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1 Introduction

This user’s guide for the MareNostrum4 cluster is intended to provide the minimum amount of information needed by a new user of this system. As such, it assumes that the user is familiar with many of the standard features of supercomputing as the Unix operating system.

Here you can find most of the information you need to use our computing resources and the technical documentation about the machine. Please read carefully this document and if any doubt arises do not hesitate to contact us (Getting help (chapter 7)).

2 System Overview

MareNostrum4 is a supercomputer based on Intel Xeon Platinum processors from the Skylake generation. It is a Lenovo system composed of SD530 Compute Racks, an Intel Omni-Path high performance network interconnect and running SuSE Linux Enterprise Server as operating system. Its current Linpack Rmax Performance is 6.2272 Petaops.

This general-purpose block consists of 48 racks housing 3456 nodes with a grand total of 165,888 processor cores and 390 Terabytes of main memory. Compute nodes are equipped with:

- 2 sockets Intel Xeon Platinum 8160 CPU with 24 cores each @ 2.10GHz for a total of 48 cores per node
- L1d 32K; L1i cache 32K; L2 cache 1024K; L3 cache 33792K
- 96 GB of main memory 1.880 GB/core (216 nodes high memory, 10368 cores with 7.928 GB/core)
- 100 Gbit/s Intel Omni-Path HFI Silicon 100 Series PCI-E adapter
- 10 Gbit Ethernet
- 200 GB local SSD available as temporary storage during jobs ($TMPDIR=/scratc/h[tmp/[jobid])

The processors support well-known vectorization instructions such as SSE, AVX up to AVX-512.

2.1 Compilation for the architecture

To generate code that is optimized for the target architecture and the supported features such as SSE, MMX, AVX instruction sets you will have to use the corresponding compile flags. For compilations of MPI applications an MPI installation needs to be loaded in your session as well. For example Intel MPI via module load impi/2017.4

Intel Compilers

The latest Intel compilers provide the best possible optimizations for the Xeon Platinum architecture. By default, when starting a new session on the system the basic modules for the Intel suite will be automatically loaded. That is the compilers (intel/2017.4), the Intel MPI software stack (impi/2017.4) and the math kernel libraries MKL (mkl/2017.4) in their latest versions. We highly recommend linking against MKL where supported to achieve the best performance results.

To separately load the Intel compilers please use

```
module load intel/2017.4
```

The corresponding optimization flags for icc are `-xCORE-AVX512 -mtune=skylake`.

As the login nodes are of the exact same architecture as the compute node you can also use the flag `-xHost` which enables all possible optimizations available on the compile host.

2.2 Intel Compiler Licences

For reasons of licensing we recommend compiling using either login1 or the partition interactive. We currently have node locked licences installed that allow unlimited compilations in the machines login1 and the ones available via the queue interactive (login 4 and 5). To compile in the rest of the compute and login nodes we have a limited amount of floating licences available. Should all of them be in use when trying to compile, you will experience a delay when the compiler starts and tries to checkout a licence.

In this case an error message like the one below will appear. In this case please switch to Login 1, Login 4 or Login 5 to compile without limitations and licencing issues.

```
ifort: error #10052: could not checkout FLEXlm license
Error: A license for Comp-CL is not available (-9,57).
License file(s) used were (in this order):
  1. Trusted Storage
  ** 2. /gpfs/apps/MN4/INTEL/2017.4/compilers_and_libraries_2017.4.196/linux/bin/intel64/../../Licenses
  ** 3. /home/bsc18/bsc18888//Licenses
  ** 4. /opt/intel/Licenses
  ** 5. /Users/Shared/Library/Application Support/Intel/Licenses
  ** 6. /gpfs/apps/MN4/INTEL/2017.4/compilers_and_libraries_2017.4.196/linux/bin/intel64/license.lic
  ** 7. /gpfs/apps/MN4/INTEL/2017.4/compilers_and_libraries_2017.4.196/linux/bin/intel64/login1_COM_L___1.lic
  ** 8. /gpfs/apps/MN4/INTEL/2017.4/compilers_and_libraries_2017.4.196/linux/bin/intel64/login4_COM_L___1.lic
  ** 9. /gpfs/apps/MN4/INTEL/2017.4/compilers_and_libraries_2017.4.196/linux/bin/intel64/login5_COM_L___1.lic
Please refer http://software.intel.com/sites/support/ for more information.
```

GCC

The GCC provided by the system is version 4.8.5. For better support of new hardware features we recommend to use the latest version that can be loaded via the provided modules. Currently the latest version available in MareNostrum is GCC 7.1.0

```
module load gcc/7.1.0
```

The corresponding flags are `CFLAGS=-march=skylake-avx512`

2.3 Login Nodes

You can connect to MareNostrum using three public login nodes. Please note that only incoming connections are allowed in the whole cluster. The logins are:

```
  mn1.bsc.es
  mn2.bsc.es
  mn3.bsc.es
```

Note: Due to the upgrade of MareNostrum the actual login nodes and their configuration changed. If you had access to the system before and the SSH identification of the logins stored in your _known_hosts_ file you might receive the following warning:

```
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
@ WARNING: REMOTE HOST IDENTIFICATION HAS CHANGED! @
@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@
IT IS POSSIBLE THAT SOMEONE IS DOING SOMETHING NASTY!
Someone could be eavesdropping on you right now (man-in-the-middle attack).
It is also possible that a host key has just been changed.
```
The fingerprint for the RSA key sent by the remote host is
SHA256:sLS2WHI4/tz/dlKt+-9Pn9VUcD4HFI/Gg/fGRjNRejkc.
Please contact your system administrator.
Add correct host key in /home/mlopez12/.ssh/known_hosts to get rid of this message.
Offending RSA key in /home/mlopez12/.ssh/known_hosts:73
remove with:
ssh-keygen -f "/home/mlopez12/.ssh/known_hosts" -R mn1.bsc.es

RSA host key for mn1.bsc.es has changed and you have requested strict checking.
Host key verification failed.

This might happen the first time you connect. To solve this issue follow the hint given to remove
the offending key by executing the following command

```
ssh-keygen -f "/home/mlopez12/.ssh/known_hosts" -R mn1.bsc.es
```

Afterwards you will have the new key stored and the warning should not appear again.

