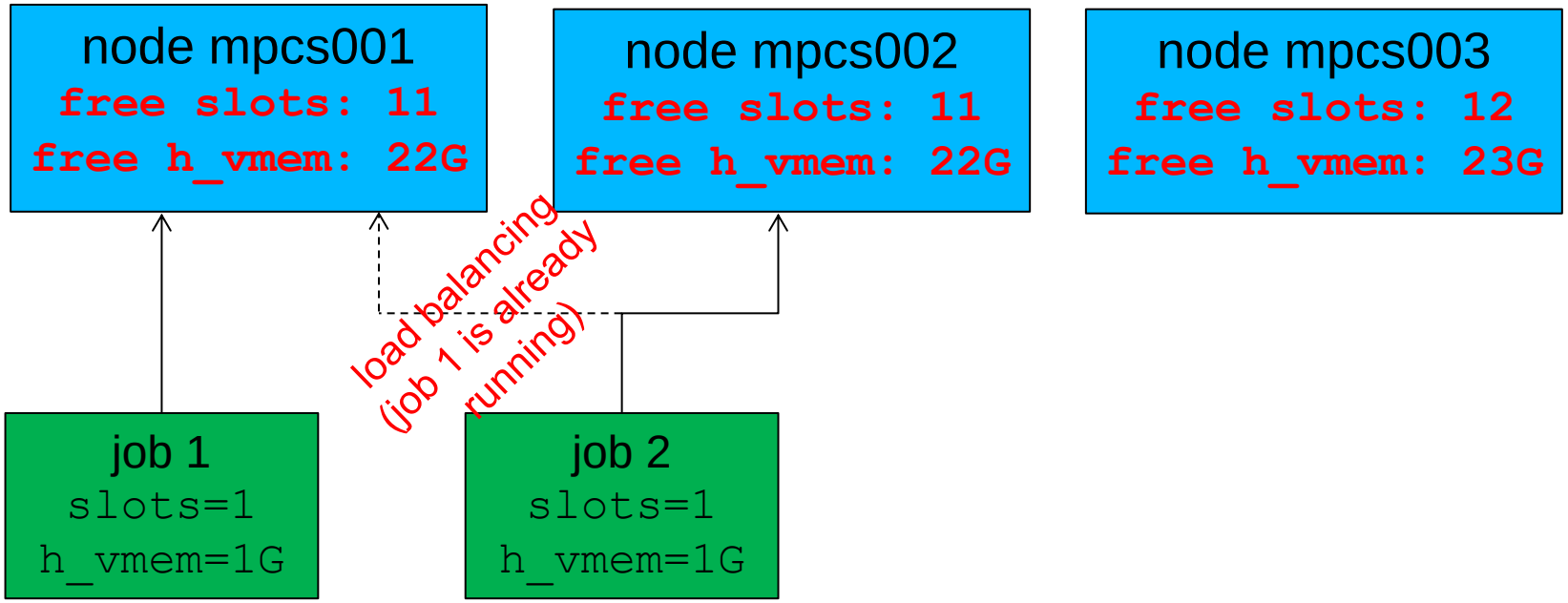

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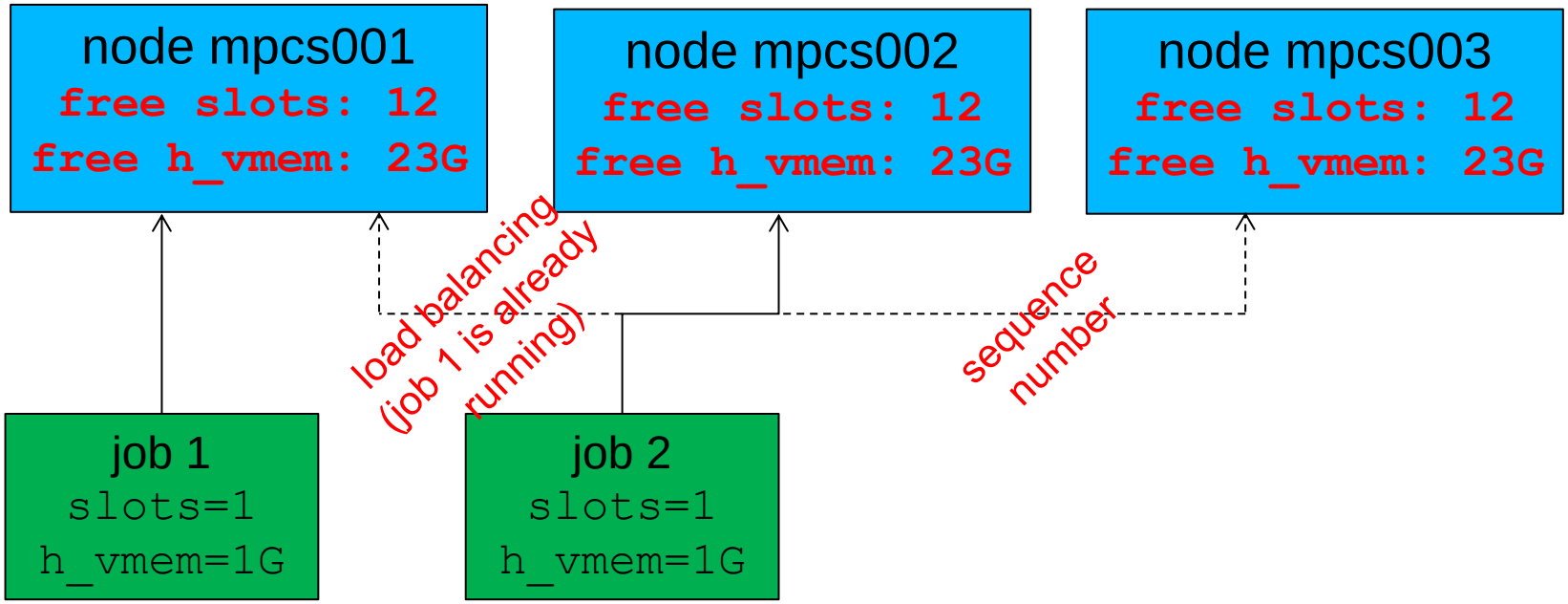
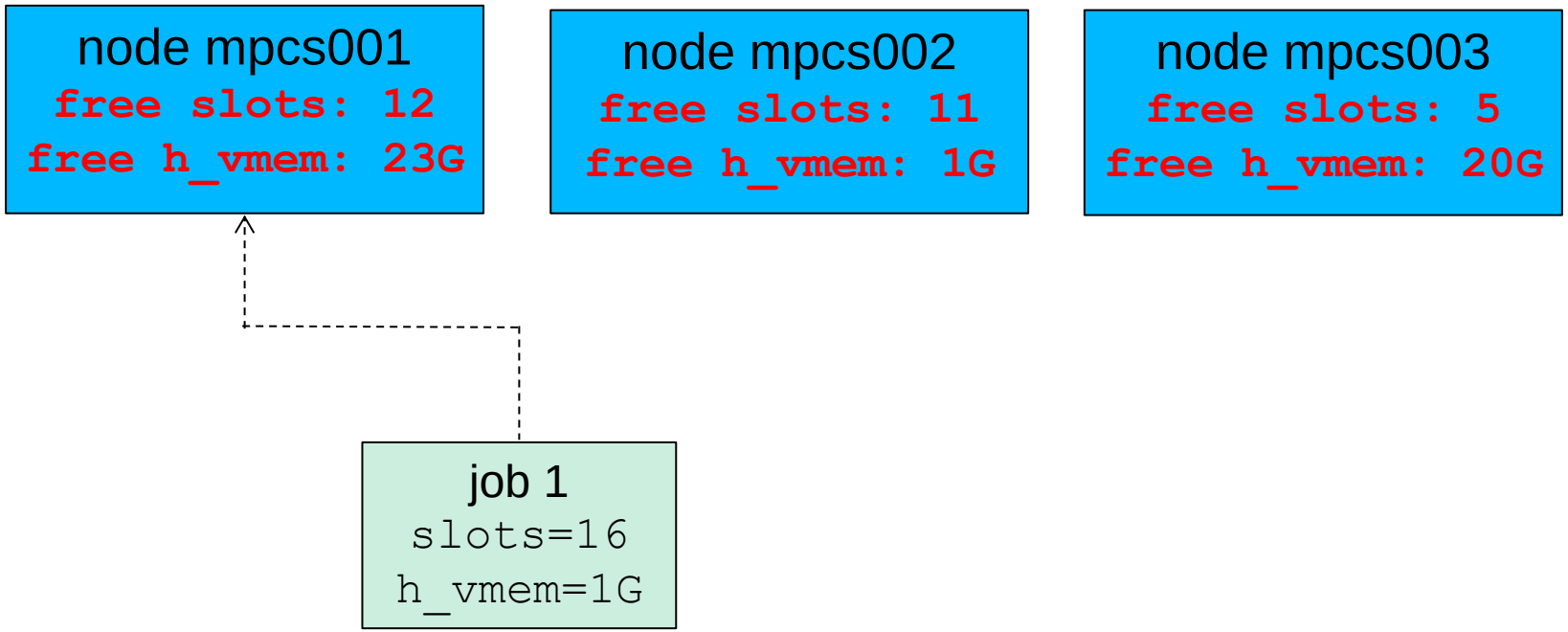


