



جامعة الملك عبد الله  
للعلوم والتقنية  
King Abdullah University of  
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# Ibex Documentation and Support

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# Increase your productivity

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## **Don't reinvent the wheel!!**

- Check the documentation website
- Use the installed packages
- Contact the team for any help/issue
  - Don't be shy, ask the team for any questions or issues

# Follow the guidance

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Logins are for editing and compiling, not for running

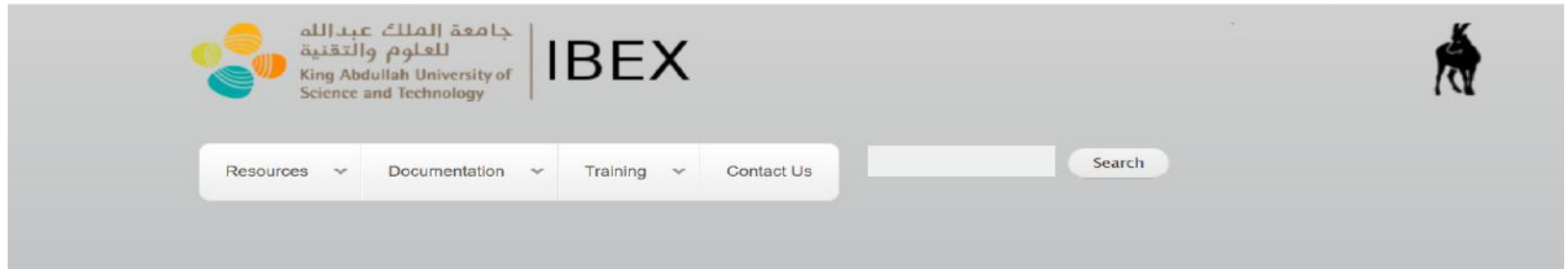
- Submit your job scripts

Follow the policy of the utilization

- Ibox is a shared resource
- Send a detailed justification for exceeding the quota/wallclock time

# IBEX Website

<https://www.hpc.kaust.edu.sa/ibex>



## Quick Links

- [New User?](#)
- [Applications](#)
- [F.A.Q.](#)
- [Training](#)
- [Jobscript Generator](#)

## Latest news from @KAUST\_HPC

### Tweets by @KAUST\_HPC

 KAUST HPC  
Retweeted

 **Bilel Hadri**  
@mnoukhiya

Replying to @jorgascon and 5 others

Kudos for the discovery using @KAUST\_News @kaust\_corelabs equipment like @KAUST\_HPC Supercomputing resources @cray\_inc.

## Welcome to Ibex

Ibex is a heterogeneous group of nodes, a mix of AMD, INTEL and Nvidia GPUs with different architectures that gives the users a variety of options to work on.

Ibex is made up of 864 nodes that are constantly monitored by the systems team.

Operating System on nodes: CentOS 7.5

Scheduler : SLURM version 18.08


Appstacks:

1. Computational Bioscience Research Centre's software stack: /cbrc/software (What used to be on the Dragon cluster)
2. Ibex's latest applications are installed on /sw/csXX appstack ,where XX is replaced by a(AMD), i(Intel), g(GPU), gv(GPU Volta) or is(Intel Skylakes) built with different compilers: like Intel and GNU.

Make sure you check the [FAQ](#) and [Applications](#) pages for further info or send us a query using the [Contact Us](#) page.

## HELP NEEDED?

 [» R | T «](#)

 [Join us on Stack!](#)

