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Working on the curie machine

1. Online users manual

- The command curie.info returns all useful information on the curie machine. Keep it in mind and use it often.
- The TGCC's storage spaces are visible from the curie machine: \$HOME , \$CCCWORKDIR and \$CCCSTOREDIR
- The \$SCRATCHDIR space only exists for the curie machine. Be careful, this space is often cleaned and only files that are less than 40 days are stored.
- You will find the users manual provided by TGCC Left-berg : provide your TGCC/CCRT login and password in the tab for TGCC.

2. Job manager commands

- ccc_msub mon_job -> submit a job
- ccc_mdel ID -> kill the job with the specified ID number
- ccc_mstat -u login -> display all jobs submitted by login
- ccc_mpp -> display all jobs submitted on the machine. ccc_mpp -n to avoid colors.
- ccc_mpp -u \$(whoami) ->display your jobs.

3. Before starting a job

3.1. Specify the project name

Since January 2013, you must specify in the header from which project you will use computing time:

#MSUB -A genxxx

3.2. QoS test

QoS (Quality of Service) is a test queue. You can have a maximum of 2 jobs in test queue, each of them is limited to 30min and 8 nodes (= 256tasks). In the job header you must add:

#MSUB -Q test

and change the CPU time limit

#MSUB -T 1800

4. Other job manager commands

• ccc_mpeek ID -> display the output listing of a job. Note that the job outputs are visible while the job is running.

ccc_mpinfo to find out about the classes status and about the computing requirements of the associated processors. For example (11/26/2012):

/usr/bin/ccc_mpinfo														
			CP	US			NOI	ES						
PARTITION	STATUS	TOTAL	DOWN	USED	FREE	TOTAL	DOWN	USED	FREE	MpC	CpN S	Nq	ps I	'pC
standard	up	80368	32	77083	3253	5023	1	4824	198	4000	16	2	8	1
xlarge	up	10112	128	1546	8438	79	1	14	64	4000	128	16	8	1
hybrid	up	1144	0	264	880	143	0	33	110	2900	8	2	4	1

detail of a running job. One command per line ccc_mprun :

ccc_mstat	-н 375309					
JobID	JobName Partitio ReqCPU	Account	Start	Timelimit	Elapsed	State ExitCode

375309 v3.histor+ standard	0	gen0826@standard 2012-05-11T16:27:53 1-00:00:00	01:49:03	RUNNING	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T16:28:16	00:14:19	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T16:42:47	00:12:54	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T16:55:59	00:13:30	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T17:09:31	00:13:22	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T17:24:06	00:13:36	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T17:37:54	00:13:31	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T17:51:28	00:14:19	COMPLETED	0:0
375309+ p86maf_ru+	32	gen0826@standard 2012-05-11T18:05:57	00:10:59	RUNNING	0:0

information about the error code of jobs: ccc_macct nqsid

• this job ran successfully:

> ccc_macct 698214 Jobid : 698214 : v5.historicalCMR4.452 Jobname : p86maf : gen2211@s+ Account : time = 1-00:00:00 , memory/task = Unknown : submit=06/09/2012 17:51:56, start=06/09/2012 17:51:57 , end= 07/09/2012 02:20:28 Execution : partition = standard , QoS = normal Resources : ncpus = 53 , nnodes = 4Nodes=curie[2166,5964,6002,6176] Memory /step Resident (Mo) Virtual (Go) Max (Node:Task) AveTask JobID Max (Node:Task) AveTask -----_____ _____ 0(: 0) 0 25(curie2166 : 0) 0 952(curie2166 : 0) 0 0(: 0) 25(curie2166 : 0) : 0) 0.00(0.00(curie2166 : 0) 698214.batch 0.00 3.00(curie2166 : 1) 698214.0 0.00 . . . 698214.23 952(curie2166 : 0) 0 3.00(curie2166 : 2) 0.00 Accounting / step JobName Ncpus Nnodes Ntasks JobID Elapsed State ExitCode -----1 698214 v5.historic+ 53 4 08:28:31 COMPLETED 1 1 53 4 698214.batch batch 08:28:31 COMPLETED 698214.batch batch 698214.0 p86maf_run_+ 698214.1 p86maf_run_+ 53 00:20:53 COMPLETED 53 00:20:20 COMPLETED p86maf_run_+ 53 4 . . . 53 4 53 00:21:06 COMPLETED 698214.23 p86maf_run_+

