Steps to run a serial/OpenMP/MPI benchmark in the cluster moore.udl.cat

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1. Install the suite NPB3.3.1

1. Download the set of NAS Parallel Benchmarks (NPB3.3.1) from the Virtual Campus of the subject. This file can be located in the folder: *COMPUTACIÓ D'ALTES PRESTACIONS (103084-1920) Resources/ Chapter2-Introduction to Parallel Processing and Benchmarking/*NAS_Benchmarks/

2. Copy the file NPB3.3.1.zip from the folder where you have downloaded the file NPB3.3.1.zip to your "*moore.udl.cat*" cluster account. You can use the tool "*sftp*" and the command "*put*":
    a. *sftp* your_user@moore.udl.*cat*
    b. *put NPB3.3.1.zip*
3. Once you have the file "*NPB3.3.1.zip*" in your account "*/home/your_account*", your should connect to your account:
    a. *ssh your_account@moore.udl.cat*
4. Next, you should uncompress the file NPB3.3.1.zip by means of the following command:
    a. *unzip NPB3.3.1.zip*
5. Now, you have created a folder with the name NPB3.3.1, which contains the set of benchmarks in three different versions: serial , OpenMP and MPI. The following image shows the content of the main folder.

```
[sisco@moore ~]$ cd NPB3.3.1
[sisco@moore NPB3.3.1]$ ls
Changes.log  NPB3.3-HPF.README  NPB3.3-JAV.README  NPB3.3-MPI  NPB3.3-OMP  NPB3.3-SER  README
[sisco@moore NPB3.3.1]$
```

Figura 1. Content of the main folder NPB3.3.1

2. Configure the Serial, OpenMP and MPI versions

1. Now, we should configure the set of benchmarks according to the kind of compiler used in the cluster *moore.udl.cat*. According to this, you should download the following configuration files:

    - make.def.ser
    - make.def.omp
    - make.def.MPI

    which are located in the folder of the Virtual Campus:

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2.1. Configure the Serial Version

2. Rename the file "*make.def.ser*" to "make.def" and copy the file "*make.def*" into the following folder of your cluster account using the command "*sftp*":

   /home/sisco/NPB3.3.1/NPB3.3-SER/config

3. Go to the folder: /home/sisco/NPB3.3.1/NPB3.3-SER/ and compile the serial benchmarks. For instance, if we want to compile the serial benchmark EP in the CLASSES A, B and C respectively, we will write the following commands:
   a. make EP CLASS=A
   b. make EP CLASS=B
   c. make EP CLASS=C
4. The compiled benchmarks (ep.A.x, ep.B.x and ep.C.x) will be stored in the folder of the moore cluster:

   /home/sisco/NPB3.3.1/NPB3.3-SER/bin

2.2. Configure the OpenMP version

5. Now, we will configure the OpenMP benchmarks. According to this, we will repeat the previous steps 2, 3 and 4 .
6. Rename the file "*make.def.omp*" to "*make.def*" and copy the file "*make.def*" into the following folder of your cluster account using the command "*sftp*":

   /home/sisco/NPB3.3.1/NPB3.3-OMP/config

7. Go to the folder: /home/sisco/NPB3.3.1/NPB3.3-OMP/ and now, we can compile OpenMP benchmarks. For instance, if we want to compile the OpenMP benchmark EP in the CLASSES A, B and C, respectively we will write the following commands:
   a. make EP CLASS=A
   b. make EP CLASS=B
   c. make EP CLASS=C
8. The compiled benchmarks (ep.A.x, ep.B.x and ep.C.x) will be stored in the folder of the *moore* cluster:

   /home/sisco/NPB3.3.1/NPB3.3-OMP/bin

2.3. Configure the MPI benchmarks

9. Now, we will configure MPI benchmarks. According to this, we will repeat previous steps 2, 3 and 4.
10. Rename the file "*make.def.mpi*" to "make.def" and copy the file "*make.def*" into the following folder of your cluster account using the command "*sftp*":