How does SGE places jobs on execution host?

Parallel jobs

- SGE try to fill up nodes (configured for FLOW/HERO)
- e.g. parallel job with 16 slots on HERO



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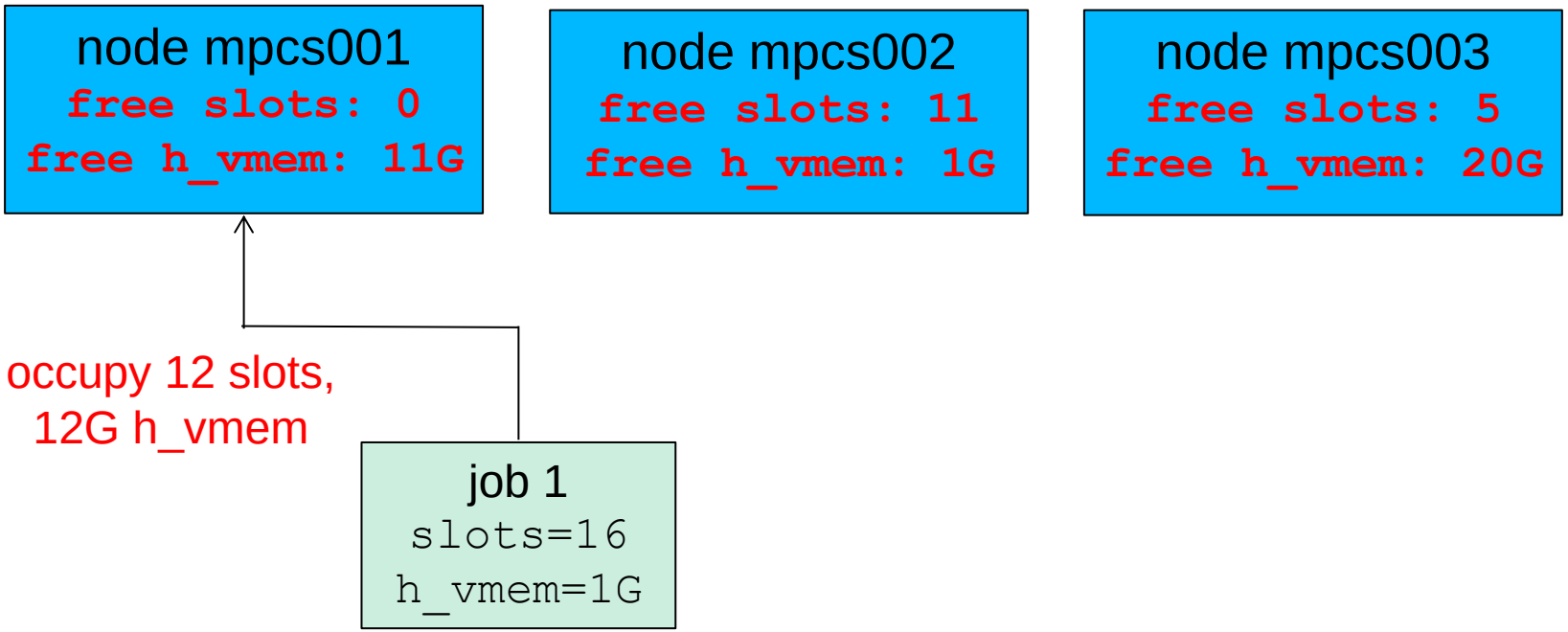

