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Introduction to MareNostrum IV

LifeSciences startup guide

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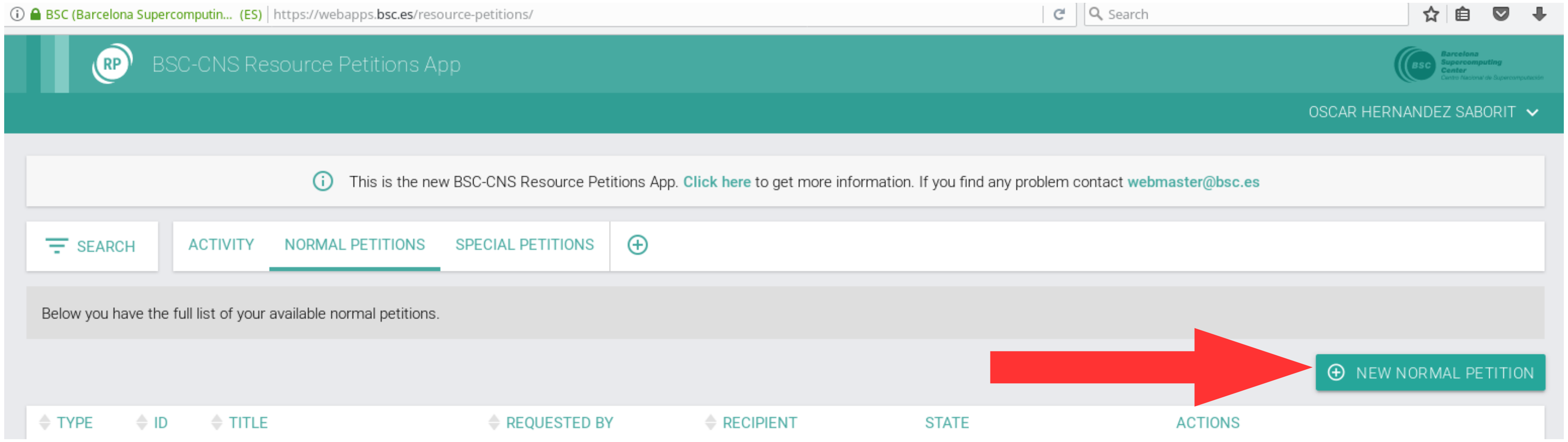
Requesting supercomputing resources

- Through the “resource petitions” app avilabe at:

  https://webapps.bsc.es/resource-petitions/



BSC (Barcelona Supercomputin... (ES) | https://webapps.bsc.es/resource-petitions/

BSC-CNS Resource Petitions App

OSCAR HERNANDEZ SABORIT

This is the new BSC-CNS Resource Petitions App. Click here to get more information. If you find any problem contact webmaster@bsc.es

SEARCH | ACTIVITY | NORMAL PETITIONS | SPECIAL PETITIONS

Below you have the full list of your available normal petitions.

NEW NORMAL PETITION

TYPE	ID	TITLE	REQUESTED BY	RECIPIENT	STATE	ACTIONS

- Team leaders can issue “special petitions”

  Intended for non-BSC personeel

BSC HPC access

- Access through SSH
  - OpenSSH for Linux / OSX
  - PuTTY for Windows
- On the facilities granted you can authenticate by:
  - password
  - SSH public keys

Shared Credentials

- Shared users among:
  - Data Transfer (dt01.bsc.es) >> Data management
  - MareNostrum IV (mn1.bsc.es) >> 48 core nodes | 166000cpus
  - Ultraviolet (bscsmp02.bsc.es) >> 96 cpus | 1.5 TB RAM
  - CTE-POWER (plogin1.bsc.es) >> P8(160 cpus) | 2xTesla P100
  - CTE-KNL (klogin1.bsc.es) >> 16*64 core xeon-phi
  - Nord3 (nord3.bsc.es) >> 16 core nodes|
  - Minotauro (mt01.bsc.es) >> 16/12 core nodes | 2* M2090/K80
- Same $HOME, $USER and password

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General Parallel Filesystem (GPFS)

