

## **Using K2: The incomplete getting started guide for serial programs:**

### **Access:**

As always, only text ssh access through the IUAC NKN gateway is possible. First: ssh <username>@gate.iuac.res.in . Next: ssh k2

### **Compiling code:**

The default compiler is the Intel Composer XE 2013 suite, which provides the icc and ifort compilers. The compilers are installed in the /opt/intel/bin directory, but the path should be defined by default and just icc / ifort should work. The default math library is the Intel MKL.

Gcc and gfortran are also available, but GSL or any other compatible math library has not been installed. Unless there are major code porting issues, we recommend you use the Intel compilers.

### **Running MPI programs:**

As usual, jobs should be submitted only through the scheduler. The scheduler for K2 is now SGE (not SLURM as in the previous incarnation). The usual SGE commands (qsub, qstat, qdel) should work. So should their man pages. If they don't, paths have not been defined: please source /etc/profile.

A sample qsub file for serial (non-MPI) jobs is on the next page; please tweak this to suit your requirements. The queue definition for serial jobs should always be serial.q. This queue should never be used for parallel jobs using mpirun.

If you need to run MPI jobs, please see the compilation instructions and qsub script in the getting started guide for MPI programs.

### **Sample qsub script:**

```
#!/bin/bash
#$ -S /bin/bash
#$ -cwd
#$ -N hello
#$ -j y
#$ -o $JOB_ID.out
#$ -q serial.q
##$ -binding linear:1
#$ -V
```

```
# If your binary is on a path defined in /etc/profile, uncomment:
# For instance, system-wide applications kept in /opt
# source /etc/profile
```

```
# The actual command line you would run without the SGE
```

```
./a.out
# To submit, qsub script_file (this being the script_file)
```

```
# In the above, the lines starting with #$ are directives to SGE
#     hello is the job name given to SGE
#     $JOB_ID is the job number returned by SGE when you qsub
#     serial.q is SGE queue asked for; only one configured for now
#     -cwd looks for input, and puts output and err, in cwd
#     -j y combines output and error in the same file $JOB_ID.out; if you want to separate
#         the two, replace this line with -e $JOB_ID.err or some such.
#     -S specifies shell; if not /bin/bash, change /etc/profile line
```

### **Statutory warning:**

I know we are too civilized to do all this, but ... Please don't run executable files directly to try programs out. Ever. It works. It also confuses SGE, slows other users' jobs, and sometimes leaves running processes behind. Please don't log in to compute nodes to run programs, or put your files away. With SGE, unlike with the earlier SLURM install, you can. Same effect. And gate.iuac.res.in is just that: a gateway system. Please don't leave your data there, or compile or run programs. Will bring the system to its knees.