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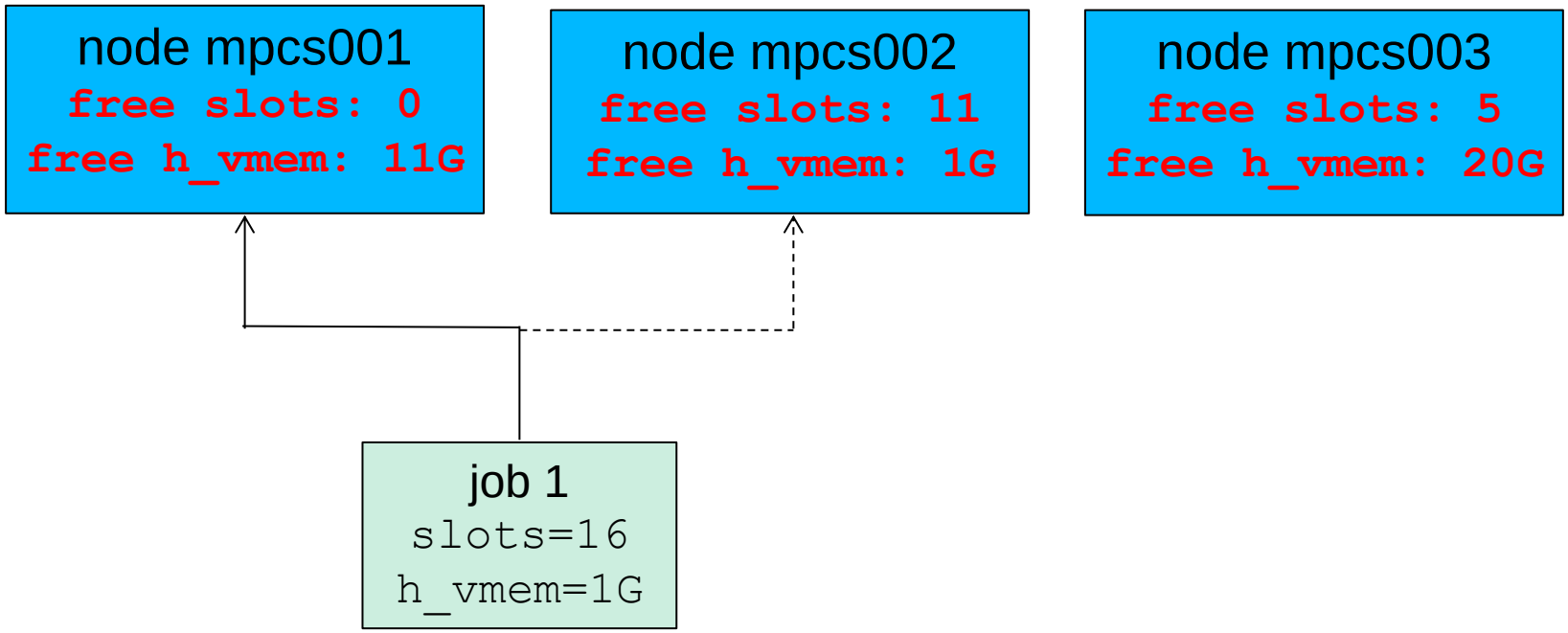

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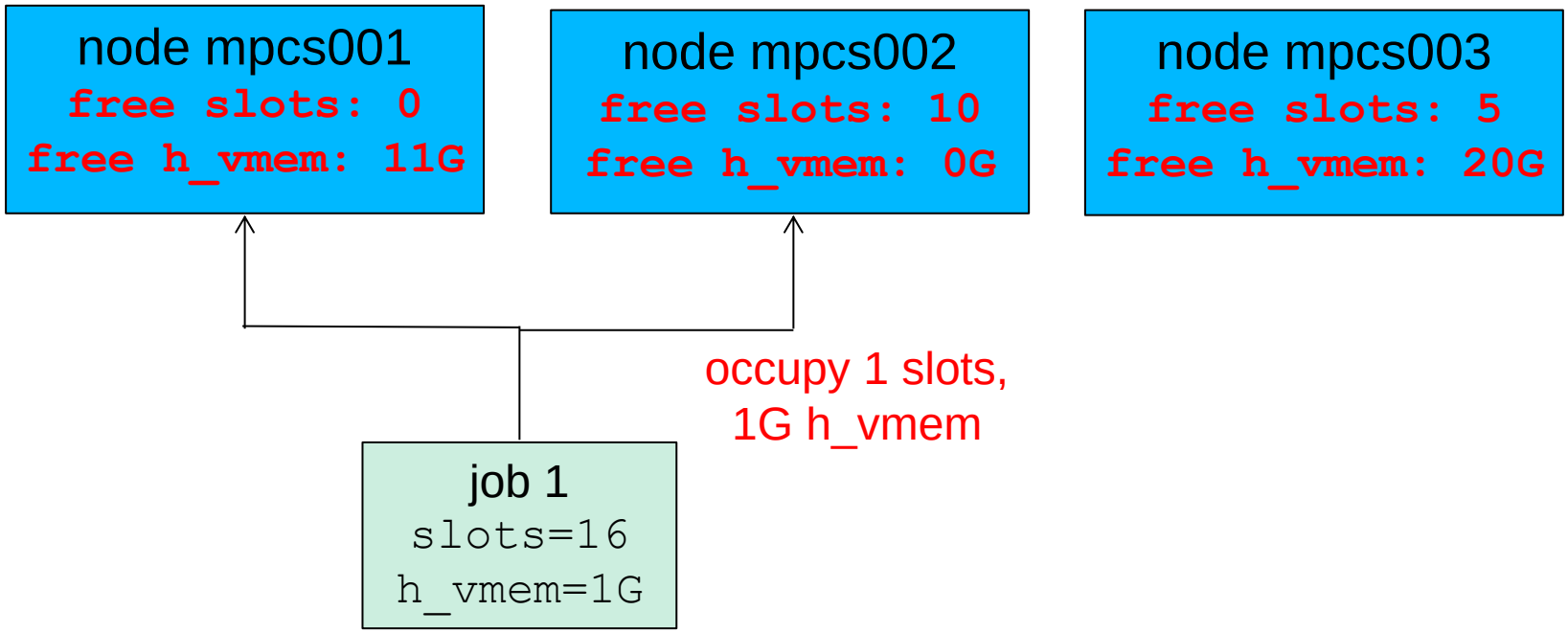