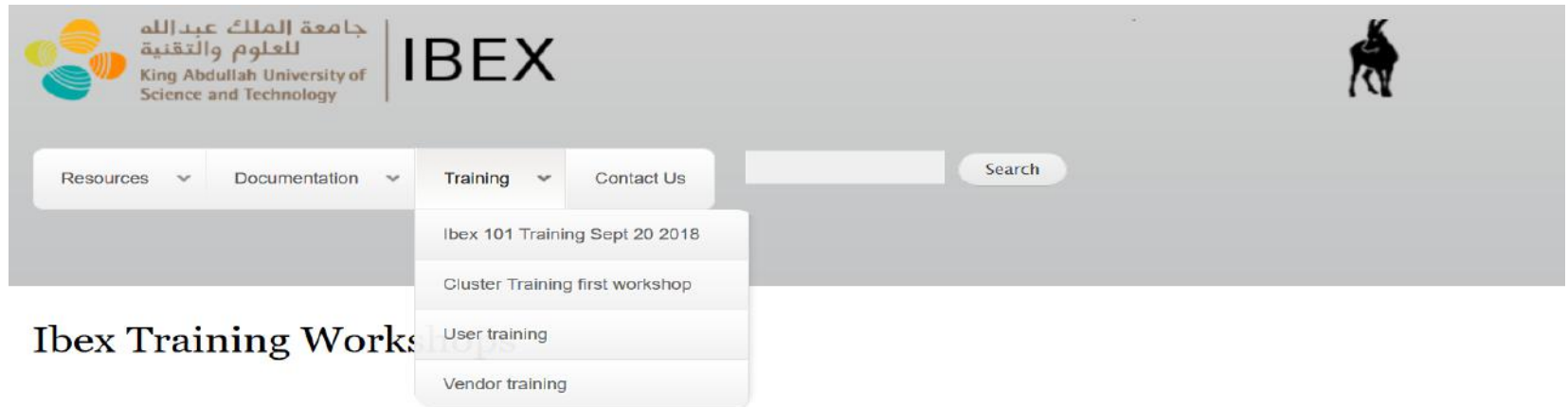
 [FEEDBACK](#)

## KSL Events Calendar

« **January** »

S	M	T	W	T	F	S
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

# Training materials



## Ibex Training Works

### Sessions

What	When	Registration/Slides
<b>Getting upto speed with Ibex cluster</b>	Nov 26, 2018	<ol style="list-style-type: none"> <li>1. <a href="#">IBEX Cheat sheet</a></li> <li>2. <a href="#">Getting upto speed with IBEX</a></li> <li>3. <a href="#">IBEX Hardware and Software stack</a></li> <li>4. <a href="#">How to run a job in IBEX</a></li> <li>5. Application software examples               <ol style="list-style-type: none"> <li>(a) <a href="#">How to run Gaussian 09</a></li> <li>(b) <a href="#">How to run Fluent application on the cluster</a></li> </ol> </li> <li>6. <a href="#">IBEX Documentation and Support</a></li> </ol>
Ibex 101 Training	Sep 20 2018	<a href="#">Slides</a>
Overview on HPC Numerical Libraries	Jan 30, 2018	<a href="#">Slides</a>
Second Workshop "Boost your efficiency when dealing with multiple jobs on Shaheen and Ibex"	Dec 12, 2017	<a href="#">Slides</a>
October 17 - Cluster Training Workshop	Oct 17, 2017	<a href="#">Slides</a>

# Almost all Applications are listed

Check the installed packages:  
module avail name\_package



Applications installed on Ibox

sort by name **sort by category**

R	RStudio Desktop	conda	gnuplot
netcdf	octave	flex	polyrate
bedtools	bedtools	blast	bowtie
bowtie2	braker	bwa	empanada
jvarkit	maker	mocat	samtools
tophat2	trinity	unicycler	snpe-seq
openfoam	flex	siesta	vasp
wland3	cambridge	ncn	flow
blast	gnss	rbc	kyote
igmpack	libbinder	libsig	openblas
glances	openmpi	lib	octave
machine-learning	nccl	tensorflow	mathematica
cuda	gimpick	laminar	open

# How to write a job script

## <https://www.hpc.kaust.edu.sa/ibex/job>

Resources ▾

Documentation ▾

Training ▾

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### IBEX Jobscript generator