## 2.4 Password Management

In order to change the password, you have to login to a different machine (dt01.bsc.es). This connection
must be established from your local machine.

```
% ssh -l username dt01.bsc.es
username@dtransfer1:~> passwd
Changing password for username.
Old Password:
New Password:
Reenter New Password:
Password changed.
```

Mind that that the password change takes about 10 minutes to be effective.

## 2.5 Transferring files

There are two ways to copy files from/to the Cluster:

- Direct scp or sftp to the login nodes
- Using a Data transfer Machine which shares all the GPFS filesystem for transferring large files

### Direct copy to the login nodes.

As said before no connections are allowed from inside the cluster to the outside world, so all scp and
sftp commands have to be executed from your local machines and never from the cluster. The usage
dependencies are in the next section.

On a Windows system, most of the secure shell clients come with a tool to make secure copies or
secure ftp's. There are several tools that accomplish the requirements, please refer to the Appendices
chapter 8, where you will find the most common ones and examples of use.

### Data Transfer Machine

We provide special machines for file transfer (required for large amounts of data). These machines
are dedicated to Data Transfer and are accessible through ssh with the same account credentials as
the cluster. They are:

- dt01.bsc.es
- dt02.bsc.es

These machines share the GPFS filesystem with all other BSC HPC machines. Besides scp and
sftp, they allow some other useful transfer protocols:

- scp
Data Transfer on the PRACE Network

PRACE users can use the 10Gbps PRACE Network for moving large data among PRACE sites. To get access to this service it’s required to contact “support@bsc.es” requesting its use, providing the local IP of the machine from where it will be used.

The selected data transfer tool is [Globus/GridFTP] which is available on dt02.bsc.es

In order to use it, a PRACE user must get access to dt02.bsc.es:

% ssh -l pr1eXXXX dt02.bsc.es

Load the PRACE environment with ‘module’ tool:

% module load prace globus

Create a proxy certificate using ‘grid-proxy-init’:

% grid-proxy-init
Your identity: /DC=es/DC=irisgrid/O=bsc-cns/CN=John.Foo
Enter GRID pass phrase for this identity:

Creating proxy ........................................... Done
Your proxy is valid until: Wed Aug 7 00:37:26 2013
pr1eXXXX@dttransfer2:

The command ‘globus-url-copy’ is now available for transferring large data.

globus-url-copy [-p <parallelism>] [-tcp-bs <size>] <sourceURL> <destURL>

Where:

- **-p**: specify the number of parallel data connections should be used (recommended value: 4)
- **-tcp-bs**: specify the size (in bytes) of the buffer to be used by the underlying ftp data channels (recommended value: 4MB)

- Common formats for sourceURL and destURL are:
  - file:// (on a local machine only) (e.g. file://home/pr1eXX00/pr1eXXXX/myfile)
  - gsiftp:// (e.g. gsiftp://supermuc.lrz.de/home/pr1dXXXX/mydir/)
  - remember that any url specifying a directory must end with /.

All the available PRACE GridFTP endpoints can be retrieved with the 'prace_service' script:

```
% prace_service -i -f bsc
gftp.prace.bsc.es:2811
```

More information is available at the [PRACE website](http://www.prace-ri.eu/Data-Transfer-with-GridFTP-Details)

### 2.6 Active Archive Management

Active Archive (AA) is a mid-long term storage filesystem that provides 3.7 PB of total space. You can access AA from the Data Transfer Machine (section 2.5) (dt01.bsc.es and dt02.bsc.es) under /gpfs/archive/your_group.

**NOTE**: There is no backup of this filesystem. The user is responsible for adequately managing the data stored in it.

To move or copy from/to AA you have to use our special commands:

- **dtcp, dtmv, dtsync, dttar**

These commands submit a job into a special class performing the selected command. Their syntax is the same than the shell command without ‘dt’ prefix (cp, mv, rsync, tar).

- **dtq, dtcancel**

  dtq shows all the transfer jobs that belong to you. (works like mnq)
  dtcancel works like mncancel (see below) for transfer jobs.

- **dttar**: submits a tar command to queues. Example: Tarring data from /gpfs/to /gpfs/archive

  ```
  % dttar -cvf /gpfs/archive/usertest/outputs.tar ~/OUTPUTS
  ```

- **dtcp**: submits a cp command to queues. Remember to delete the data in the source filesystem once copied to AA to avoid duplicated data.

  ```
  # Example: Copying data from /gpfs/to /gpfs/archive
  % dtcp -r ~/OUTPUTS /gpfs/archive/usertest/
  
  # Example: Copying data from /gpfs/archive to /gpfs
  % dtcp -r /gpfs/archive/OUTPUTS ''/
  ```

- **dtmv**: submits a mv command to queues.

  ```
  # Example: Moving data from /gpfs/to /gpfs/archive
  % dtmv ''/OUTPUTS /gpfs/archive/usertest/
  ```
# Example: Moving data from /gpfs/archive to /gpfs

% dtmv /gpfs/archive/usertest/OUTPUTS ~/

Additionally, these commands accept the following options:

- **-blocking**: Block any process from reading file at final destination until transfer completed.
- **-time**: Set up new maximum transfer time (Default is 18h).

It is important to note that these kind of jobs can be submitted from both the ‘login’ nodes (automatic file management within a production job) and ‘dt01.bsc.es’ machine. AA is only mounted in Data Transfer Machine [section 2.5]. Therefore if you wish to navigate through AA directory tree you have to login into dt01.bsc.es

3 File Systems

**IMPORTANT**: It is your responsibility as a user of our facilities to backup all your critical data. We only guarantee a monthly backup of user data under /gpfs/home and /gpfs/projects.

Each user has several areas of disk space for storing files. These areas may have size or time limits, please read carefully all this section to know about the policy of usage of each of these filesystems. There are 3 different types of storage available inside a node:

- **Root filesystem**: Is the filesystem where the operating system resides
- **GPFS filesystems**: GPFS is a distributed networked filesystem which can be accessed from all the nodes and Data Transfer Machine [section 2.5]
- **Local hard drive**: Every node has an internal hard drive

3.1 Root Filesystem

The root file system, where the operating system is stored doesn't reside in the node, this is a NFS filesystem mounted from one of the servers.