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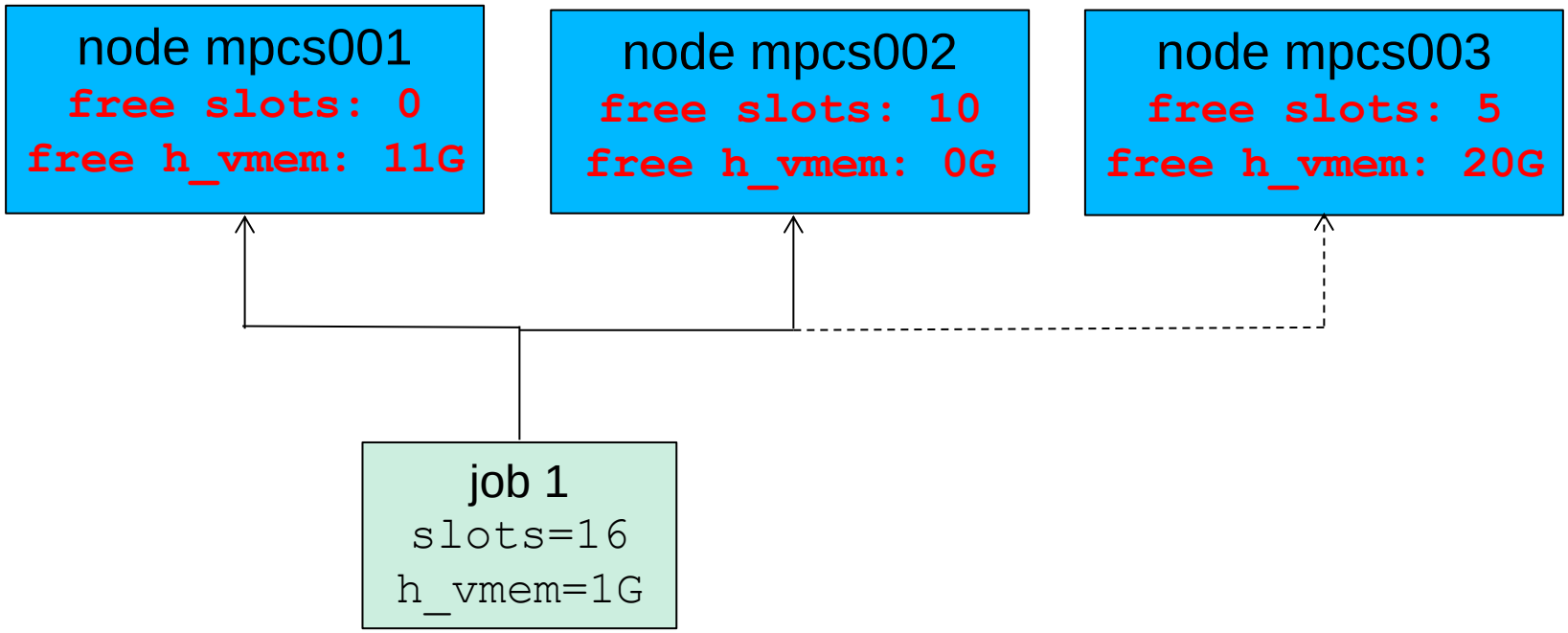

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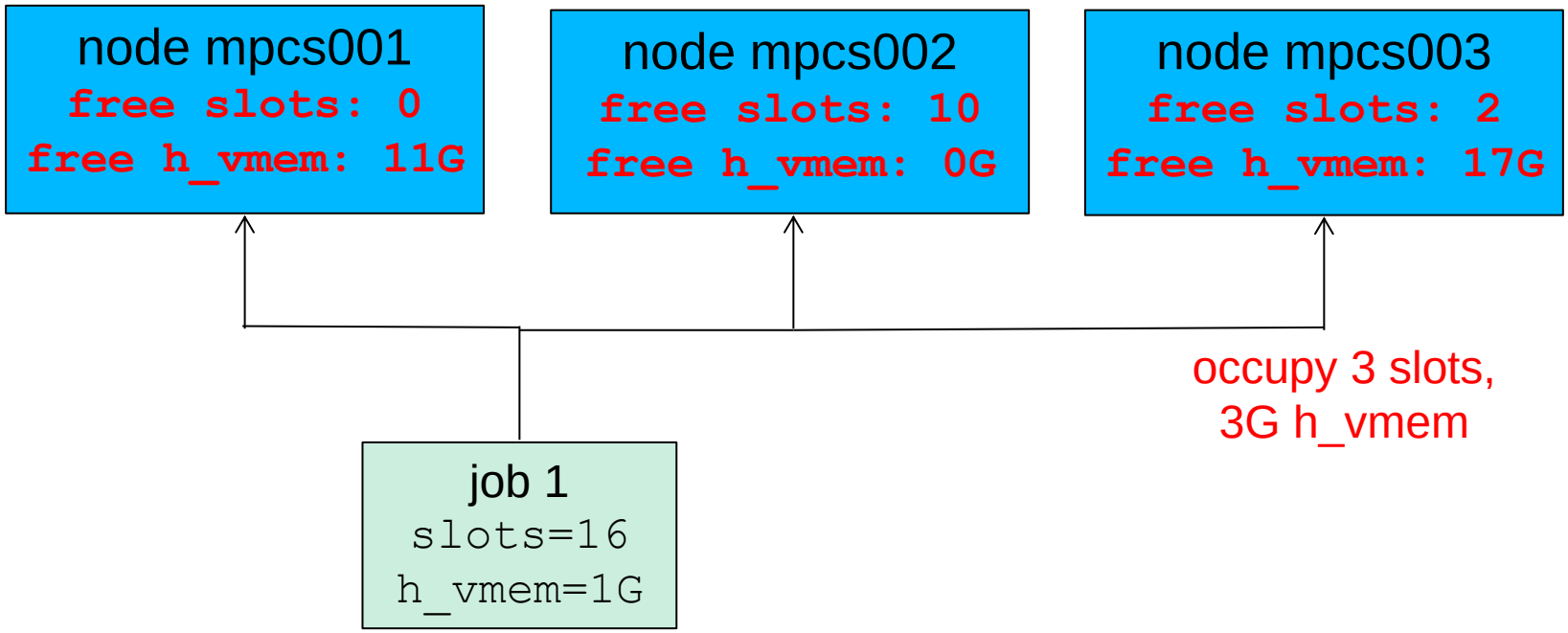