- High performance parallel filesystem
- GPFS Filesystems on the cluster
  - /gpfs/apps (Support vetted applications)
  - /gpfs/home (User's home, backup)
  - /gpfs/projects (Inputs, custom installations, backup)
  - /gpfs/scratch (Temporary files, NO backup)
  - /gpfs/archive (Long term storage, batch interaction)

Filesystem limits (Quota)

- Filesystem limit per user and/or group.
- Check with: bsc_quota
- Typical related problems:
  - Job submission failure when $HOME is over quota
  - Job execution failure when writing to over-quota filesystem
- Group-shared quota on /gpfs/projects and /gpfs/scratch

/gpfs/home Filesystem usage

- Few space (~40 GB per user)
- /gpfs/home Do:
  - Store source code
  - Store personal scripts
- /gpfs/home Don't:
  - Use as production directory

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/gpfs/archive Filesystem usage

- You can check availability with bsc_quota and dtquota
- /gpfs/archive Do:
  - Store data you are not going to use soon
  - Store processed final results
- /gpfs/archive Don't:
  - Execute commands interactively (cp, mv, …)
  - Try to put ACLs

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Data Transfer Commands

- Set of commands to send data transfer jobs to queues
  - Available in MareNostrum and dt01 & dt02
- Commands
  - File movement: dtcp & dtmv
  - Archiving & synchronizing: dttar & dtrsync
  - Job control: dtq & dtcancel

Node's local disk (/scratch)

- All nodes have disk for temporary files
  - Accessible via $TMPDIR
  - Not shared between nodes (different to /gpfs/scratch)
  - Content erased after execution
- Useful for temporary files
  - Temporal data from MPI communication
- 200 GB disk

MareNostrum logins

- 3 external accessible logins:
  - mn1.bsc.es
  - mn2.bsc.es
  - mn3.bsc.es

- 2 internal accessible logins:
  - Login4
  - Login5

- No outgoing connections
  - No downloads or uploads
  - 5 minutes cpu time limit

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Login usage

✓	⛔
Manage & edit files	Run production executions
Small & medium compilations	Copy large amount of files
Submit jobs to batch system	Long and heavy load graphical interfaces
Check results and prepare scripts	

Compilers

- Intel and GNU compiler suites available
- Intel compilers available in:
  - login1
  - Interactive nodes ($ salloc -p interactive)
- Several versions, managed by modules
  - Fortran, C, C++
  - Intel (licensed)
  - GCC (Free Software)

- MPI compilation also managed by modules through wrappers
  - mpicc, mpifort...

Module Environment (I)

- Open Source project
- Environment variables and software dependencies management
- Several versions of same program side-to-side (/gpfs/apps only)
- Typical dependencies:
  - MPI libraries
  - Mathematical libraries

Module Environment (II)

- Module commands:

Command	Option	Example	Info
avail	[program]	module avail	List modules available
list		module list	List loaded modules
purge		module purge	Unload all modules
load	<program[/version]>	module load gcc/5.1.0	Load a module
switch	<old> <new>	module switch intel gcc	Change a module by another

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Batch System

- MareNostrum IV uses Platform SLURM as batch system
- Benefits of using jobscripts
  - Defines resources needed
  - Reusable
  - Documents needs and requests
  - Jobscripts are shellscripts with special markings
- Each submission is a job

slurm
workload manager

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SLURM commands

- Submit a job defined in job_script.cmd
  - sbatch job_script.cmd
- Check status of jobs submitted:
  - User's: squeue
- Cancel a job:
  - scancel JobID

SLURM Common Parameters

Option	Comment	Example
-n | -ntasks	Number of tasks	#SBATCH -n 32
-t |--time	Wallclock limit	#SBATCH -t 01:00
-J | --job-name	Job name	#SBATCH -J myjob
-o | --output	Output file	#SBATCH -o %j.out
-e | --error	Error file	#SBATCH -e %j.err
--qos	Queue	#SBATCH --qos debug
--exclusive	Exclusive mode	#SBATCH --exclusive
-D | --workdir	Current working dir	#SBATCH -D= /my/path/
--reservation	Reservation	#SBATCH --reservation reserv_name

SLURM Extra Parameters: Process layout

- How to define spicific load balance configurations:

Option	Comment	Example
--ntasks-per-core	Tasks per core	#SBATCH --ntasks-per-core 1
--ntasks-per-node	Tasks per node	#SBATCH --ntasks-per-node 48
-c |--cpus-per-task	Cpus per task	#SBATCH -c 1