As this is a remote filesystem only data from the operating system has to reside in this filesystem. It is NOT permitted the use of /tmp for temporary user data. The local hard drive can be used for this purpose as you could read in Local Hard Drive [section 3.3].

3.2 GPFS Filesystem

The IBM General Parallel File System (GPFS) is a high-performance shared-disk file system providing fast, reliable data access from all nodes of the cluster to a global filesystem. GPFS allows parallel applications simultaneous access to a set of files (even a single file) from any node that has the GPFS file system mounted while providing a high level of control over all file system operations. In addition, GPFS can read or write large blocks of data in a single I/O operation, thereby minimizing overhead.

An incremental backup will be performed monthly only for /gpfs/home and /gpfs/projects (not for /gpfs/scratch).

These are the GPFS filesystems available in the machine from all nodes:

- **/apps**: Over this filesystem will reside the applications and libraries that have already been installed on the machine. Take a look at the directories to know the applications available for general use.

- **/gpfs/home**: This filesystem has the home directories of all the users, and when you log in you start in your home directory by default. Every user will have their own home directory to store own developed sources and their personal data. A default quota [section 3.4] will be enforced on all users to limit the amount of data stored there. Also, it is highly discouraged to run jobs from this filesystem. **Please run your jobs on your group’s /gpfs/projects or /gpfs/scratch instead.**
• /gpfs/projects: In addition to the home directory, there is a directory in /gpfs/projects for each group of users. For instance, the group bsc01 will have a /gpfs/projects/bsc01 directory ready to use. This space is intended to store data that needs to be shared between the users of the same group or project. A quota (section 3.4) per group will be enforced depending on the space assigned by Access Committee. It is the project’s manager responsibility to determine and coordinate the better use of this space, and how it is distributed or shared between their users.

• /gpfs/scratch: Each user will have a directory over /gpfs/scratch. Its intended use is to store temporary files of your jobs during their execution. A quota (section 3.4) per group will be enforced depending on the space assigned.

### 3.3 Local Hard Drive

Every node has a local solid state (SSD) hard drive (HDD) that can be used as a local scratch space to store temporary files during executions of one of your jobs. This space is mounted over /scratch/tmp/$JOBID directory and pointed out by $TMPDIR environment variable. The amount of space within the /scratch filesystem is about 200 GB. All data stored in these local hard drives at the compute nodes will not be available from the login nodes. You should use the directory referred to by $TMPDIR to save your temporary files during job executions. This directory will automatically be cleaned after the job finishes.

### 3.4 Quotas

The quotas are the amount of storage available for a user or a groups’ users. You can picture it as a small disk readily available to you. A default value is applied to all users and groups and cannot be outgrown.

You can inspect your quota anytime you want using the following command from inside each filesystem:

```
% bsc_quota
```

The command provides a readable output for the quota. Check BSC Commands (section 5.4) for more information.

If you need more disk space in this filesystem or in any other of the GPFS filesystems, the responsible for your project has to make a request for the extra space needed, specifying the requested space and the reasons why it is needed. For more information or requests you can Contact Us (chapter 7).

### 4 Running Jobs

Slurm is the utility used for batch processing support, so all jobs must be run through it. This section provides information for getting started with job execution at the Cluster.

**Important notice:** All jobs requesting 48 or more cores will automatically use all requested nodes in exclusive mode. For example if you request 49 cores you will receive two complete nodes (48 cores * 2 = 96 cores) and the consumed runtime of these 96 cores will be reflected in your budget.

### 4.1 Queues

There are several queues present in the machines and different users may access different queues. All queues have different limits in amount of cores for the jobs and duration. You can check anytime all queues you have access to and their limits using:

```
% bsc_queues
```

The standard configuration and limits of the queues are the following

For longer and/or larger executions special queues are available upon request and will require proof of scalability and application performance. To solicit access to these special queues please contact us (chapter 7).
### Queue Maximum number of nodes (cores) Maximum wallclock

<table>
<thead>
<tr>
<th>Queue</th>
<th>Maximum number of nodes (cores)</th>
<th>Maximum wallclock</th>
</tr>
</thead>
<tbody>
<tr>
<td>Debug</td>
<td>16 (768)</td>
<td>2 h</td>
</tr>
<tr>
<td>Interactive</td>
<td>(max 4 cores)</td>
<td>2 h</td>
</tr>
<tr>
<td>BSC</td>
<td>50 (2400)</td>
<td>48 h</td>
</tr>
<tr>
<td>RES Class A</td>
<td>200 (9600)</td>
<td>72 h</td>
</tr>
<tr>
<td>RES Class B</td>
<td>200 (9600)</td>
<td>48 h</td>
</tr>
<tr>
<td>RES Class C</td>
<td>32 (1536)</td>
<td>24 h</td>
</tr>
<tr>
<td>PRACE</td>
<td>400 (19200)</td>
<td>72 h</td>
</tr>
</tbody>
</table>

## 4.2 Submitting jobs

The method for submitting jobs is to use the SLURM `sbatch` directives directly.

A job is the execution unit for SLURM. A job is defined by a text file containing a set of directives describing the job’s requirements, and the commands to execute.

In order to ensure the proper scheduling of jobs, there are execution limitations in the number of nodes and cores that can be used at the same time by a group. You may check these limits using command ‘bsc_queues’. If you need to run an execution bigger than the limits already granted, you may [Contact Us]

### SBATCH commands

These are the basic directives to submit jobs with `sbatch`:

```
sbatch <job_script>
```

submits a “job script” to the queue system (see Job directives (section 4.4)).

```
squeue
```

shows all the submitted jobs.

```
scancel <job_id>
```

remove the job from the queue system, canceling the execution of the processes, if they were still running.

## 4.3 Interactive Sessions

Allocation of an interactive session in the interactive partition has to be done through SLURM:

```
salloc -partition=interactive
```
or

```
salloc -p interactive
```

## 4.4 Job directives

A job must contain a series of directives to inform the batch system about the characteristics of the job. These directives appear as comments in the job script and have to conform to either the `sbatch` syntaxes.