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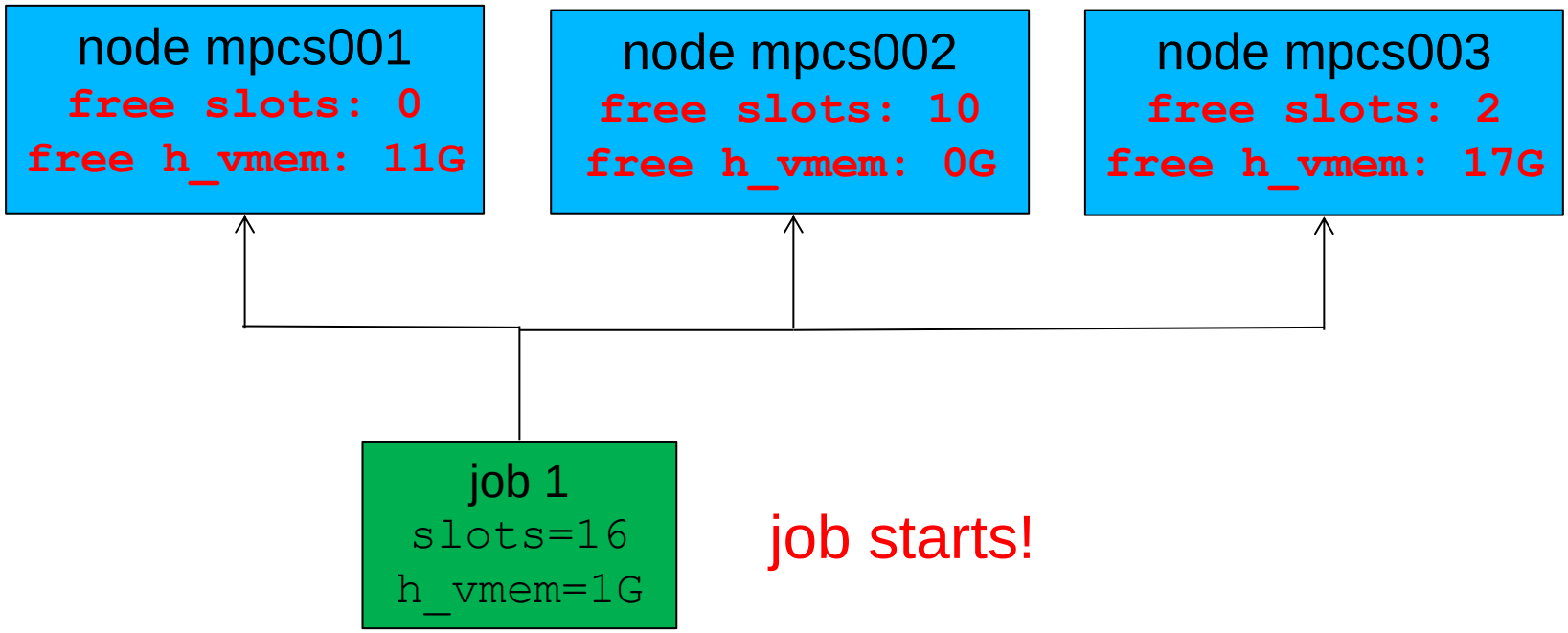

How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW

- for parallel jobs nodes will be used exclusively (nodes will be flagged that no other job can use the resources anymore, except serial jobs started before the parallel job runs on a node)
- for serial jobs/job arrays the nodes can be shared by other jobs

Serial/Parallel jobs on HERO

- for parallel jobs nodes will ***not*** be used exclusively by default. To activate exclusive usage use

```
#$ -l exclusive=true
```

- for serial jobs/job arrays the nodes can be shared by other jobs

How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW

- on FLOW nodes are always fully occupied
- e.g. several jobs on FLOW

node cfd001	node cfd002	node cfd003
free slots: 12	free slots: 12	free slots: 12
free h_vmem: 23G	free h_vmem: 23G	free h_vmem: 23G
excl_flow: True	excl_flow: True	excl_flow: True

job 1	job 2	job 3
slots=16	slots=16	slots=4
h_vmem=1G	h_vmem=1G	h_vmem=1G
excl_flow=True	excl_flow=True	excl_flow=True

How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW

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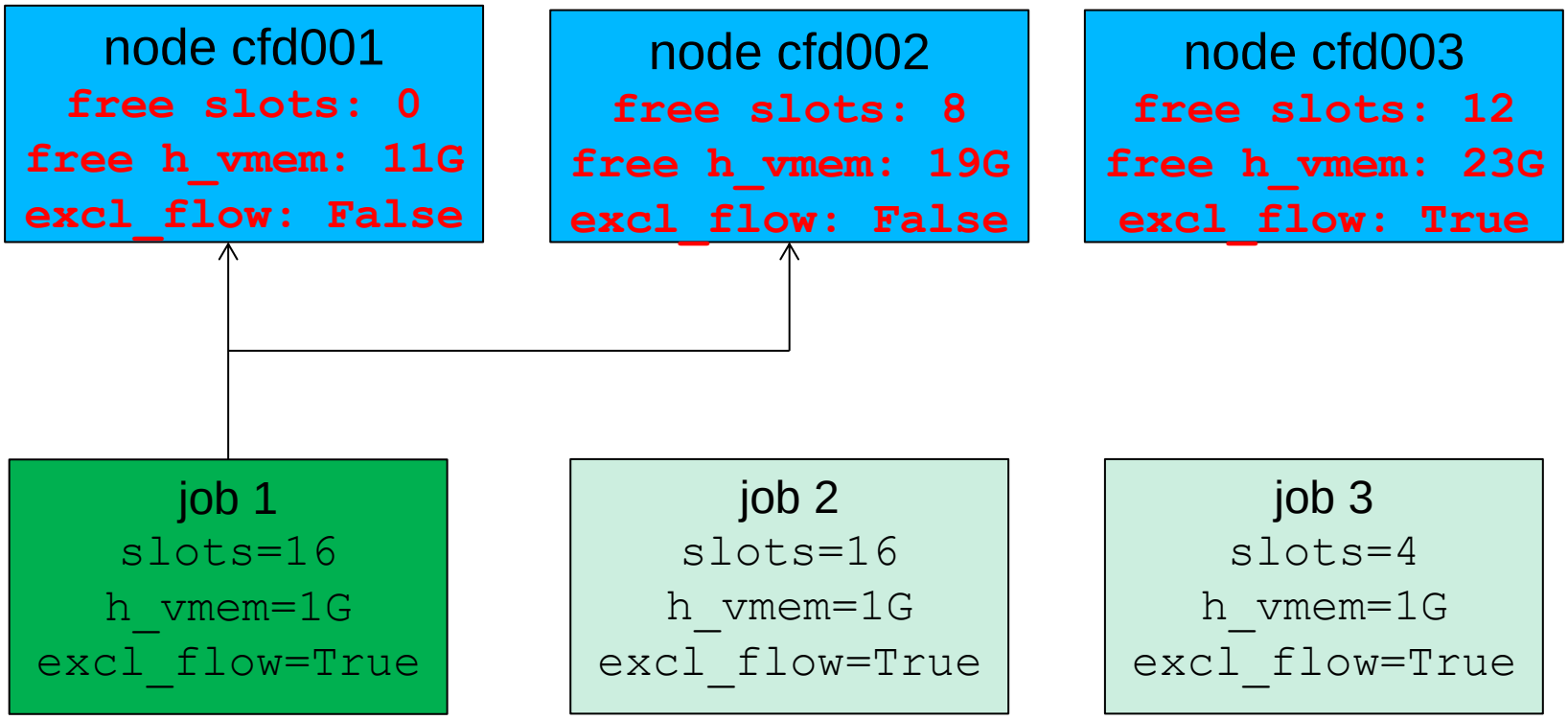