• this job failed with an error code:

> ccc_macct 680580

Jobid : 680580

Jobname : v5.historicalCMR4

User : p86maf

Account : gen2211@s+

Limits : time = 1-00:00:00 , memory/task = Unknown

Date : submit=30/08/2012 17:10:06, start=01/09/2012 04:11:30 , end= 01/09/2012 04:42:48

Execution : partition = standard , QoS = normal

Resources : ncpus = 53 , nnodes = 5

Nodes=curie[2097,2107,4970,5413,5855]

Memory /step										
	Res	ident	(Mo)		Vi	irtual	. (Go)	
JobID	Max (Node	:Task)			AveTask					Ave
680580	0 (:	0)	0	0.00(:		0)	0.00
680580.batch	28(curie	2097	:	0)	0	0.00(curie209	97 :		0)	0.00
680580.0	952(curie	2097	:	0)	0	3.00(curie209	97 :		1)	0.00
680580.1	316(curie	2097	:	8)	0	2.00(curie209	97 :		8)	0.00
Accounting / st	cep									
JobID	JobName	Ncpus	Nn (odes	Ntasks	Elapsed	S	Sta	te Ex	xitCode
680580 v	.historic+	5	3	 5		00:31:18	COMP	LE	TED	0:9
680580.batch	batch		1	1	1	00:31:18	COMP	LE	TED	
680580.0 p8	36maf_run_+	5	3	5	53	00:19:48	COMP	LE	TED	
680580.1 p	36maf_run_+	5	3	5	53	00:10:06 CA	ANCELL	ĿΕD	b+	

5. Fat nodes / Thin nodes

Fat nodes for the IPSLCM5A-LR coupled model are slower than titane (130%). Thin nodes are two times faster than fat nodes for computations; they are as fast as fat nodes for post processing.

We decided to use thin nodes for computations and fat nodes for post processing. Be careful! Since November 21st 2012, you must use at least libIGCM_v2.0_rc1 to perform post processing on fat nodes.

The job header must include #MSUB -q standard to use thin nodes.

The job header must include #MSUB -q xlarge to use fat nodes.

5.1. SSD on standard node: how to use it for rebuild job

SSD usage could accelerate rebuild job. It's very usefull for medium and high resolution configuration like IPSLCM5A-MR. You have only to change header and RUN_DIR_PATH in rebuild.job. Take care you will run faster but cost will be multiplicated by a factor of 16 because standard node ie 16 cpus are dedicated. Beware of the size of the /tmp (64GB/node): if you have configuration with very high resolution and very high output frequency, the /tmp of standard node could be too small; in this case see below.

```
#MSUB -q standard # thin nodes
#MSUB -x # exclusive node
RUN_DIR_PATH=/tmp/REBUILD_DIR_MR_$$
```

5.2. RAM on fat node: how to use it for rebuild job

If /tmp of standard node (64GB) is too small for you, you can use fat node. You have to know the /tmp of fat node is also of 64GB. You have to use the RAM disk which is 250GB/node. You have only to change header and RUN_DIR_PATH in rebuild.job. Take care you will run faster but cost will be multiplicated by a factor of 128 because fat node ie 128 cpus are dedicated.

```
#MSUB -q xlarge # fat nodes
#MSUB -x # exclusive node
RUN_DIR_PATH=/dev/shm/REBUILD_DIR_MR_$$
```

