

How to run Python code on NERSC

Running Serial Python code.

- Load build-in modules : module load python (numpy, scipy, matplotlib and ipython).
- Import your own modules.

```
export PYTHONPATH=/Dir/to/your/own/modules:${PYTHONPATH}
```

- Example of sub-script.

```
#!/bin/bash -l
#PBS -q serial
#PBS -l walltime=00:05:00
#PBS -l vmem=0.1GB
#PBS -e tmp.err
#PBS -o tmp.out
module load python
export PYTHONPATH=/dir/to/my/modules:${PYTHONPATH}
cd $PBS_0_WORKDIR
python ./ex0.py
```

How to run Python code on NERSC

Using mpi4py on NERSC.

- module load mpi4py
- Get ranks and nprocs.

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
nprocs = comm.Get_size()
rank = comm.Get_rank()
```

- Example of sub-script :

```
#!/bin/bash -l
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=00:05:00
#PBS -e tmp.err
#PBS -o tmp.out
cd $PBS_0_WORKDIR
module load python
module load mpi4py
aprun -n 48 python-mpi ./ex1.py 200
```

How to run Python code on NERSC

Using mpi4py to run Multiple Serial Jobs.

- Import mpi4py and subprocess.
- Connect your code with python :

```
import subprocess as sp
input_cmd_sh= "./a.out " + arg1 + " " + arg2 + " " + arg3
sp.check_output(input_cmd_sh, shell=True)
```

- Example of sub-script:

```
#!/bin/bash -l
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=00:05:00
#PBS -e tmp.err
#PBS -o tmp.out
cd $PBS_0_WORKDIR
module load python
module load mpi4py
aprun -n 48 python-mpi ./ex2.py 200
```