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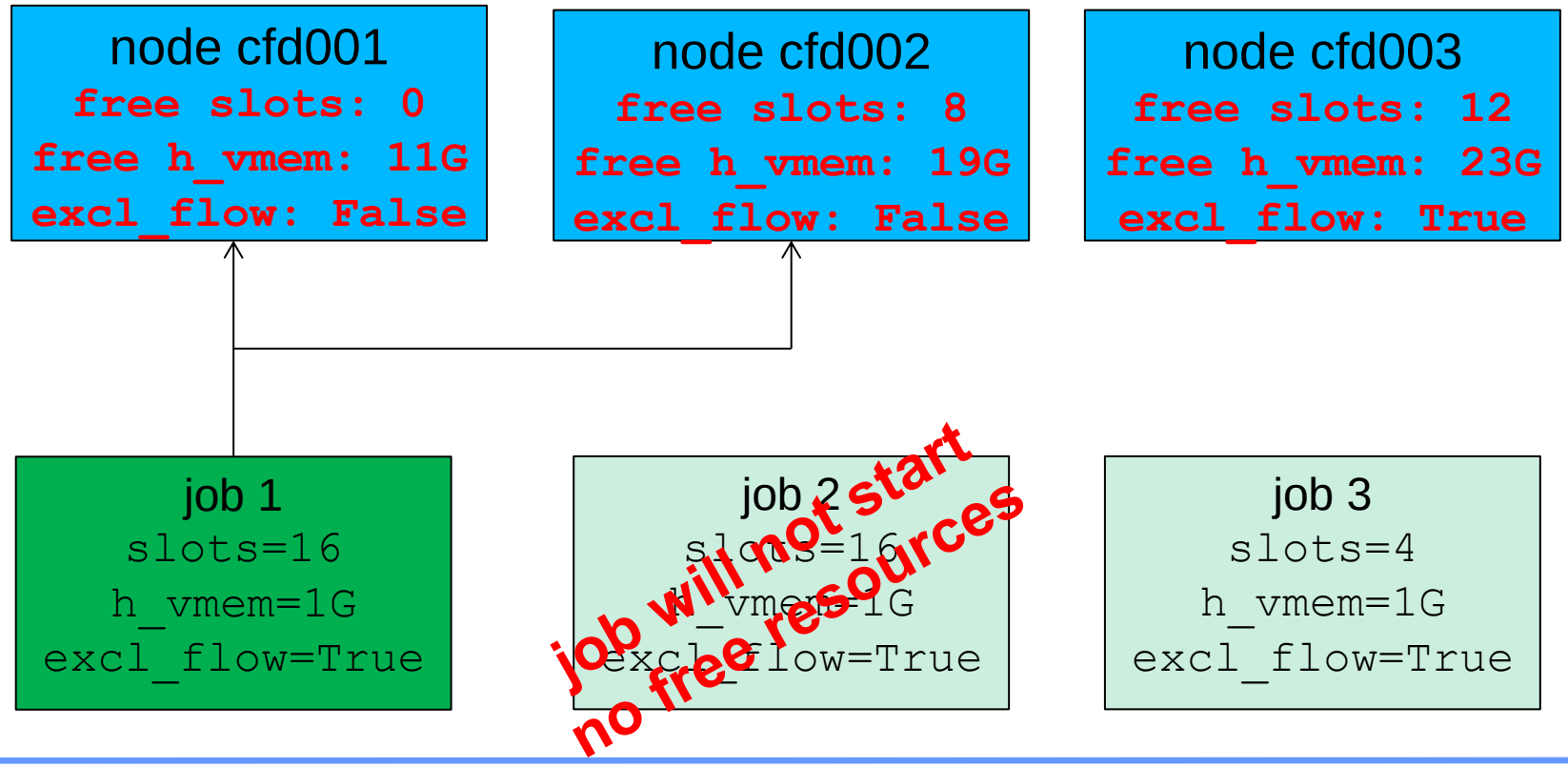

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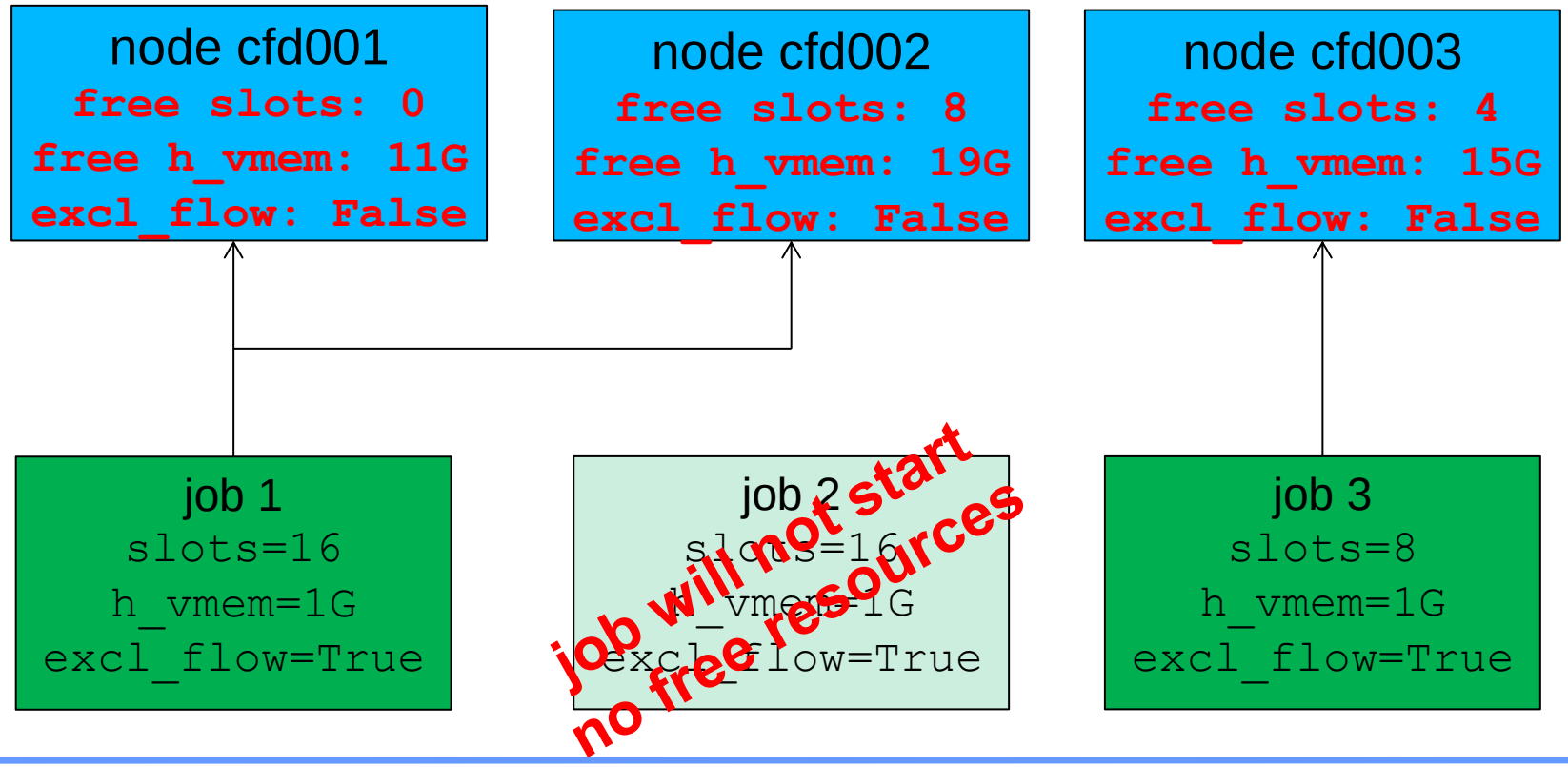