6. Job Header for MPI - MPI/OMP with libIGCM

6.1. Forced model

6.1.1. MPI

To launch a job on XXX MPI tasks

```
#MSUB -r MyJob

#MSUB -o Script_Output_MyJob.000001  # standard output

#MSUB -e Script_Output_MyJob.000001  # error output

#MSUB -eo

#MSUB -n XXX  # number of MPI task

#MSUB -T 86400  # Wall clock limit (seconds)

#MSUB -q standard  # thin nodes

#MSUB -A gen****

BATCH_NUM_PROC_TOT=$BRIDGE_MSUB_NPROC
```

6.1.2. hybrid MPI-OMP

Hybrid version are only available with _v6 configurations

To launch a job on XXX MPI tasks and YYY threads OMP on each task

• first you need to modify your config.card

```
ATM= (gcm.e, lmdz.x, XXXMPI, YYYOMP)
```

· second you need to modify your job header

```
#MSUB -r MyJob

#MSUB -o Script_Output_MyJob.000001  # standard output

#MSUB -e Script_Output_MyJob.000001  # error output

#MSUB -eo

#MSUB -n XXX  # number of MPI task

#MSUB -c YYY  # number of threads OMP by task

#MSUB -T 86400  # Wall clock limit (seconds)

#MSUB -q standard  # thin nodes

#MSUB -A gen****

BATCH_NUM_PROC_TOT=XXX * YYY # number of MPI task * OMP threads
```

6.2. Coupled model

6.2.1. MPI

To launch a job on XXX MPI tasks

```
#MSUB -r MyCoupledJob
#MSUB -o Script_Output_MyCoupledJob.000001  # standard output
#MSUB -e Script_Output_MyCoupledJob.000001  # error output
#MSUB -eo
#MSUB -n XXX  # number of MPI task
#MSUB -T 86400  # Wall clock limit (seconds)
#MSUB -q standard  # thin nodes
#MSUB -A gen****
BATCH_NUM_PROC_TOT=$BRIDGE_MSUB_NPROC
```

6.2.2. hybrid MPI-OMP

Hybrid version are only available with _v6 configurations

To launch a job on XXX MPI tasks and YYY threads OMP on each task

• first you need to modify your config.card

```
ATM= (gcm.e, lmdz.x, 24MPI, 20MP)

SRF= ("" ,"" )

SBG= ("" ,"" )

OCE= (opa, opa.xx , 7MPI)

ICE= ("" ,"" )

MBG= ("" ,"" )

CPL= ("", "" )

IOS= (xios_server.exe, xios.x, 1MPI)
```

second you need to modify your job header

```
#MSUB -r MyCoupledJob

#MSUB -o Script_Output_MyCoupledJob.000001  # standard output

#MSUB -e Script_Output_MyCoupledJob.000001  # error output

#MSUB -eo

#MSUB -n XXX * YYY  # Number of cores

#MSUB -N (XXX * YYY) / 16  # Number of nodes (16 cores per node)

#MSUB -x  # exclusive node

#MSUB -E '--cpu_bind=none'

#MSUB -T 86400  # Wall clock limit (seconds)

#MSUB -q standard  # thin nodes

#MSUB -A gen***
```

7. Tricks

- export LANG=C to correctly display curie.info (by default for new logins)
- use [SHIFT] [CTL] C to copy part of a text displayed by curie.info
- ccc_quota gives usage of HOME, WORK, STORE and SCRATCHDIR. ccc_quota gives also detailed informations about CCCSTOREDIR usage.
 These informations are updated once a day at 1pm.