Application Executable	<input type="text" value="Myapp"/>	<p>-- Corresponding ibex SLURM script --</p> <pre>#!/bin/bash #SBATCH -N 1 #SBATCH --partition=batch #SBATCH -J Myjob #SBATCH -o Myjob.%j.out #SBATCH -e Myjob.%j.err #SBATCH --time=01:30:00 #SBATCH --mem=100M  #run the application: Myapp</pre>
Job Name	<input type="text" value="Myjob"/>	
Email Address to get notified	<input type="text" value="@kaust.edu.sa"/>	
Wallclock Time (duration of job)	<input type="text" value="1"/> h <input type="text" value="30"/> m	
Partition	<input type="text" value="batch"/>	
Processor	<input type="text" value="Intel or AMD"/>	
Local Storage	<input type="text" value="No preference"/>	
memory	<input type="text" value="100"/> <input type="text" value="MB"/> per node	
EXCLUSIVE	<input type="checkbox"/>	
MPI	<input type="checkbox"/>	
OpenMP	<input type="checkbox"/>	
Array	<input type="checkbox"/>	
<input type="button" value="Generate Script"/>		

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

### To Login:

Intel nodes:

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

AMD nodes:

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

GPU nodes (non-Volta):

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

Intel Skylake nodes:

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

GPU nodes (Volta):

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

### Application installation :

All compilers, libraries and applications are installed on each login node due to variation in the system architecture. Intel, AMD and GPU based architecture specific applications are available through modules.

### Application availability:

```
$module avail
$module avail <ApplicationName>
```

### Application loading:

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

### Job Submission (batch mode):

To set memory requirement: `--mem=<in MB>`

To select architecture specific node type:

```
--constraint=intel|amd
```

```
--gres=gpu:<$$$>:<#>", where: <$$$> is
```

the GPU architecture and <#> is for number of GPUs. For example, "`--gres=gpu:gtx1080ti:4`" is for 4 GTX GPUs

To set number of nodes: `--nodes`

To set number of tasks (for parallel processing): `--ntasks`

To set the number of core per tasks: `--cpus-per-task`

To set wall clock time: `--time`

To set the node as dedicated for the job: `--exclusive`

To set the file name for standard err: `--error`

To set the file name for standard out: `--output`

**Tunable job script generator for IBEX is available in:**

<https://www.hpc.kaust.edu.sa/ibex/job>

### Example Job Script:

```
#!/bin/bash
## SLURM Resource requirement:
#SBATCH --nodes=1
#SBATCH --cpus-per-task=8
#SBATCH --job-name=spades
#SBATCH --output=myjob.%J.out
#SBATCH --error=myjob.%J.err
#SBATCH --time=8:00:00
```

```
## Required software list:
module load gaussian09/d.01/precompiled
## Run the application:
echo "This job ran on $SLURM_NODELIST dated
`date`;
srun g09 < testgau.inp > testgau.out
```

### Job Submission queues:

There are 2 queues, the default batch is for production runs and the debug is for interactive debugging the jobs.

### To use debug queue (for example):

```
salloc --time=5:00 --nodes=1 \
--partition=debug
```

### Other Slurm Commands:

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

### General Tips:

- Do to run on the logins nodes, always submit your jobs through scripts.
- Logins are designed for compilations and edits.
- 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.

### Contact for Help/Support:

[ibex@hpc.kaust.edu.sa](mailto:ibex@hpc.kaust.edu.sa)

### Our website:

<https://www.hpc.kaust.edu.sa/ibex>





# SLURM Job Script Cheat Sheet

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*Check out the print outs and you can find them available on our website*

# TIPS

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- Ibex is a shared resource be patient
- Adjust your wall clock time accordingly
- Choose the right resource
  - Workstation/ Ibex/ Shaheen

# Feedback and Contribution

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- We really appreciate your feedback on the website and also on the team.
- Monthly prize for the best tips and tricks on any application of use.
- All the best and useful tips will be added to the website with your names.

# Contact for Help /Support

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Application installation/failure/support or System issues  
/failure/support :

- [cluster@hpc.kaust.edu.sa](mailto:cluster@hpc.kaust.edu.sa)
- [ibex@hpc.kaust.edu.sa](mailto:ibex@hpc.kaust.edu.sa)

Our website : <https://www.hpc.kaust.edu.sa/ibex>

Slack : <https://kaust-ibex.slack.com/> - Use #general for simple queries

# Questions ?

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