How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW, 2nd example

- full occupation doesn't work perfectly
- e.g. several jobs on FLOW

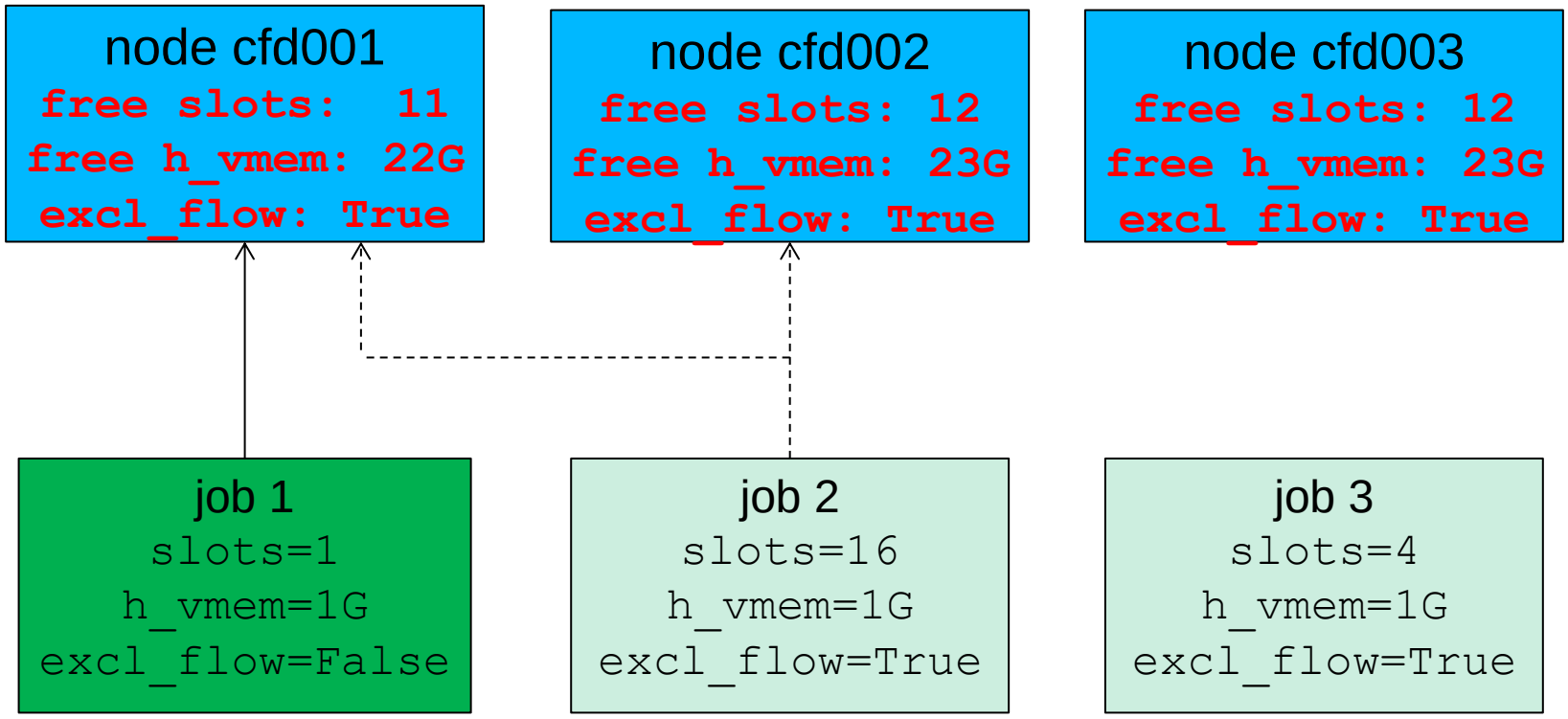
node cfd001	node cfd002	node cfd003
free slots: 12 free h_vmem: 23G excl_flow: True	free slots: 12 free h_vmem: 23G excl_flow: True	free slots: 12 free h_vmem: 23G excl_flow: True

job 1	job 2	job 3
slots=1 h_vmem=1G excl_flow=False	slots=16 h_vmem=1G excl_flow=True	slots=4 h_vmem=1G excl_flow=True