    /home/sisco/NPB3.3.1/NPB3.3-MPI/config

11. Go to the folder: /home/sisco/NPB3.3.1/NPB3.3-MPI/ and now, we can compile MPI benchmarks. For instance, if we want to compile the MPI benchmark EP to be executed with 4 different tasks in the CLASSES A, B and C respectively, we will write the following commands:
    a. make EP NPROCS =4 CLASS=A
    b. make EP NPROCS=4 CLASS=B
    c. make EP NPROCS=4 CLASS=C
12. The compiled benchmarks (ep.A.4, ep.B.4 and ep.C.4) will be stored in the folder of the *moore* cluster:

    /home/sisco/NPB3.3.1/NPB3.3-MPI/bin

3. Execute the Serial, OpenMP and MPI benchmarks in the *moore* cluster using the SGE sytem queue management

1. Now, we should download the scripts that contain SGE commands to run the benchmarks in the *cluster moore.udl.cat*. According to this, you should download the following scripts:

    - run-simple-serial.sh
    - run-simple-omp.sh
    - run-extended-mpi.sh

    which are located in the folder of the Virtual Campus:

COMPUTACIÓ D'ALTES PRESTACIONS (103084-2122) recursos Chapter2-Introduction Parallel Processing and benchmarking SGE System Scripts

3.1. Execute the Serial benchmarks

1. Copy the script *run-simple-serial.sh* into the following folder of your cluster account using the command "*sftp*":

    /home/sisco/NPB3.3.1/NPB3.3-SER/bin

2. Edit the file *run-simple-serial.sh* using the command *vim* or another text editor:

run-simple-serial.sh

run-simple-serial.sh 〉 No Selection

```
1  #!/bin/bash
2
3  ## Specifies the interpreting shell for the job.
4  #$ -S /bin/bash
5
6  ## Specifies that all environment variables active within the qsub utility be
       exported to the context of the job.
7  #$ -V
8
9  ## Specifies the parallel environment if it is needed
10
11 ## Execute the job from the current working directory.
12 #$ -cwd
13
14 ## The  name  of  the  job.
15 #$ -N EP_A
16
17 ##send an email when the job ends
18 #$ -m e
19
20 ##email addrees notification
21 #$ -M Your_email@alumnes.udl.cat
22
23
24 ## In this line you have to write the command that will execute your application.
25 ./ep.A.x
26
```

Figura 2. Content of the serial SGE script.

3. **This script is ready to run the benchmark named ep.A.x. If you want to change the benchmark to be executed, you should only change the lines 15 and 25 with the corresponding new benchmark name. Likewise, you should change the line 21 with your UdL email.**
4. From the folder */home/sisco/NPB3.3.1/NPB3.3-SER/bin* of the moore cluster, you can run the *ep.A.x* using the following SGE command:
    a. *qsub run-simple-serial.sh*
5. When the execution of the *ep.A.x* is finished, the following two new files will be created automatically:
    a. EP_A.o7380: This file shows the output of the benchmark. Figure 3 shows an example.
    b. EP_A.e7380: This file contains the error messages. Usually, this is empty.