8. How to use the ddt debuger for the coupled model (or any other MPMD mode)

8.1. MPI only

- compile the model you wish to debug with the -g option (necessary in order to have access to sources from the ddt interface)
- create a debug directory which includes the model executables and the input files required by the model
- create a simplified debug job which allows you to start a run in the debug directory
- add the command "module load ddt" to your job
- add the creation of configuration run_file
- add a ddt start command in your job
- delete the environment variable SLURM_SPANK_AUKS : unset SLURM_SPANK_AUKS

```
...
module load ddt
unset SLURM_SPANK_AUKS

echo "-np 1 ${DDTPATH}/bin/ddt-client ${TMPDIR_DEBUG}/oasis" > run_file
echo "-np 26 ${DDTPATH}/bin/ddt-client ${TMPDIR_DEBUG}/lmdz.x" >> run_file
echo "-np 5 ${DDTPATH}/bin/ddt-client ${TMPDIR_DEBUG}/opa.xx" >> run_file
ddt
```

- connect yourself to curie in SSH mode with graphic export (option -X) and enter your password (if you have SSH keys on the front-end machine, move the ~/.ssh/authorized_keys* files outside of the directory, disconnect and reconnect yourself)
- start the job with graphic export : ccc_msub -X Job
- when the ddt window appears:

- · click on "Run and Debug a Program"
- in Application select one of the 3 model executables (which one does not matter)
- in MPI Implementation choose the "OpenMPI (Compatibility)" mode
- in mpirun arguments put "--app \${TMPDIR_DEBUG}/run_file" with TMPDIR_DEBUG = debug directory
- · click on "Run" then on the "play" key in the upper left corner

8.2. Hybrid MPI-OpenMP (use of mpirun -rankfile method)

- · compile the model you wish to debug with the -g option (necessary in order to have access to sources from the ddt interface)
- create a debug directory which includes the model executables and the input files required by the model
- create a simplified debug job which allows you to start a run in the debug directory
- add the command "module load ddt" to your job
- example with 4 OpenMP threads for Imdz and 1 OpenMP thread for nemo :

```
ddt -start -n 51 -mpiargs "-rankfile rankfile.txt --tag-output \
    -np 20 -x KMP_STACKSIZE=3g -x KMP_LIBRARY=turnaround -x MKL_SERIAL=YES -x OMP_NUM_THREADS=4 ./lmdz.x : \
    -np 31 -x OMP_NUM_THREADS=1 ./opa.xx
    "
```

- start the job with graphic export : ccc_msub -X Job
- if not default option, select "Autoselect Bullx MPI" in Options and relaunch the job.

9. Errors on curie when running simulations

9.1. Job error: KILLED ... WITH SIGNAL 15

```
slurmd[curie1006]: error: *** STEP 639264.5 KILLED AT 2012-08-01T17:00:29 WITH SIGNAL 15 ***
```

This error message means that the time limit is exceeded. To solve the problem type clean_month, increase the time limit (or decrease PeriodNb) and restart.

9.2. Isn't there restart files for LMDZ?

Problem:

If the coupled model does not run successfully, the whole chain of commands stops because there is no restart file for LMDZ. Read carefully the
out_execution file.

Solution:

- look if a file like *error exists in the Debug subdirectory. It contains clear message errors.
- in the executable directory \$SCRATCHDIR/RUN_DIR/xxxx/IPSLCM5A/xxxx look for the out_execution file. If it contains:

```
srun: First task exited 600s ago
srun: tasks 0-40,42-45: running
srun: task 41: exited abnormally
srun: Terminating job step 438782.1
slurmd[curiel150]: *** STEP 438782.1 KILLED AT 2012-06-10T18:45:41 WITH SIGNAL 9 ***
slurmd[curiel151]: *** STEP 438782.1 KILLED AT 2012-06-10T18:45:41 WITH SIGNAL 9 ***
srun: Job step aborted: Waiting up to 2 seconds for job step to finish.
slurmd[curiel150]: *** STEP 438782.1 KILLED AT 2012-06-10T18:45:41 WITH SIGNAL 9 ***
slurmd[curiel151]: *** STEP 438782.1 KILLED AT 2012-06-10T18:45:41 WITH SIGNAL 9 ***
```

don't ask questions! Type clean_month and restart the simulation.