Generic MNIV example:

```
#SBATCH --ntasks-per-core 1
#SBATCH --ntasks-per-node 48
```

SLURM Extra Parameters: Memory layout

2 nodetypes:

- HIGH MEMORY NODES

  - Total of 384GBytes per node (8G per core)

  - Only 216 nodes available

  #SBATCH --constraint=highmem

- LOW MEMORY NODES

  - Total of 96GBytes per node (2G per core)

  - Deafult nodes

Job queues

- Jobs are assigned to queues (QoS)
- Default queue automatically selected.
- Specify when special need: debug, interactive, graphical...
- Different queues have different limits and goals
- Check your available queues and their limits:
  - bsc_queues
- Example: #SBATCH --qos debug

Job Examples: Sequential

- Sequential

```
#!/bin/bash
 #SBATCH -n 1
 #SBATCH -o %J.out
 #SBATCH -e %J.err
 #SBATCH -t 01:00

 hostname
```

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Job Examples: Threaded

- Threaded (OpenMP, pthreads, ...)

```
#!/bin/bash
 #SBATCH -n 1
 #SBATCH --exclusive
 #SBATCH -o %j.out
 #SBATCH -e %j.err
 #SBATCH -t 01:00

 export OMP_NUM_THREADS=16
 ...
```

Job Examples: Typical MPI

- MPI (multiple nodes, OpenMPI)

```
#!/bin/bash
 #SBATCH -n 96
 #SBATCH -o %j.out
 #SBATCH -e %j.err
 #SBATCH -t 01:00
 module purge
 module load openmpi
 mpirun ...
```

Job Examples: MPI + OpenMP

- MPI + Threads

```
#!/bin/bash
 #SBATCH -n 96
 #SBATCH -o %j.out
 #SBATCH -e %j.err
 #SBATCH --ntasks-per-node=4
 #SBATCH -t 01:00
 export OMP_NUM_THREADS=4
 module purge
 module load openmpi
 mpirun ...
```

Container executions

- We do know that it is a common practice

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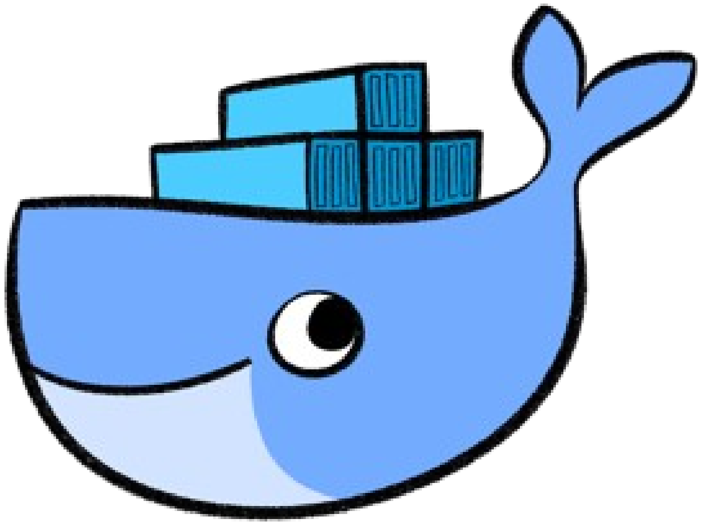
  Docker the most used platform



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- Root priveleges

- High level abstraction features

Singularity

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more info at http://singularity.lbl.gov/faq

We suggest

- Install singularity locally

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- Generate and edit your containers locally

  $ sudo singularity shell --writable container.img

  Always create folders in container for mountpoints:

  $mkdir /gpfs/home /gpfs/scratch /gpfs/projects /gpfs/apps

We suggest

- Install singularity locally

  Available via git

- Generate and edit your containers locally

  $ sudo singularity shell --writable container.img

- Upload them to GPFS for production runs

  $ scp /local/path/container bscXX@dt01.bsc.es:/gpfs/path

  - > Singularity run [container]
  - > Singularity exec [container] [executable + args]