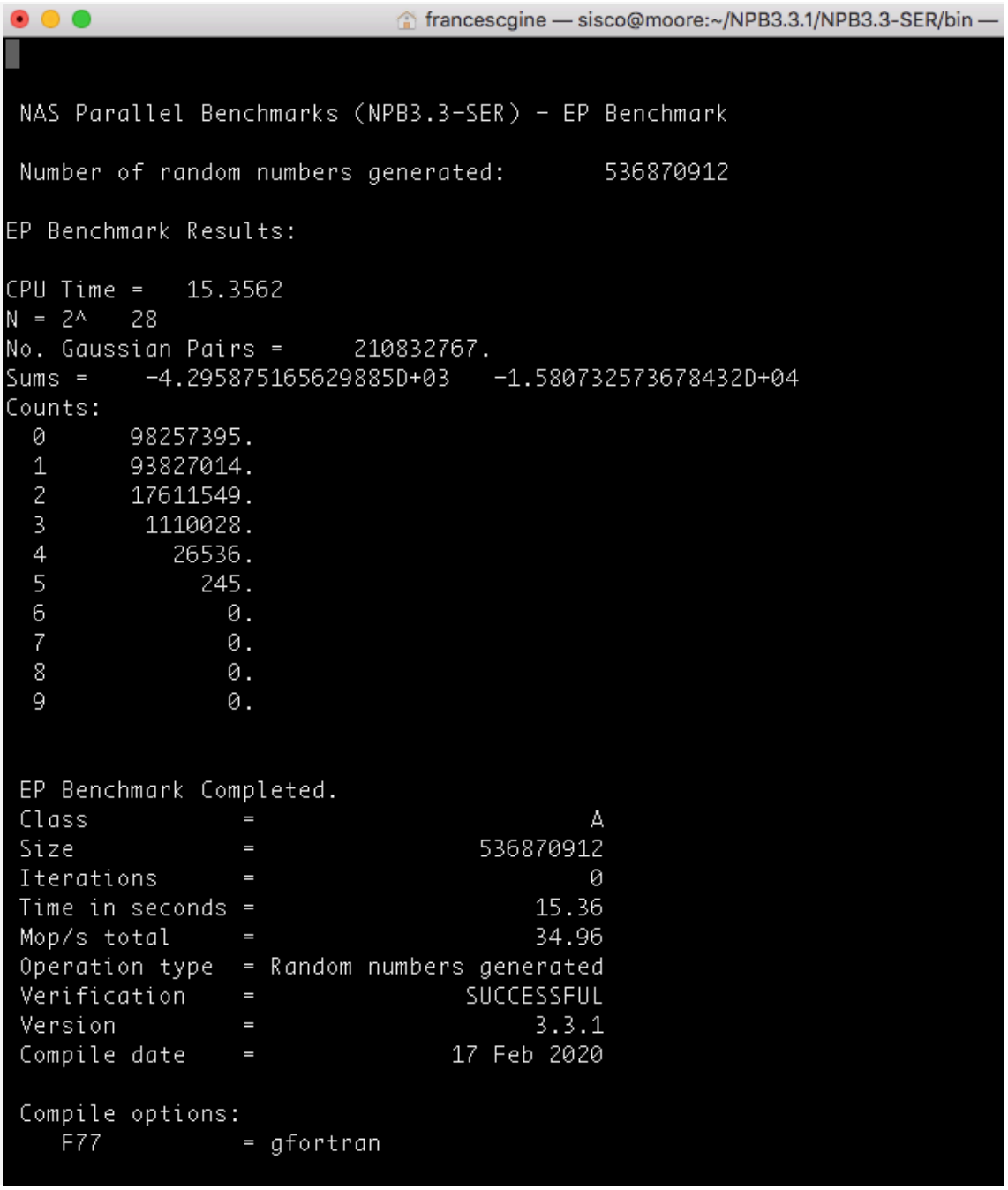

Figura 3. Example of the output of the serial ep.A.x benchmark.

3.2. Execute the OpenMP benchmarks

6. Copy the script *run-simple-omp.sh* into the following folder of your cluster account using the command "*sftp*":

   /home/sisco/NPB3.3.1/NPB3.3-OMP/bin

7. Edit the file *run-simple-omp.sh* using the command *vim* or another text editor:

run-simple-omp.sh — Edited

run-simple-omp.sh 〉 No Selection

```
1  #!/bin/bash
2
3  ## Specifies the interpreting shell for the job.
4  #$ -S /bin/bash
5
6  ## Specifies that all environment variables active within the qsub utility be
       exported to the context of the job.
7  #$ -V
8
9  ## Specifies the parallel environment
10 #$ -pe smp 4
11
12 ## Execute the job from the current working directory.
13 #$ -cwd
14
15 ## The  name  of  the  job.
16 #$ -N EP_B
17
18 ##send an email when the job ends
19 #$ -m e
20
21 ##email addrees notification
22 #$ -M Your_email@alumnes.udl.cat
23
24 ##Passes an environment variable to the job
25 #$ -v  OMP_NUM_THREADS=4
26
27 ## In this line you have to write the command that will execute your application.
28 ./ep.B.x
```

Figura 4. Content of the OpenMP SGE script.

