High Performance Computing for the VPH

A practical introduction to HPC usage

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Introduction to HPC in Computational Modelling

HANDS ON

Getting the training material

The material for this course is available at:
http://bit.ly/HPC_CBM

Transfer the zip file to MarenostrumIV

```
~> scp IntroHPC_CBM-master.zip nct00004@mn1.bsc.es:
```

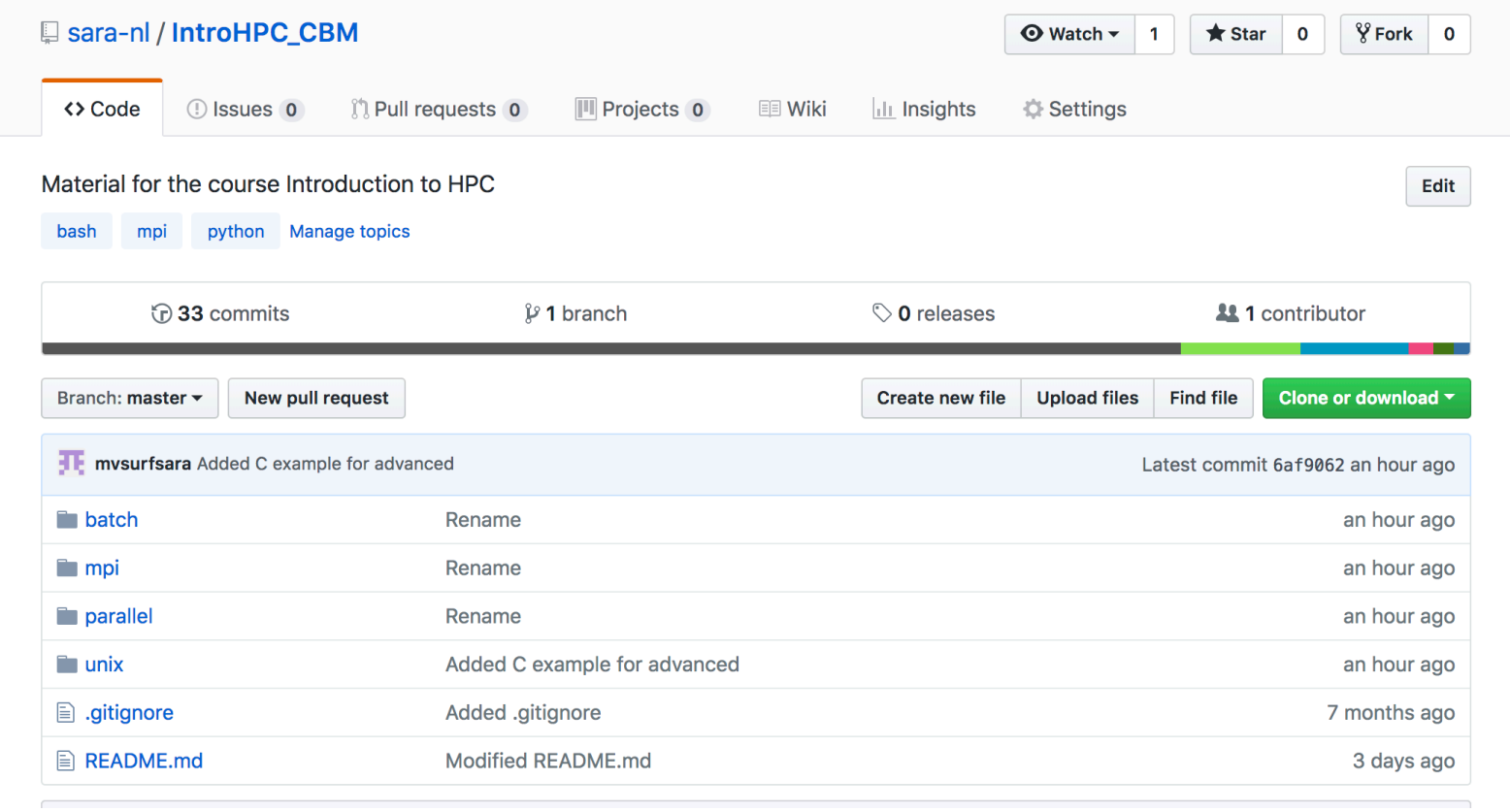
(Windows users can use MobaXterm or Winscp)

Extract the zip in your home:

```
nct00004@login1:~> unzip IntroHPC_CBM-master.zip
```

Getting the training material

Hands on material **http://bit.ly/HPC_CBM**



Bash scripting

Simple bash script

unix/simple.sh

```
#!/bin/bash

echo "Hi, I'm your first script."
echo


lscpu --help > cpu.log
lscpu >> cpu.log


echo "I've left something for you."
echo "Ciao"
```

Use "`nano simple.sh`" to visualize the file. Ctrl-X to exit .