How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW, 2nd example

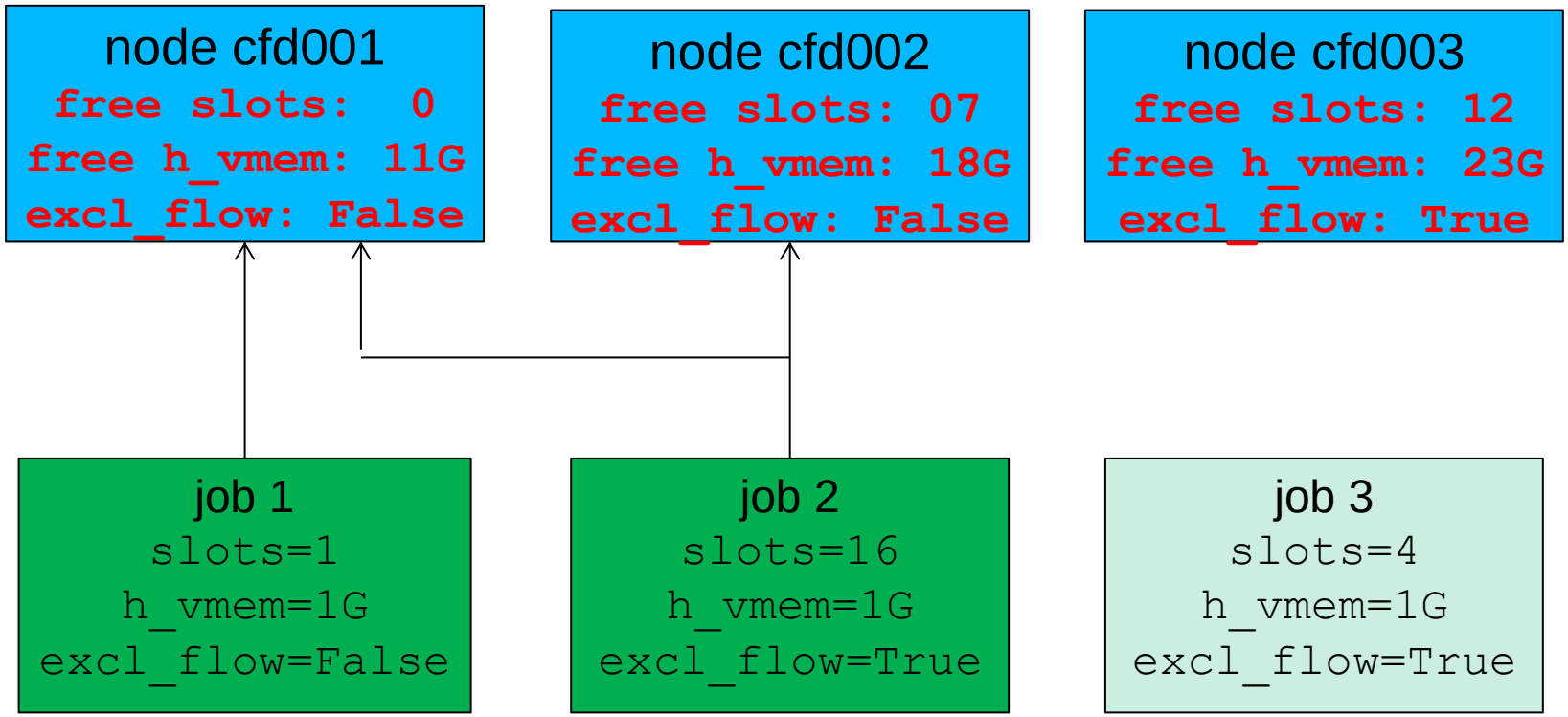
- full occupation doesn't work perfectly
- e.g. several jobs on FLOW



How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW, 2nd example

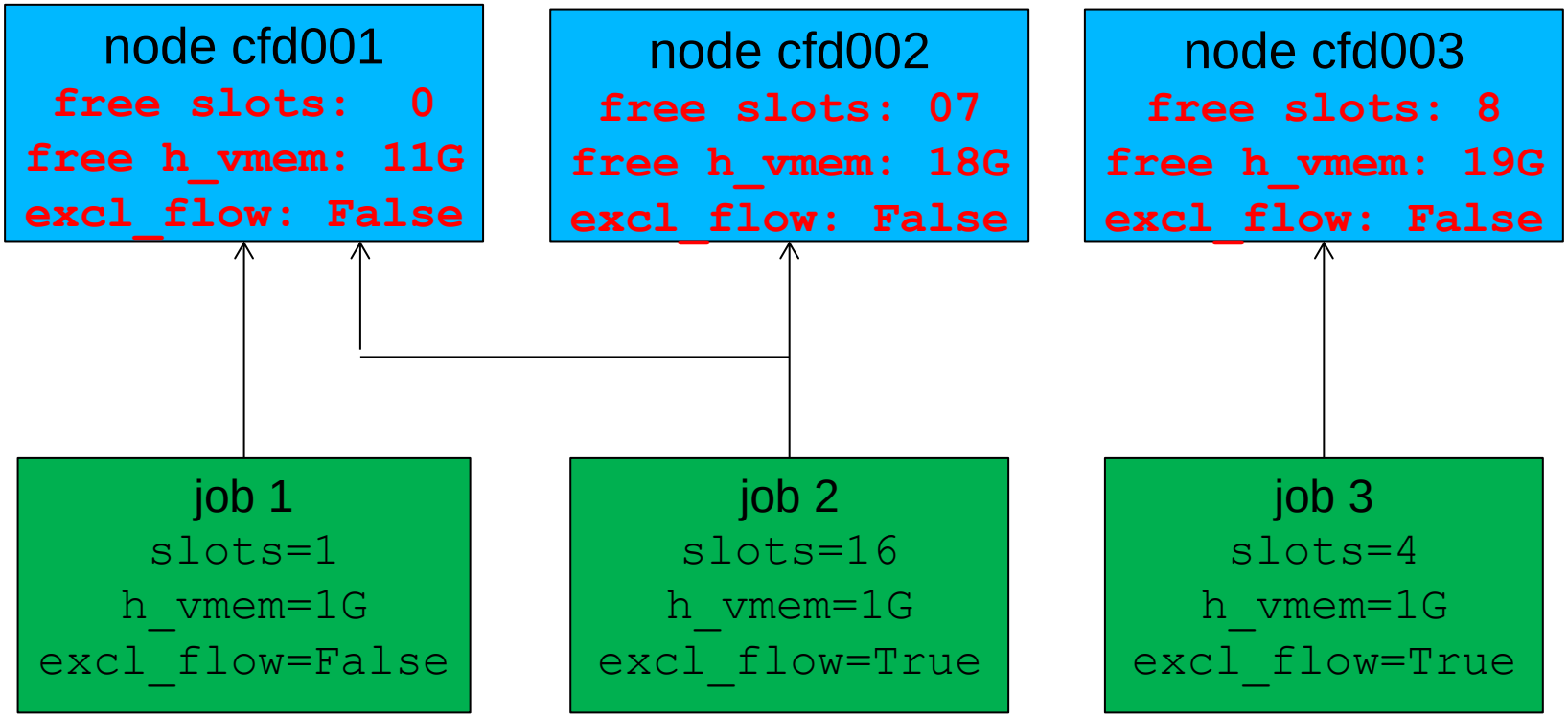
- full occupation doesn't work perfectly
- e.g. several jobs on FLOW



How does SGE places jobs on execution host?

Serial/Parallel jobs on FLOW, 2nd example

- full occupation doesn't work perfectly
- e.g. several jobs on FLOW



Thanks a lot for your attention!

For further information please visit the HPC Wiki

http://wiki.hpcuser.uni-oldenburg.de

Exercises

- Login to FLOW/HERO
  `ssh -XY abcd1234@flow.hpc.uni-oldenburg.de`
  `ssh -XY abcd1234@hero.hpc.uni-oldenburg.de`
- Create a simple serial job script
  - e.g. with commands `date; sleep 60; date`
  - or your own application
- submit job
- monitor job
  - how many resources you need?
- have a lock at the output files

HPC Wiki: http://wiki.hpcuser.uni-oldenburg.de