8. **This script is ready to run the benchmark named ep.B.x with 4 threads. If you want to change the benchmark to be executed, you should only change the lines 16 and 28 with the corresponding new benchmark name. Note that line 25 specifies the number of threads to be created. So, if you want to modify the number of threads, you should modify this. However, remember that each node of the moore cluster has only 4 cores; so, if there is no sense to use more than 4**

threads (1thread/core). Likewise, you should change the line 21 with your UdL email.

9. From the folder */home/sisco/NPB3.3.1/NPB3.3-OMP/bin* of the moore cluster, you can run the *ep.B.x* using the following SGE command:
    a. *qsub run-simple-omp.sh*
10. When the execution of the *ep.B.x* is finished, the following two new files will be created:
    a. EP_B.o7381: This file shows the output of the benchmark. Figure 5 shows an example.
    b. EP_B.e7381: This file contains the error messages. Usually, this file is empty.

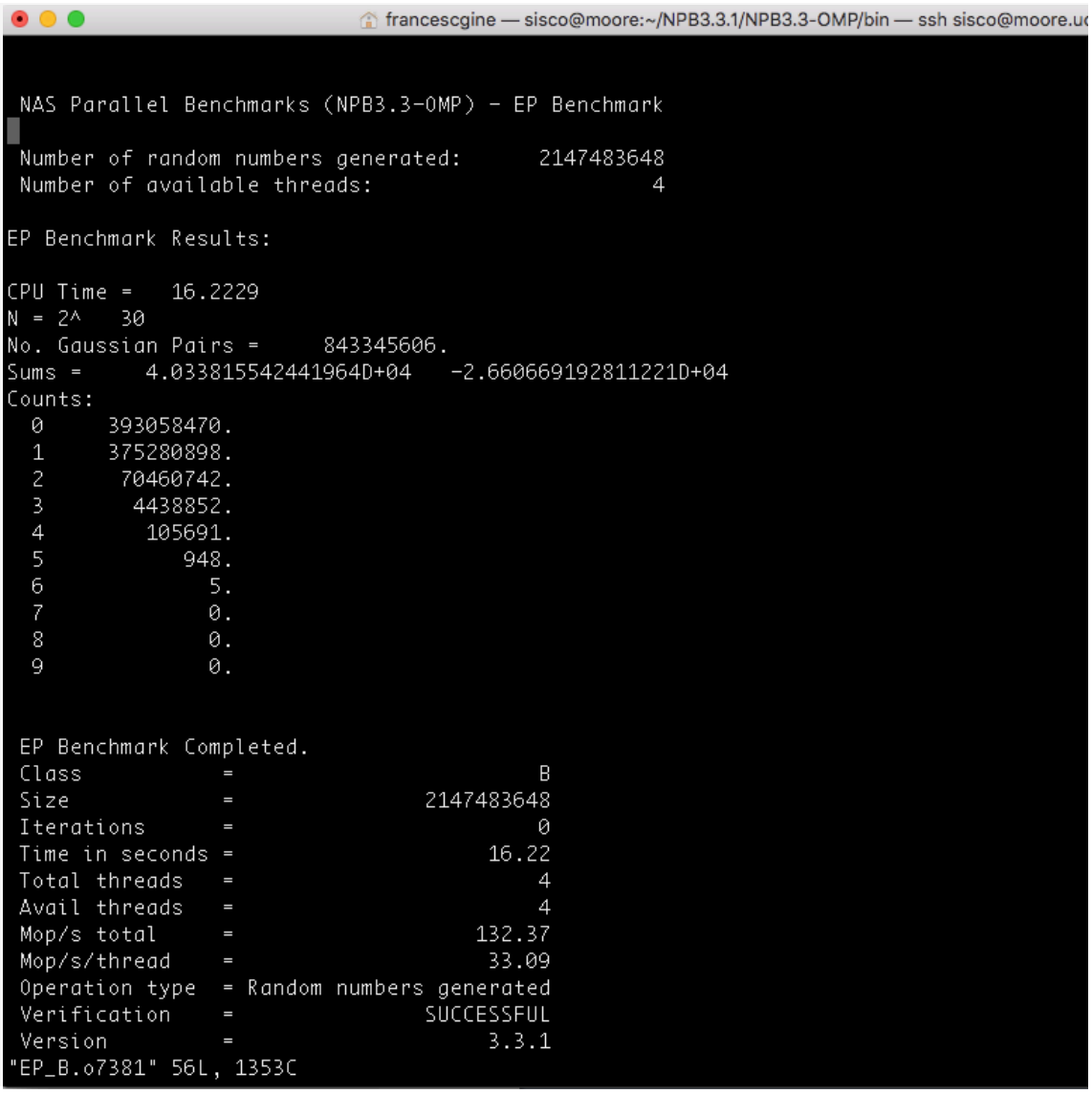

Figura 5. Content of the EP_B.o7381 file.

