جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology
IBEX

IBEX CHEAT SHEET

Ibex is a heterogeneous cluster with a mix of AMD, INTEL and NVIDIA GPUs.

Operating System	Centos 7
Scheduler	SLURM
Number of Nodes	864

To Login:

Intel nodes:

```
ssh -X <UserName>@ilogin.ibex.kaust.edu.sa
```

AMD nodes:

```
ssh -X <UserName>@alogin.ibex.kaust.edu.sa
```

GPU nodes:

```
ssh -X <UserName>@glogin.ibex.kaust.edu.sa
```

Software Installation (APP-STACK):

Previous Cluster AppStacks are available on IBEX . Check the AppStack available on each login node after logging in.

Note: Appstacks are different on each login node.

Software Availability:

```
$module avail
$module avail <ApplicationName>
$module avail <ApplicationName>/<version>
```

Software Loading:

```
$module load <ApplicationName>
$module load <ApplicationName>/<version>
```

Job Submission (batch mode):

To set minimum memory: --mem
To select node type: --constraint=intel|amd
--gres=gpu
To select a specific gpu node:
Example: --gres=gpu:p100:1
To set number of nodes: --nodes
To set number of tasks: --ntasks
To set wall clock time: --time
To set node usage mode: --exclusive
To set the file name for standard err: --err
To set the file name for standard out: --output

Sample Job Script:

```
#!/bin/bash
#SBATCH --partition=batch
#SBATCH --job-name="vasp-example"
#SBATCH --constraint=intel
#SBATCH --mem=60000
#SBATCH --nodes=2
#SBATCH --ntasks=32
#SBATCH --time=4:00:00
#SBATCH --exclusive
#SBATCH --err= JOB.%j.err
#SBATCH --output= JOB.%j.out
#-------------------------------------------------------#
module load intel/2016
module load vasp/5.4.1/ompi211-intel1602
module load openmpi/2.1.1/icc16.0.2
export OMP_NUM_THREADS=1
touch WAVECAR CHGCAR
srun --ntasks=32 --hint=nomultithread ${VASP_HOME}/vasp_std
```

Job Submission (interactive mode):

salloc --time=2:00:00 --nodes=2 --exclusive

Other Slurm Commands:

sbatch: to run jobs
sinfo: to check node availability
squeue: to check job status
scancel job#: to cancel jobs

General Tips:

- Never ssh to a compute node
- Always run your jobs from the scratch
- Remember to clean up your scratch

Filesystem:

- /home/<UserName>: *Home directory for important data backup.*
- Always use the /scratch filesystem to *submit jobs from amd/intel/gpu* nodes.
- Use /fscratch if your jobs require a high number of IOPS.

Need Help:

cluster-apps@hpc.kaust.edu.sa
cluster-systems@hpc.kaust.edu.sa
cluster-vm@hpc.kaust.edu.sa

Visit Our Wiki Page for info on each application, Job Generator, tutorials and more:
https://www.hpc.kaust.edu.sa/cluster