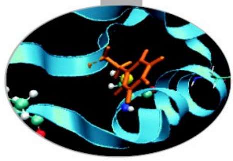
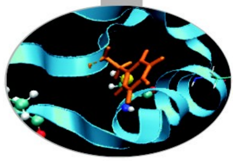


GROMACS su cluster ibridi: produzione e analisi dei dati

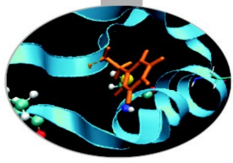
A. Grottesi (CINECA)

This afternoon you will learn...



- How to set up a protein topology using GROMACS
- How to prepare your submission script
- How to submitt your job to the PBS queueing system on Eurora
- Tutorial:
  - Example: small peptide in solution
  - Domain vs. Particle Decomposition

How to become a CINECA user



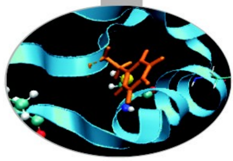
- Please fill out the form on:

  https://userdb.hpc.cineca.it/user/register

- You'll receive userdb credentials: Then
  - Click on “HPC Access” and follow the on-screen instructions
  - You'll be asked to upload an image of a valid ID document
  - Ask your PI or send an email to superc@cineca.it to be included on an active project.

- When everything is done an automatic procedure sends you (via 2 separate emails) the username/password to access HPC systems

How to log in

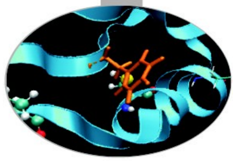


- Establish a ssh connection

  ssh a08traXX@login.eurora.cineca.it **(XX = 49 to 72)**

- Remarks:
  - **ssh** available on all linux distros
  - **Putty** (free) or **Tectia** ssh on Windows
  - *secure shell plugin* for Google Chrome!
  - important messages can be found in the *message of the day*

Check the **user guide**! http://www.hpc.cineca.it/content/eurora-user-guide

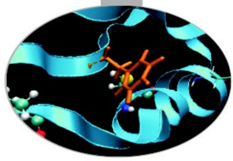


Launching jobs

- Now that we have our executable, it's time to learn how to prepare a job for its execution
- Eurora uses **PBS** scheduler.
- The job script scheme is:

```
#!/bin/bash
#PBS keywords
variables environment
execution line
```

Environment setup and execution line



The execution line starts with mpirun: Given: `./myexe arg_1 arg_2`

```
mpirun –n 24 ./myexe arg_1 arg_2
```

–n is the number of **cores** you want to use

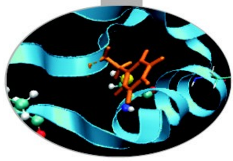
arg_1 arg_2 are the normal arguments of myexe

In order to use mpirun, **openmpi** (or **intelmpi**) has to be loaded. Also, if you linked dynamically, you have to remember to load every library module you need (automatically sets the LD_LIBRARY_PATH variable).

The environment setting usually starts with "**cd $PBS_O_WORKDIR**". That's because by default you are launching on your home space the executable may not be found.

$PBS_O_WORKDIR points to the directory from where you're submitting the job .

PBS keywords



```
#PBS –N jobname                                    # name of the job
#PBS -o job.out                                    # output file
#PBS -e job.err                                    # error file
#PBS -l select=1:ncpus=16:mpiprocs=16:mem=ngpus=2  # resources
#PBS -l walltime=1:00:00                           # hh:mm:ss
#PBS -q <queue>                                    # chosen queue
#PBS -A <my_account>                               # name of the account
```

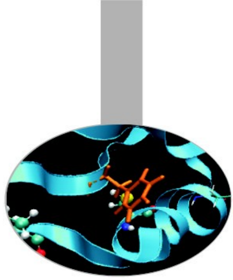
select = number of chunk requested

ncpus = number of cpus per chunk requested

mpiprocs = number of mpi tasks per chunk

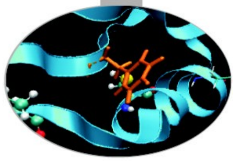
mem = RAM memory per chunk

job script template



```
#!/bin/bash
#PBS -l walltime=1:00:00
#PBS -l select=1:ncpus=16:mpiprocs=16:ngpus=2:mem=14GB
#PBS -o job.out
#PBS -e job.err
#PBS -q parallel
#PBS -A <account_no>
#PBS -m mail_events ==> specify email notification
                    (a=aborted,b=begin,e=end,n=no_mail)
#PBS -M user@email.com

cd $PBS_O_WORKDIR
module load autoload openmpi
module load somelibrary

mpirun ./myprogram < myinput
```

PBS commands



qsub

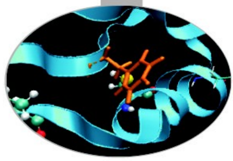
qsub <job_script>

Your job will be submitted to the PBS scheduler and executed when there will be nodes available (according to your priority and the queue you requested)

qstat

qstat

Shows the list of all your scheduled jobs, along with their status (idle, running, closing, …) Also, shows you the job id required for other qstat options