9.3. Errors when creating or transfering files

The file system \$CCCWORKDIR, \$CCCSTOREDIR, \$SCRATCHDIR are delicate. The error messages look like:

```
Input/output error
Cannot send after transport endpoint shutdown
```

Don't ask question and resubmit the job.

9.4. Job error: Segmentation fault

```
/var/spool/slurmd/job637061/slurm_script: line 534: 458 Segmentation fault /bin/ksh -x ${TEMPO_SCRIPT}
```

If you have this kind of message don't ask question and resubmit the job.

9.5. Error when submitting jobs

This message:

```
error: Batch job submission failed: Job violates accounting policy (job submit limit, user's size and/or time limits)
```

means that you have submitted too many jobs (wait for the jobs to end and resubmit), that your headers are not properly written, or that you did not specify on which genci project the computing time must be deducted. The ccc_mqinfo command returns the maximum number of jobs (to this day: 300 for 24h-max jobs, 8 for 72h-max jobs and 2 for test jobs (30 min and max 8 nodes)):

ccc_mqinfo											
Name	Priority	MaxCPUs	MaxNodes	MaxRun	MaxSub	MaxTime					
long	18	1024		2	8	3-00:00:00					
normal	20				300	1-00:00:00					
test	40		8		2	00:30:00					

9.6. Long waiting time before a job execution

The computation of the users priority is based on 3 cumulated criteria:

- Selected QOS (test or not)
- · The fair-share value of the account (computed from the project and/or partner computation share and the previous use)
- Job's age

If your job is far down the waiting list and if you are working on different projects, use the project with the least computing time used.

This computation is not satisfying because we would prefer to encourage long simulations. We are looking for real examples of anormal waiting situations. Please take the time to give us your feedback.

9.7. Disk quota exceeded

Be careful to quotas on /scratch! Monitor them with the command ccc_quota. Destroy the temporary directories created by jobs that ended too early and that did not clear the \$SCRATCHDIR/TMPDIR_IGCM and \$SCRATCHDIR/RUN_DIR directories. You should have a 20 To quota on curie.

> ccc_quota								
Disk quotas	for user xxxx:							
-		VOLUME				INODE		
Filesystem	usage	soft	hard	grace	files	soft	hard	grace
scratch	3.53T	20T	20T	-	42.61k	2M	2M	-
store	-	-	-	-	93.76k	100k	101k	-
work	232.53G	1T	1.1T	-	844.8k	1.5M	1.5M	-

10. **REDO**

Simulations with the IPSLCM5A coupled model are reproducible if you use the same Bands file for LMDZ. See trusting TGCC/curie on this webpage: http://webservices.ipsl.jussieu.fr/trusting/

11. Feedback

11.1. On November 20th 2012

The maintenance has noticed and corrected the last two problems.

11.2. In June 2012

The 100-yr simulation of piControl in June 2012:

- 9% of jobs were resubmitted manually (3/34).
- 0,6 % of the jobs and post processing were resubmitted manually (4/694).

11.3. Error to watch in the post processing: WARNING Intra-file non-monotonicity. Record coordinate "time_counter" does not monotonically increase

- To identify quickly: grep -i monoton create_ts* | awk -F: '{print \$1}' |sort -u
 - (Command to type in \${SCRATCHDIR}/IGCM_OUT/\${TagName}/\${SpaceName}/\${ExperimentName}/\${JobName}/Out.
 - For example /ccc/scratch/cont003/dsm/p25mart/IGCM_OUT/IPSLCM5A/DEVT/lgm/LGMBR03/Out)
- · Example:

+ IGCM_sys_ncrcat --hst -v lon,lat,plev,time_counter,time_counter_bnds,zg v3.rcp45GHG1_20160101_20161231_HF_histhfNMC.nccat: WARNING Intra-file non-monotonicity. Record coordinate "time_counter" does not monotonically increase between (

Check the non monotonic time axis:

Solution: rm the TS files created and restart with TimeSeries_Checker