Batch system

Run “simple.sh” interactively

Give execution permissions to the script:

```
nct00004@login1:~> chmod u+x simple.sh
```

Run the script:

```
nct00004@login1:~> ./simple.sh
```

```
nct00004@login1:~> bash simple.sh
```

Bash scripting

Advanced bash script

unix/advanced.sh

```
#!/bin/bash
# <- this is a comment and everything that follow is ignored

args=$# # Number of args passed.

if [ $args = 0 ]
then
 echo "This script needs a number as argument input."
 echo "Ex: ./advanced.sh 10"
 exit
fi
```

Bash scripting

unix/advanced.sh (cont'd)

```
num=$1 # First argument passed.

echo "The input number is:" $1
echo

cd src

gcc -o ../fact.exe fact.c 1> compile.log 2> compile.err
# Redirect stdout and stderr to files

cd ..

./fact.exe $num | tee fact.log # Pipe output into command

echo
echo "Done"
```

Batch system

Run “advanced.sh” interactively

Give execution permissions to the script:

```
nct00004@login1:~> chmod u+x advanced.sh
```

Run the script:

```
nct00004@login1:~> ./advanced.sh 10
```

```
nct00004@login1:~> ls –l *.log
```

Batch jobs

batch/slurm1.sub

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

echo "Who am I?"
whoami
echo "Where ?"
srun hostname

sleep 600
echo "Ciao"
```

batch/slurm2.sub

```
#!/bin/bash
#SBATCH --job-name="test_multinode"
#SBATCH --nodes=2
#SBATCH --tasks-per-node=3
#SBATCH --time=00:02:00
#SBATCH --workdir=.
#SBATCH --output=multinode_%j.out
#SBATCH --error=multinode_%j.err

echo "Who am I?"
whoami
echo "Where ?"
srun hostname

sleep 600
echo "Ciao"
```

Batch system

Submitting jobs with SLURM

Submits a “job script” to the queue system:

```
nct00004@login1:~> sbatch slurm1.sub
```

Check the status of the submitted jobs:

```
nct00004@login1:~> squeue

JOBID   PARTITION   NAME  USER    ST  TIME  NODES  NODELIST(REASON)
2262040      main test_s nct00001 PD  0:00      2  (None)
```

MPI jobs

Running an MPI application

mpi/run_wave (I)

```
...

SCRATCH=/gpfs/scratch/nct00/$USER/$SLURM_JOBID

mkdir –p $SCRATCH || exit 1

cp wave $SCRATCH
...

cd $SCRATCH
```

MPI jobs

Running an MPI application

mpi/run_wave (II)

```
...
# if wave was compiled with OpenMPI support, set the number of
threads
# export OMP_NUM_THREADS=4

srun ./wave $m $n $dx $dy $nt $dt $c $zeta \
           $f0x0 $f0y0 $f0r0 $nt_i $outfile

perl h52anim.pl wave.h5 u

cp wave.h5 wave.h5.gif $SLURM_SUBMIT_DIR
```

Batch system

Prepare and runs mpi example

Read the README.md for more information:

```
nct00004@login1:~> nano README.md
```

Requires compilers, MPI, HDF5, perl:

```
nct00004@login1:~> module load hdf5
nct00004@login1:~> module load mpi
nct00004@login1:~> module load perl
nct00004@login1:~>
```

Batch system

Prepare and run mpi example

The code needs to be compiled and linked to right libraries:

```
nct00004@login1:~> nano Makefile
nct00004@login1:~> make
```

Submit to the batch:

```
nct00004@login1:~> sbatch run_wave
```

Check that it runs:

```
nct00004@login1:~> squeue
```

Batch system

Prepare and run mpi example

It generates a gif that we can copy back at the end:

```
~> scp nct00004@mn1.bsc.es:IntroHPC_CBM-master/mpi/wave.h5.gif .
```

Or can be visualized remotely:

```
~> ssh –X nct00004@mn1.bsc.es
```

```
nct00004@login1:~> display IntroHPC_CBM-master/mpi/wave.h5.gif
```