PBS commands

qstat

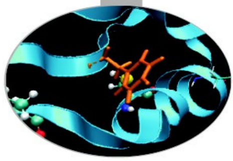
```
qstat -f <job_id>
```

Provides a long list of informations for the job requested.
In particular, if your job isn’t running yet, you'll be notified about its estimated start time or, if you made an error on the job script, you will learn that the job won’t ever start

qdel

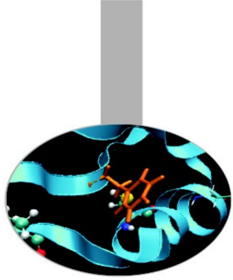
```
qdel <job_id>
```

Removes the job from the scheduled jobs by killing it



Scripts for running MD codes on Eurora

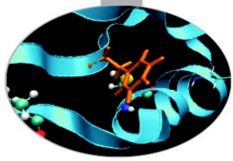
Gromacs 4.6.5, pure MPI on Eurora



```
>module load autoload gromacs/4.6.5
>module help gromacs/4.6.5

#!/bin/bash
#PBS -N gmx
#PBS -l select=1:ncpus=16:mpiprocs=16:mem=14GB
#PBS -q <queue>
#PBS -l walltime=1:00:00
#PBS -A <account_nr>

cd $PBS_O_WORKDIR                     ==> change to current dir

module load profile/advanced
module load autoload gromacs/4.6.5

export OMP_NUM_THREADS=1              ==> set nr. Of OpenMP threads per MPI proc to1

mdrun=$(which mdrun_mpi)
cmd="$mdrun -s topol.tpr -v -maxh 1.0 -nb cpu"
mpirun -np 16 $cmd
```

exclusive mode:
whole node allocated

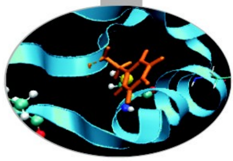
Gromacs 4.6.5 MPI+CUDA on Eurora



```
>module load autoload gromacs/4.6.5
>module help gromacs/4.6.5

#!/bin/bash
#PBS -N gmx
#PBS -l select=1:ncpus=16:mpiprocs=2:ngpus=2:mem=14GB
#PBS -q <queue>
#PBS -l walltime=1:00:00
#PBS -A <account_nr>

cd $PBS_O_WORKDIR                      ==> change to current dir

module load profile/advanced
module load autoload gromacs/4.6.5

export OMP_NUM_THREADS=1               ==> set nr. Of OpenMP threads to 1
#                                      ==> set total mpi tasks = 2 and bind to two GPUs

mdrun=$(which mdrun_mpi_cuda)
cmd="$mdrun -s topol.tpr -v -maxh 1.0 -gpu_id 01 "
mpirun -np 2 $cmd
```

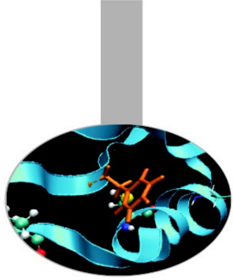
exclusive mode:
whole node allocated

NAMD 2.9 MPI+CUDA on Eurora



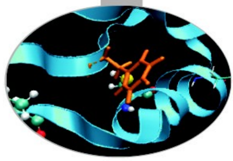
```
>module load profile/advanced autoload namd/2.9
>module help namd/2.9

#!/bin/bash
#PBS -l select=1:ncpus=16:mpiprocs=16:ngpus=2:mem=14GB
#PBS -l walltime=0:30:00
#PBS -o namd.out
#PBS -e namd.err
#PBS -A <account_no>
#PBS -q <queue>

cd $PBS_O_WORKDIR                    ==> change to current dir

module load profile/advanced
module load autoload namd/2.9

namd=$(which namd2_cuda)             ==> set path to namd executable

mpirun $namd +idlepoll md.namd       ==> run CUDA version of NAMD
```

Amber-14 on Eurora (pure MPI version)



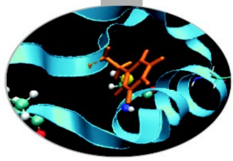
```
>module load autoload amber/14
>module help amber/14

#!/bin/bash
#PBS -A <account_no>
#PBS -N amber
#PBS -l walltime=1:00:00
#PBS -l select=1:ncpus=16:mpiprocs=16:mem=14GB
#PBS -o job.out
#PBS -q <queue>

cd $PBS_O_WORKDIR                    ==> change to current dir
module load autoload amber/14

cmd="pmemd.MPI -O -i mdin -o mdout -p prmtop -c inpcrd -r restrt -x mdcrd"
mpirun -np 16 $cmd
```

Amber 14 – MPI+CUDA version



```
#!/bin/bash
#PBS -A <account_no>
#PBS -l select=1:ncpus=2:mpiprocs=2:ngpus=2
#PBS -l walltime=1:00:00
#PBS -o job.out
#PBS -q longpar

cd $PBS_O_WORKDIR
module load autoload amber/12

# for best performance use 1 mpi task/1 gpu.  In this example we have 1*2 gpus = 2 MPI tasks.

cmd="pmemd.cuda.MPI -O -i mdin -o mdout -p prmtop -c inpcrd -r restrt -x mdcrd"

mpirun -np 2 $cmd
```

Tutorial 2: small peptide in water



- Copy gzipped file from here:

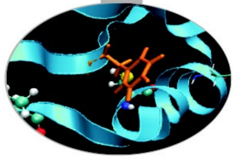
  https://hpc-forge.cineca.it/files/CoursesDev/public/2015/High_Performance_Molecular_Dynamics/Rome/February/Tutorial2.tar.gz

  Alternativelly, copy gzipped tar file from here:

  /gpfs/scratch/userinternal/agrottes/Corsi/Tutorial2.tar.gz

- Generate topol.top using starting file: Peptide.pdb
- Minimize peptide structure using file steep.mdp
- Run a small run (10000 steps) using file pure MPI, MPI+CUDA and MPI_OpenMP+CUDA
- Analyze runs using Gromacs log files and determine speed up curves
- Optional: domain vs. particle decomposition: compare performances

Tutorial 3: small peptide in water



Parameters for running tutorials on Eurora:

- queue = R1598562
- PBS keyword: #PBS -A train_cmd12015
  #PBS -l select=1:ncpus=N:mpiprocs=M:ngpus=2