3.3. Execute the MPI benchmarks

11. Copy the script *run-extended-mpi.sh* into the following folder of your cluster account using the command "*sftp*":

    /home/sisco/NPB3.3.1/NPB3.3-MPI/bin

12. Edit the file *run-extended-mpi.sh* using the command *vim* or another text editor

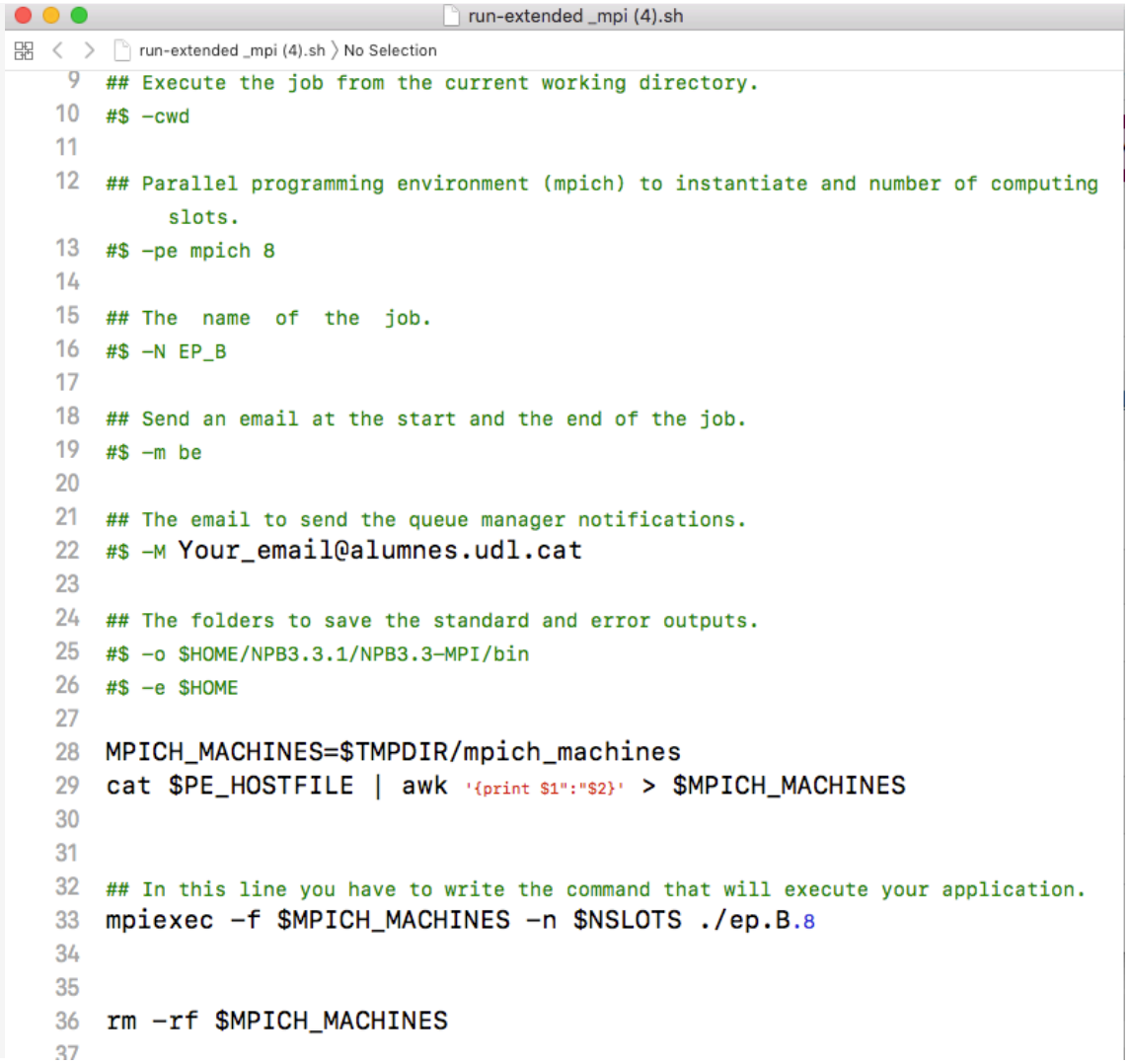

Figura 6. Content of the MPI SGE script.

13. **This script is ready to run the benchmark named ep.B.8 with 8 tasks. If you want to change the benchmark to be executed, you should only change the lines 16 and 33 with the corresponding new benchmark name. Note that line 13 specifies the number of cores used to run the**

MPI benchmark. So, if you want to modify the number of cores, you should modify this. However, remember that the number of used cores must to coincide with the number of tasks specified in line 33 (name of the benchmark: ep.B.8). Likewise, you should change line 21 with your UdL email.