`sbatch` syntax is of the form:

```
#SBATCH --directive=value
```

Additionally, the job script may contain a set of commands to execute. If not, an external script may be provided with the ‘executable’ directive. Here you may find the most common directives for both syntaxes:

```
#SBATCH --qos=debug
```
To request the queue for the job. If it is not specified, Slurm will use the user’s default queue. The debug queue is only intended for small test.

```
#SBATCH --time=DD-HH:MM:SS
```

The limit of wall clock time. This is a mandatory field and you must set it to a value greater than real execution time for your application and smaller than the time limits granted to the user. Notice that your job will be killed after the time has passed.

```
#SBATCH --workdir=pathname
```

The working directory of your job (i.e. where the job will run). If not specified, it is the current working directory at the time the job was submitted.

```
#SBATCH --error=file
```

The name of the file to collect the standard error output (stderr) of the job.

```
#SBATCH --output=file
```

The name of the file to collect the standard output (stdout) of the job.

```
#SBATCH --nodes=number
```

The number of requested nodes.

```
#SBATCH --ntasks=number
```

The number of processes to start. Optionally, you can specify how many threads each process would open with the directive:

```
#SBATCH --cpus-per-task=number
```

The number of cores assigned to the job will be the total _tasks number * cpus _per_task number.

```
#SBATCH --tasks-per-node=number
```

The number of tasks assigned to a node.

```
#SBATCH --ntasks-per-socket=number
```

The number of tasks assigned to a socket.

```
#SBATCH --constraint=highmem
```

Select which configuration to run your job on, for example “highmem” to run the job on a HighMem node with 7928 MB per core. Without this directive the jobs will be sent to standard nodes that have 1880 MB of RAM per core. There are only a limited number of high memory nodes available, 216 nodes (10368 cores) out of 3456 nodes (165888 cores) in total. Therefore when requesting these nodes you can expect significantly longer queueing times to fulfill the resource request before your job can start.

The accounting for one core hour in standard and highmem nodes is the same, e.g. 1 core hour per core per hour will be budgeted. For faster turnaround times in the queues you can also use standard nodes and run less processes per node. For this you will need to use more cores per task, as every cores requested comes with its 2 GB RAM. You can do this by specifying the flag `#SBATCH --cpus-per-task=number` and your budget will get charged for all cores requested.

```
#SBATCH --x11=batch
```
If it is set the job will be handled as graphical and Slurm will assign the necessary resources to the job, so you will be able to execute a graphical command and if you do not close the current terminal you will get a graphical window.

```bash
#SBATCH --reservation=reservation_name
```

The reservation where your jobs will be allocated (assuming that your account has access to that reservation). In some occasions, node reservations can be granted for executions where only a set of accounts can run jobs. Useful for courses.

```bash
#SBATCH --switches=number@timeout
```

By default, Slurm tries to schedule a job in order to use the minimum amount of switches. However, a user can request a maximum of switches for their jobs. Slurm will try to schedule the job for `timeout` minutes. If it is not possible to request number switches (each rack has 3 switches, every switch is connected to 24 nodes) after `timeout` minutes, Slurm will schedule the job by default.

```bash
#SBATCH --array=<indexes>
```

Submit a job array, multiple jobs to be executed with identical parameters. The indexes specification identifies what array index values should be used. Multiple values may be specified using a comma separated list and/or a range of values with a "-" separator. Job arrays will have two additional environment variable set. `SLURM_ARRAY_JOB_ID` will be set to the first job ID of the array. `SLURM_ARRAY_TASK_ID` will be set to the job array index value. For example:

```bash
sbatch --array=1-3 job.cmd
Submitted batch job 36
```

Will generate a job array containing three jobs and then the environment variables will be set as follows:

```bash
# Job 1
SLURM_JOB_ID=36
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=1
# Job 2
SLURM_JOB_ID=37
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=2
# Job 3
SLURM_JOB_ID=38
SLURM_ARRAY_JOB_ID=36
SLURM_ARRAY_TASK_ID=3
```

```bash
#SBATCH --cpu-freq=<number>
```

Request that job steps initiated by srun commands inside this sbatch script be run at some requested frequency if possible, on the cores selected for the step on the compute node(s). Available frequency steps: 2.10 GHz, 2.00 GHz, 1.90 GHz, 1.80 GHz, 1.70 GHz, 1.60 GHz, 1.50 GHz, 1.40 GHz, 1.30 GHz, 1.20 GHz, 1.10 GHz, 1 GHz

The value is being given in KHz and therefore you will need to specify the values from 2100000 to 1000000.

By default both the turbo boost and speed step technologies are activated in MareNostrum4.

```bash
#SBATCH --exclusive
```

To request an exclusive use of a compute node without sharing the resources with other users. This only applies to jobs requesting less than one node (48 cores). All jobs with $\geq 48$ cores will automatically use all requested nodes in exclusive mode.

For more information:

```bash
man sbatch
man srun
man salloc
```
<table>
<thead>
<tr>
<th>Variable</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLURM_JOBID</td>
<td>Specifies the job ID of the executing job</td>
</tr>
<tr>
<td>SLURM_NPROCS</td>
<td>Specifies the total number of processes in the job</td>
</tr>
<tr>
<td>SLURM_NNODES</td>
<td>Is the actual number of nodes assigned to run your job</td>
</tr>
<tr>
<td>SLURM_PROCID</td>
<td>Specifies the MPI rank (or relative process ID) for the current process. The range is from 0-(SLURM_NPROCS-1)</td>
</tr>
<tr>
<td>SLURM_NODEID</td>
<td>Specifies relative node ID of the current job. The range is from 0-(SLURM_NNODES-1)</td>
</tr>
<tr>
<td>SLURM_LOCALID</td>
<td>Specifies the node-local task ID for the process within a job</td>
</tr>
</tbody>
</table>

### 4.5 Examples

**sbatch examples**

Example for a sequential job:

```bash
#!/bin/bash
#SBATCH --job-name="test_serial"
#SBATCH --workdir=
#SBATCH --output=serial_%j.out
#SBATCH --error=serial_%j.err
#SBATCH --ntasks=1
#SBATCH --time=00:02:00
./serial_binary> serial.out
```

The job would be submitted using:

```bash
> sbatch ptest.cmd
```

Examples for a parallel job:

- Running a pure OpenMP job on one MN4 node using 48 cores on the debug queue:

  ```bash
  #!/bin/bash
 #SBATCH --job-name=omp
 #SBATCH --workdir=
 #SBATCH --output=omp_%j.out
 #SBATCH --error=omp_%j.err
 #SBATCH --cpus-per-task=48
 #SBATCH --ntasks=1
 #SBATCH --time=00:10:00
 #SBATCH --qos=debug
  ./openmp_binary
  ```

- Running on two MN4 nodes using a pure MPI job

  ```bash
  #!/bin/bash
 #SBATCH --job-name=mpi
 #SBATCH --output=mpi_%j.out
 #SBATCH --error=mpi_%j.err
 #SBATCH --ntasks=96
  srun ./mpi_binary
  ```

- Running a hybrid MPI+OpenMP job on two MN4 nodes with 24 MPI tasks (12 per node), each using 4 cores via OpenMP:

  ```bash
  #!/bin/bash
 #SBATCH --job-name=mpi
 #SBATCH --output=mpi_%j.out
 #SBATCH --error=mpi_%j.err
 #SBATCH --ntasks=96
  srun ./mpi_binary
  ```
• Running on four high memory MN4 nodes with 1 task per node, each using 48 cores:

4.6 Resource usage and job priorities

Projects will have assigned a certain amount of compute hours or core hours that are available to use. One core hour is the computing time of one core during the time of one hour. That is a full node with 48 cores running a job for one hour will use up 48 core hours from the assigned budget. The accounting is solely based in the amount of compute hours used.

The priority of a job and therefore its scheduling in the queues is being determined by a multitude of factors. The most important and influential ones are the fairshare in between groups, waiting time in queues and job size. MareNostrum is a system meant for and favouring large executions so that jobs using more cores have a higher priority. The time while waiting in queues for execution is being taken into account as well and jobs gain more and more priority the longer they are waiting. Finally our queue system implements a fairshare policy between groups. Users who did not run many jobs and consumed compute hours will get a higher priority for their jobs than groups that have a high usage. This is to allow everyone their fair share of compute time and the option to run jobs without one group or another being favoured. You can review your current fair share score using the command

```
sshare -la
```

Notifications

It is currently not possible to be notified about the status of jobs via email. To check if your jobs are being executed or have finished you will need to connect to the system and verify their status manually. For the future it is being planned to enable automatic notifications.

5 Software Environment

All software and numerical libraries available at the cluster can be found at /apps/. If you need something that is not there please contact us to get it installed (see Getting Help (Chapter 7)).

5.1 C Compilers

In the cluster you can find these C/C++ compilers:

```
ic /icpc -> Intel C/C++ Compilers
```
 gcc /g++ -> GNU Compilers for C/C++

All invocations of the C or C++ compilers follow these suffix conventions for input files:

- .C, .cc, .cpp, or .cxx -> C++ source file.
- .c -> C source file
- .i -> preprocessed C source file
- .so -> shared object file
- .o -> object file for ld command
- .s -> assembler source file

By default, the preprocessor is run on both C and C++ source files.

These are the default sizes of the standard C/C++ datatypes on the machine

<table>
<thead>
<tr>
<th>Type</th>
<th>Length (bytes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>bool (C++ only)</td>
<td>1</td>
</tr>
<tr>
<td>char</td>
<td>1</td>
</tr>
<tr>
<td>wchar_t</td>
<td>4</td>
</tr>
<tr>
<td>short</td>
<td>2</td>
</tr>
<tr>
<td>int</td>
<td>4</td>
</tr>
<tr>
<td>long</td>
<td>8</td>
</tr>
<tr>
<td>float</td>
<td>4</td>
</tr>
<tr>
<td>double</td>
<td>8</td>
</tr>
<tr>
<td>long double</td>
<td>16</td>
</tr>
</tbody>
</table>

Distributed Memory Parallelism

To compile MPI programs it is recommended to use the following handy wrappers: mpicc, mpicxx for C and C++ source code. You need to choose the Parallel environment first: module load openmpi /module load impi /module load poe. These wrappers will include all the necessary libraries to build MPI applications without having to specify all the details by hand.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>% mpicc a.c -o a.exe</td>
<td></td>
</tr>
<tr>
<td>% mpicxx a.C -o a.exe</td>
<td></td>
</tr>
</tbody>
</table>

Shared Memory Parallelism

OpenMP directives are fully supported by the Intel C and C++ compilers. To use it, the flag -qopenmp must be added to the compile line.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>% icc -qopenmp -o exename filename.c</td>
<td></td>
</tr>
<tr>
<td>% icpc -qopenmp -o exename filename.C</td>
<td></td>
</tr>
</tbody>
</table>

You can also mix MPI + OPENMP code using -openmp with the mpi wrappers mentioned above.

Automatic Parallelization

The Intel C and C++ compilers are able to automatically parallelize simple loop constructs, using the option “-parallel”:

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>% icc -parallel a.c</td>
<td></td>
</tr>
</tbody>
</table>
5.2 FORTRAN Compilers

In the cluster you can find these compilers:

ifort -> Intel Fortran Compilers

```
% man ifort
```

gfortran -> GNU Compilers for FORTRAN

```
% man gfortran
```

By default, the compilers expect all FORTRAN source files to have the extension “.f”, and all FORTRAN source files that require preprocessing to have the extension “.F”. The same applies to FORTRAN 90 source files with extensions “.f90” and “.F90”.

Distributed Memory Parallelism

In order to use MPI, again you can use the wrappers mpif77 or mpif90 depending on the source code type. You can always man mpif77 to see a detailed list of options to configure the wrappers, ie: change the default compiler.

```
% mpif77 a.f -o a.exe
```

Shared Memory Parallelism

OpenMP directives are fully supported by the Intel Fortran compiler when the option “-qopenmp” is set:

```
% ifort -qopenmp
```

Automatic Parallelization

The Intel Fortran compiler will attempt to automatically parallelize simple loop constructs using the option “-parallel”:

```
% ifort -parallel
```

5.3 Modules Environment

The Environment Modules package (http://modules.sourceforge.net/) provides a dynamic modification of a user's environment via modulefiles. Each modulefile contains the information needed to configure the shell for an application or a compilation. Modules can be loaded and unloaded dynamically, in a clean fashion. All popular shells are supported, including bash, ksh, zsh, sh, csh, tcsh, as well as some scripting languages such as perl.

