

How to connect to the system

```
ssh -X z3XX@login-gfx2.hpc.cam.ac.uk
```

If you want to use Windows please download **MobaXterm**
(<http://mobaxterm.mobatek.net>)

Access all material

<https://github.com/RSE-Cambridge/2017-cuda-fortran-material>

(short url: <https://tinyurl.com/CUDAFORTRAN>)

```
git clone https://github.com/RSE-  
Cambridge/2017-cuda-fortran-material.git
```

Environment HW/SW

HW (Wilkes, Cambridge)

- dual socket 6-core Ivy Bridge (12 cores total)
- 2 NVIDIA GPU K20

SW

- PGI 16.10 (community edition)
- MKL 11.3
- Open MPI 1.10.3
- CUDA 8.0
- Few custom libraries (for QE-GPU)

Compile and link using PGI

FORTRAN: pgfortran / pgf90

C: pgcc

C++: pgc++

Important flags:

- “-Mpreprocess” = enable preprocessor
- “-mp” = enable OpenMP
- “-Mcuda=cc35,cuda8.0” = enable CUDA FORTRAN
- “-Mcuda lib=cufft,cublas ” = link CUBLAS and CUFFT
- “-pgf90libs” = runtime libraries for mixed prog lang

SLURM commands

Three command to learn ...

```
sbatch <script>
```

```
squeue -u $USER
```

```
scancel <jobid>
```

Submission scripts

- `submit-monday.sh`
- `submit-tuesday.sh`
- `submit-wednesday.sh`

- `submit-serial.sh`
- `submit.sh`

Example submission script

```
#!/bin/bash
#SBATCH -J NAME
#SBATCH -A TRAINING-GPU
#SBATCH --nodes=UUUUU
#SBATCH --ntasks=XXXXX
#SBATCH --time=0:05:00
#SBATCH --no-requeue
#SBATCH --partition=tesla
#SBATCH --reservation=cuda_fortran_mon

# EDIT ME ONLY IF YOU KNOW WHAT YOU ARE DOING #####
. /etc/profile.d/modules.sh
module purge
module load default-wilkes
module unload cuda intel/cce intel/fce intel/impi intel/mkl
module load intel/mkl/11.3.3.210
module load pgi/16.10
module load openmpi/pgi/1.10.3
module load cuda/8.0
module load custom/magma/2.0.2 custom/lib-jdr/1.0
#####

cd $SLURM_SUBMIT_DIR

export EXE="./pw.x"
export PARAMS="-input pw.in"

export OMP_NUM_THREADS=6
mpirun -np XXXXX -report-bindings -bind-to socket --map-by ppr:1:socket ${EXE} ${PARAMS}
```

Compile and run QE-GPU code

Two examples: “PW-AUSURF54” & “PW-AUSURF112” (k and gamma)

Compile

```
cd qe-gpu_mini
./configure --enable-parallel --enable-openmp --without-scalapack
cp make.inc-STELLA make.inc
make pw
```

(executable located in “PW/src/pw.x”)

Run

```
export EXE="./pw.x"
export PARAMS="-input ausurf_k.in"
```

```
export OMP_NUM_THREADS=6
mpirun -np XXXXX -report-bindings \
  -bind-to socket --map-by ppr:1:socket ${EXE} ${PARAMS}
```