14. From the folder */home/sisco/NPB3.3.1/NPB3.3-MPI/bin* of the moore cluster, you can run the *ep.B.8* benchmark using the following SGE command:
    a. *qsub run-extended-mpi.sh*
15. When the execution of the *ep.B.8* is finished, the following four new files will be created:
    a. EP_B.o7384: This file shows the output of the benchmark.
    b. EP_B.e7384: This file contains the error messages. Usually, this file is empty.
    c. EP_B.po7384: This file contains the name of the moore nodes where the benchmark has been executed. Figure 7 shows an example of the output. In this case, SGE environment has assigned two nodes given that each node contains 4 cores/node.
    d. EP_B.pe7384: This file contains the errors produced by the SGE environment. Usually, this is empty.

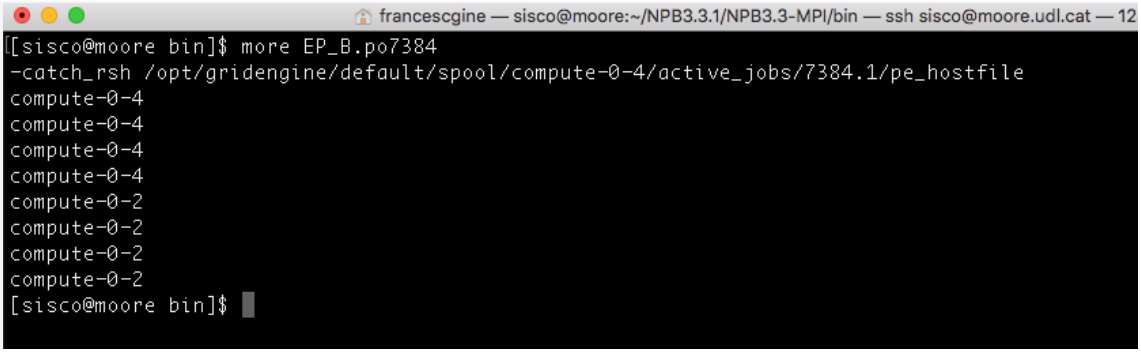

Figura 7. Content of the EP_B.po7384 file.