Installed software packages are divided into five categories:

- Environment: modulefiles dedicated to prepare the environment, for example, get all necessary variables to use openmpi to compile or run programs
- Tools: useful tools which can be used at any time (php, perl, ...)
- Applications: High Performance Computers programs (GROMACS, ...)
- Libraries: Those are tipycally loaded at a compilation time, they load into the environment the correct compiler and linker flags (FFTW, LAPACK, ...)
- Compilers: Compiler suites available for the system (intel, gcc, ...
Modules tool usage

Modules can be invoked in two ways: by name alone or by name and version. Invoking them by name implies loading the default module version. This is usually the most recent version that has been tested to be stable (recommended) or the only version available.

```
% module load intel
```

Invoking by version loads the version specified of the application. As of this writing, the previous command and the following one load the same module.

```
% module load intel/2017.4
```

The most important commands for modules are these:

- **module list** shows all the loaded modules
- **module avail** shows all the modules the user is able to load
- **module purge** removes all the loaded modules
- **module load <modulename>** loads the necessary environment variables for the selected module-file (PATH, MANPATH, LD_LIBRARY_PATH...)
- **module unload <modulename>** removes all environment changes made by module load command
- **module switch <oldmodule> <newmodule>** unloads the first module (oldmodule) and loads the second module (newmodule)

You can run “module help” any time to check the command’s usage and options or check the module(1) manpage for further information.

Module custom stack size

The stack size is 2GB by default, but there are modules that can change that value when they are loaded. That’s to prevent errors that would happen otherwise (for example, while using python threads). Here’s a list of the affected modules:

- python/3-intel-2018.2 (64 MB)
- python/2-intel-2018.2 (64 MB)
- python/2.7.13 (10 MB)
- python/2.7.13_ML (64 MB)
- python/2.7.14 (10 MB)
- python/3.6.1 (10 MB)
- python/3.6.4_ML (64 MB)
- paraview/5.4.0 (64 MB)
- paraview/5.5.2 (64 MB)
- vmd/1.9.3 (64 MB)
- vmd/1.9.3-python (64 MB)
- igv/2.3.94 (64 MB)

You can check your stack size at any time using the command:

```
% ulimit -s
```

If by any chance this stack size doesn’t fit your needs, you can add to your job script a command to have a custom set value after the module load commands. This way, you can have an appropriate stack size while using the compute nodes:

```
% ulimit -s <new_size_in_KB>
```
5.4 BSC Commands

The Support team at BSC has provided some commands useful for user’s awareness and ease of use in our HPC machines. A short summary of these commands follows:

- `bsc_queues`: Show the queues the user has access to and their time/resources limits.
- `bsc_quota`: Show a comprehensible quota usage summary for all accessible filesystems.
- `bsc_acct`: Displays accounting information on the project’s allocation usage.
- `bsc_load`: Displays job load information across all related computing nodes.

You can check more information about these commands through any of the following manpages:

```
% man bsc_commands
```

6 PRACE

A large part of MareNostrums capacities is reserved for users of the PRACE Research Infrastructure. There are regular calls ongoing to gain access to the system via this way and more information can be found here.

6.1 Compute hour allocation

PRACE projects that have been awarded compute hours are expected to **start their work and the consumption of hours immediately when the project begins**. The allocated hours are meant to be **consumed consistently and proportionally** during the projects lifetime. To aid users of the system we will regularly inform those groups by mail that are exhibiting a usage below the proportional average for their project.

To avoid the accumulation of too many hours towards the end of the project when it might be complicated to use them up fully we implement a **sliding usage window of 3 months**. This means that after 3 months the hours of the first month that have not been consumed will count as used up and deducted from the total of available compute hours. The sliding-window is moved every 3 months, so we will deduct hours on the month 3rd, 6th and 9th of the project.

For example a 12 months project has been awarded with 12 Mio core hours and starts in January. The monthly proportional consumption is therefore 1 Mio core hours. Due to a sabbatical of the PIs group in Menorca the actual usage of the project only starts in April. Therefore 1 Mio core hours from the month of January will be deducted from the total assignation. If the group continues to consume normally the remaining 11 Mio core hours can be used up entirely.

This regulation does not affect overconsumption of the awarded compute hours. Therefore you could also use up all of your hours within the first month of the project.

7 Getting help

BSC provides users with excellent consulting assistance. User support consultants are available during normal business hours, Monday to Friday, 09 a.m. to 18 p.m. (CEST time).

User questions and support are handled at: support@bsc.es

If you need assistance, please supply us with the nature of the problem, the date and time that the problem occurred, and the location of any other relevant information, such as output files. Please contact BSC if you have any questions or comments regarding policies or procedures.

Our address is:

Barcelona Supercomputing Center - Centro Nacional de Supercomputación
C/ Jordi Girona, 31, Edificio Capilla 08034 Barcelona

[http://www.prace-ri.eu/]
[http://www.prace-ri.eu/call-announcements/]
7.1 Frequently Asked Questions (FAQ)

You can check the answers to most common questions at [BSC’s Support Knowledge Center](http://www.bsc.es/user-support/). There you will find online and updated versions of our documentation, including this guide, and a listing with deeper answers to the most common questions we receive as well as advanced specific questions unfit for a general-purpose user guide.

8 Appendices

8.1 SSH

SSH is a program that enables secure logins over an insecure network. It encrypts all the data passing both ways, so that if it is intercepted it cannot be read. It also replaces the old and insecure tools like telnet, rlogin, rcp, ftp, etc. SSH is a client-server software. Both machines must have ssh installed for it to work.

We have already installed a ssh server in our machines. You must have installed an ssh client in your local machine. SSH is available without charge for almost all versions of UNIX (including Linux and MacOS X). For UNIX and derivatives, we recommend using the OpenSSH client, downloadable from [http://www.openssh.org](http://www.openssh.org) and for Windows users we recommend using Putty, a free SSH client that can be downloaded from [http://www.putty.org](http://www.putty.org). Otherwise, any client compatible with SSH version 2 can be used.