From Docker to Singularity

- Singularity supports pulling containers from docker repos
- Docker2singularity

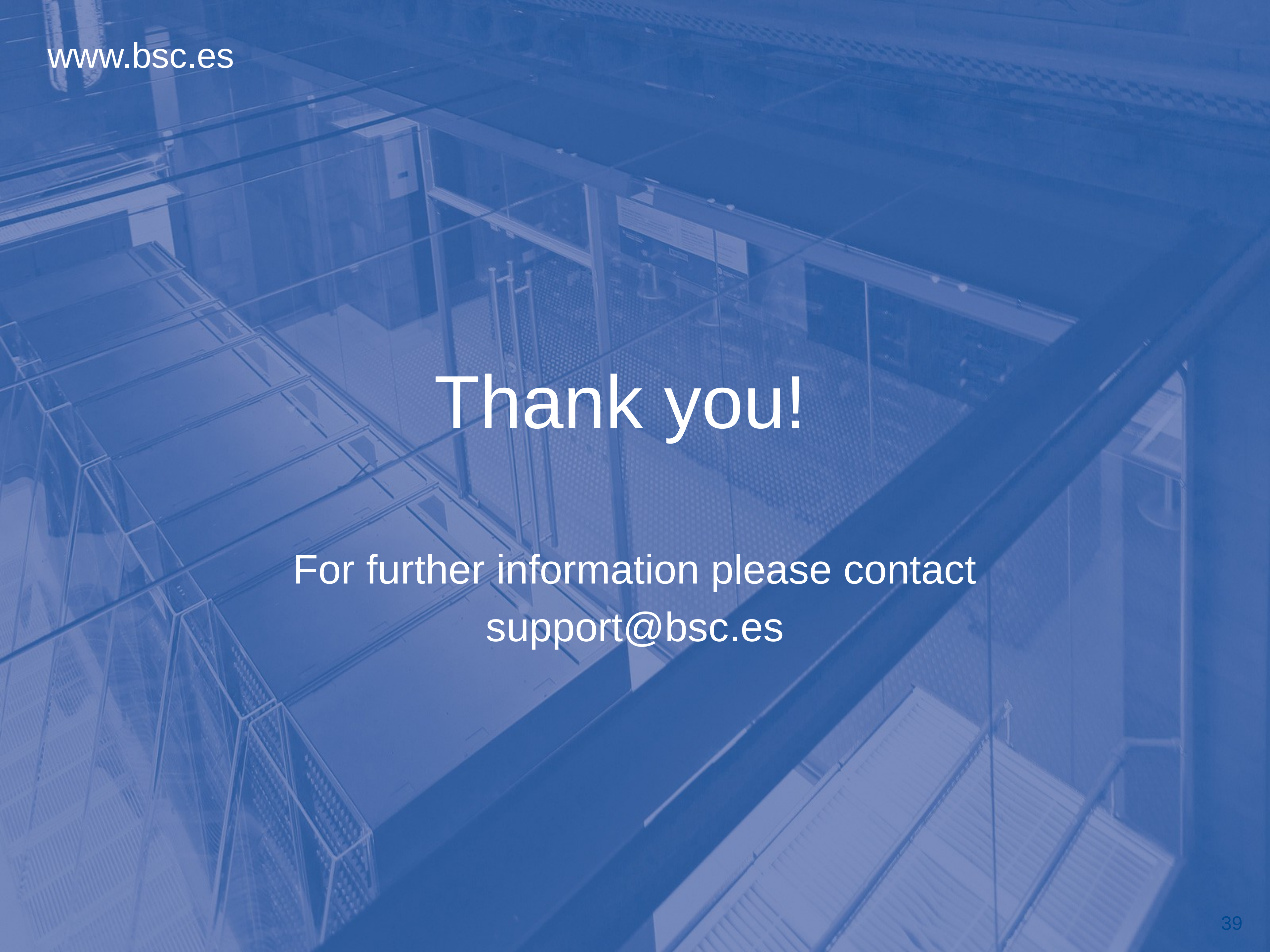
  Docker script that converts containers

  Run the following script from your local machine

https://github.com/singularityware/docker2singularity

Support Contact practices

- When contacting support remember to:
  - Specify Job Ids, software version and environment (if applies), machine, username
  - Not take for granted we know what you know, want or need
- We don't know who you are but we care you do fine
- We have no favorites



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Thank you!

For further information please contact
support@bsc.es