This section describes installing, configuring and using the client on Windows machines. No matter your client, you will need to specify the following information:

- Select SSH as default protocol
- Select port 22
- Specify the remote machine and username

For example with putty client:

![Putty Configuration](http://example.com/putty.png)

This is the first window that you will see at putty startup. Once finished, press the Open button. If it is your first connection to the machine, you will get a Warning telling you that the host key from the server is unknown, and will ask you if you are agree to cache the new host key, press Yes.
IMPORTANT: If you see this warning another time and you haven’t modified or reinstalled the ssh client, please do not log in, and contact us as soon as possible (see Getting Help (chapter 7)).

Finally, a new window will appear asking for your login and password:

8.2 Transferring files

To transfer files to or from the cluster you need a secure ftp (sftp) or secure copy (scp) client. There are several different clients, but as previously mentioned, we recommend using of Putty clients for transferring files: **psftp** and **pscp**. You can find it at the same web page as Putty ([http://www.putty.org/](http://www.putty.org/)).

Some other possible tools for users requiring graphical file transfers could be:

- WinSCP: Freeware Sftp and Scp client for Windows ([http://www.winscp.net](http://www.winscp.net))
- SSH: Not free. ([http://www.ssh.org](http://www.ssh.org))
Using PSFTP

You will need a command window to execute psftp (press start button, click run and type cmd). The program first asks for the machine name (mn1.bsc.es), and then for the username and password. Once you are connected, it’s like a Unix command line.

With command **help** you will obtain a list of all possible commands. But the most useful are:

- **get file_name**: To transfer from the cluster to your local machine.
- **put file_name**: To transfer a file from your local machine to the cluster.
- **cd directory**: To change remote working directory.
- **dir**: To list contents of a remote directory.
- **lcd directory**: To change local working directory.
- **!dir**: To list contents of a local directory.

You will be able to copy files from your local machine to the cluster, and from the cluster to your local machine. The syntax is the same that cp command except that for remote files you need to specify the remote machine:

```
Copy a file from the cluster:
> pscp.exe username@mn1.bsc.es:remote_file local_file
Copy a file to the cluster:
> pscp.exe local_file username@mn1.bsc.es:remote_file
```

### 8.3 Using X11

In order to start remote X applications you need and X-Server running in your local machine. Here is a list of most common X-servers for windows:

- Cygwin/X: [http://x.cygwin.com](http://x.cygwin.com)
- X-Win32: [http://www.starnet.com](http://www.starnet.com)
- WinaXe: [http://labf.com](http://labf.com)
- XconnectPro: [http://www.labtam-inc.com](http://www.labtam-inc.com)
- Exceed: [http://www.hummingbird.com](http://www.hummingbird.com)

The only Open Source X-server listed here is Cygwin/X, you need to pay for the others. Once the X-Server is running run putty with X11 forwarding enabled.

### 8.4 Using the DDT debugger

**Introduction to debugging with DDT**

Debugging programs that run on MPI can be fairly cumbersome without the right tools, so we have provided our systems with the DDT program.

DDT is a debugger initially developed by Allinea, now property of ARM. The debugger is specifically designed to be used in HPC environments, as its purpose is to keep track of the state of the program in every MPI node/task it uses.

With DDT you can (but not limited to): * Interactively track and debug program crashes that may occur on certain nodes. * Track memory related problems in your programs. * Use offline (non-interactive) debugging for long running jobs. * Get more information about crashes.

We’ll begin explaining how to set up your environment and job scripts for a simple debugging session.
Basic interactive debugging with DDT

To debug with DDT using an interactive session (as if it was a typical debugger), you need to do some things: you need to compile your program with a debugging flag and then modify your job script so your program is launched with the option to connect to the debugger (note that this is only one of the ways you use DDT).

Compiling your program

To compile your program for debugging purposes, you need to add the following flags to your compiler:
* -g (enabling executable debugging) * -O0 (do not apply optimizations)

For example, the compiling line would be rewritten in the following manner:

```
$ mpicc application.c -o application.exe $ mpicc -O0 -g application.c -o application.exe
```

Modifying your job script

Your job script needs to be modified so it can launch DDT when the job enters execution in the queue. To do that, you need to specify that you want to connect with the DDT debugger when the job is launched, loading the DDT module and adding these parameters to the line that launches the program:

```
module load DDT
mpirun ./application.exe ddt --connect mpirun ./application.exe
```

Launching the job script

Finally, to launch the job script with the debugger you need to load the DDT module, start the program in background mode and then launch the modified job script:

```
$ module load DDT [if not already loaded]
$ ddt &
$ sbatch your_modified_jobscript
```
We have provided a capture of a real modified job script as an example:

The DDT main screen will appear, but you have to wait until the job enters execution. To do interactive debugging, we strongly recommend using the debug queue as it normally has a shorter waiting time, but remember that you will have limited resources.

When the job enters execution, you will be prompted with the option to accept the incoming connection. It will give you some options before loading the debugger, mainly so it can know if you use OpenMP, CUDA or some sort of memory debugging.

Once the desired options are selected and the program is loaded, you will see the main GUI for the debugger.

**Quick look of common utilities and general usage**

DDT largely operates the same way than most classical debuggers for serial applications, with the distinct difference that it can effectively track the state of the execution of every MPI process involved. We’ve made a general legend of the different utilities present on the main GUI:

1. General debugging actions.
2. Process selector. You can also focus on single processes or threads of a process.
3. Project tree.
5. Variable and stack monitoring window.
6. Input/Output and general tracking utility window.
7. Evaluate window (used to view values for arbitrary expressions and global variables).

Outside the process selector, everything is like a normal debugger and is used in a similar way.
Figure 6: Debugging options

Figure 7: Main GUI
Offline debugging

As we know, jobs can take a while to complete or even get into an execution state, so an interactive debugging session may not be the best solution if we expect them to take some time. DDT offers the possibility of offline debugging, allowing us to come back whenever the execution finishes. The execution will generate a file (either a .html or .txt) where you can check the parameters of the execution and the problems that it may have encountered.

To do it, you need to follow the next steps.

Compiling the application for debugging

For this step, you have to compile the application applying the same changes we did in the previous chapter:

```
$ mpicc application.c -o application.exe  $ mpicc -O0 -g application.c -o application.exe
```

Modifying your job script

Make sure that your script loads the ddt module:

```
module load DDT
```

And now, modify your launching adding ddt and your desired flags. Note that you have the option to choose between generating a .txt or a .html. We will generate a .html in this example:

```
 ddt --offline --output=report.html  mpirun ./your_application.exe
```

Launching the job

To launch the job, you just need to launch it as if you were launching it normally. Once the execution finishes, the report file will be generated. If it was a .txt, you can check it on the login node itself. The HTML version is more user-friendly and interactive, but needs a web browser to display it, so you will need to transfer it to your local machine.
Here’s an example of a report:

It may have caught your eye that there’s a “Memory Leak Report” tab. DDT allows memory debugging with different granularities, which can be really helpful. Let’s talk more about that in the following chapter.

Enabling memory debugging with DDT

DDT can track down memory related issues like invalid pointers, abnormal memory allocation, memory leaks and more. You can enable memory debugging using two different methods, one for interactive debugging and the other for offline debugging.

Interactive debugging

You don’t have to modify anything for this. When your job requests a connection to DDT, you can check the “Memory Debugging” (which can be seen in Fig. 2) option with the desired parameters.

Offline debugging

For offline debugging you will need to add a simple flag to the execution line inside your job script. Using the line we used for the offline debugging chapter as an example, add this flag:

```bash
$ ddt --offline --mem-debug --output=report.html mpirun ./your_application.exe
```

With this, you should be able to have memory-related information inside your report.

Example of a debugging, step by step

To end this manual, we will provide you a code and we will debug it using DDT. You can follow the same procedures that we will show by yourself. You can get the source code here (copy it to your home folder and extract it):

```bash
[Assuming you’re inside your home folder]
$ cp /apps/DDT/SRC/DDT_example.tar.gz ~
$ tar xvf DDT_example.tar.gz
```

Figure 9: HTML offline report
Inside the generated folder you will see some source code files (one in C and the other one in Fortran, we’ll use the C version), a job script and a makefile alongside a solutions folder.

Compiling

Our job is to find and fix what is wrong with the source code, so the first step will be compiling our application using our makefile (feel free to check the contents). This makefile has an option to add the required compiling flags for debugging, so we’ll take advantage of it:

```bash
$ make DEBUG=1
```

This will generate the required executable files for when we launch our job script.

Adapting the job script

The job script provided is functional as it is, but we will be doing an interactive debugging session, so you could be waiting for a while. To alleviate that, we will be using the debug queue, which shouldn’t have too many waiting jobs. To achieve that, add this line to your job script:

```bash
#SBATCH --qos=debug
```

We’re almost ready to launch it!

Launching the program and the debugger

First we need to load our DDT module:

```bash
$ module load DDT
```

Once we’ve done this, we can launch DDT as a background process:

```bash
$ ddt &
```

As you read before, the DDT window will appear, but ignore it for now. Now it’s time to launch our job script:

```bash
$ sbatch job.sub
```

It may take a while, but eventually your job will enter execution and DDT will prompt you with a little window telling you there’s an incoming connection. Accept it. In the next window you don’t need to check any box, just press “Run”.

Locating the issue with the debugger

First of all, let’s talk a bit about the program we are launching. It’s a matrix multiplication implemented with MPI, following this algorithm:

1. Master initializes matrices A, B and C.
2. Master slices the matrices A and C, sends them to slaves.
3. Master and slaves perform the multiplication.
4. Slaves send their results back to master.
5. Master writes the result matrix C in an output file.
Figure 10: Data distribution

Figure 11: Program flow control bar

Figure 12: Program crash
Here you have a diagram showing the data distribution:

Reading the code you can see the detailed implementation. To see if the program works, we can just execute it without any break point. Let’s do that:

If everything works as expected (which is, that it isn’t really working), we should see that DDT prompts us with a notification that our program received a signal (SIGFPE, arithmetic exception) and stopped.

DDT will give us some hints. The first one is the nature of the problem, in this case an integer division by zero. Not only that, it also tells (and shows) the line of code that launched the error. We can deduce that there’s something wrong with the operation “size/nslices”.

Using the window to our right, we can check the values of all variables affected by the current line of code, and we can see that the problem resides in the variable “nslices”, having 0 as its value.

The variable “nslices” is a parameter given to the function “mmult” and it’s not changed anywhere inside it. That means that the value provided to our function is incorrect and we should check how the function was called. Looking through the code, we locate it:

```
  printf("%d: Processing...\n", mr);
  mmult(size, mr, mat_a, mat_b, mat_c);
  if(mr == 0)
  {
    printf("%d: Receiving result matrix...\n", mr);
  }
```

We can see the arguments that this call provided. Specifically, we’re interested in the “mr” variable, which in theory should be the one defining the number of slices used to divide the partition the data of the matrices.

Inspecting the code, we can see that the “mr” variable is not what we thought it was. Why? Because we can see that in reality is the variable that holds the identifier of our MPI rank. Our conclusion is that the error is just putting a wrong variable as a function parameter.

```
  MPI_Init (&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &mr); // my rank
  MPI_Comm_size(MPI_COMM_WORLD, &nproc); // number of processors
```

28
This explains why only process 0 is the only that gives us this problem, as it will be the only one where “mr” equals zero. We also know that the right variable is defined in the code, so we only need to find it and put it as the argument inside the “mmult” call.

**Fixing the issue**

Knowing that this program distributes the data into N slices of the matrices (one for each process), we can use the variable “nproc” shown above for that purpose. The only thing left to do is to apply the change to the function call:

```c
mmult(size, mr, mat_a, mat_b, mat_c); mmult(size, nproc, mat_a, mat_b, mat_c);
```

And with this, the program should work now. Let’s recompile it and launch it again following the same steps we did for the first version, compiler and all. Once DDT is up and running, we can directly click the continue button. This time, DDT shouldn’t give us any problems and the execution should end normally, as shown see here:

![Figure 16: Program termination without problems](https://developer.arm.com/docs/101136/0701/ddt)

And this is it. We’ve debugged our first application! Although it is a rather simple application and fix, it’s a good exercise to grasp the methodology to use with DDT. We hope you find it useful in future debugging sessions.

**Where can I know more?**

If you need more information about DDT and how to use it, check the reference manual:

[link](https://developer.arm.com/docs/101136/0701/ddt)