

Overview on Ibex Software Environment

Passant Hafez
HPC Applications Specialist
Supercomputing Core Lab

Q: Do I need to apply to use Ibex?

The answer is **NO**.

Any KAUST member should be able to login and use Ibex.

First check your credentials are correct by logging into the KAUST Portal

<https://portal.kaust.edu.sa>

or KAUST Webmail

<https://webmail.kaust.edu.sa/>



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Faculty Focus: Taous-Meriem Laleg-Kirati



Ph.D. student Jian You Wang wins outstanding poster award at International Symposium on Rice Functional Genomics



Developing sensor solutions

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Email :
ithelpdesk@kaust.edu.sa

Phone : (+966) (12) 808-0910

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If for any reason you can't access lbex using the verified credentials, you should contact IT, sometimes they don't configure Unix Attributes for new user accounts on the Active Directory.

If you experience login failures, you'll need to wait 15 mins and try again, if it still fails then contact IT.

IT Service Desk

Phone: (in KAUST) 900 option 1

Phone: (out of KAUST) +(966) 2 808 0900 option 1

Email: ithelpdesk@kaust.edu.sa

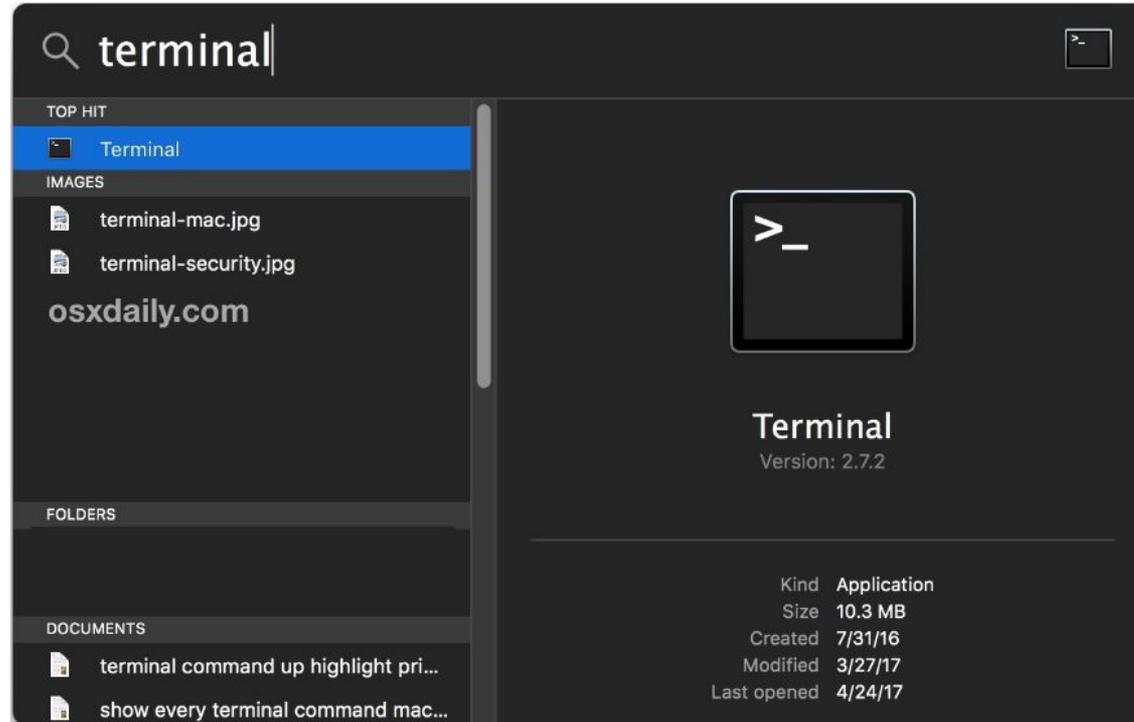
Web: <http://servicedesk.kaust.edu.sa>

How to login to Ibex from different Operating Systems?

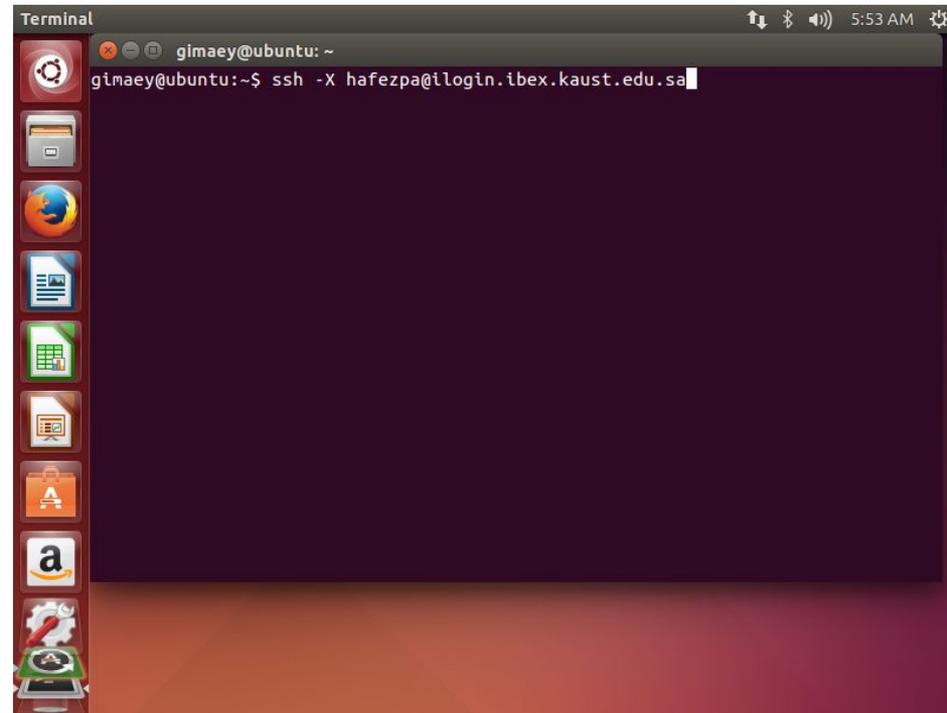
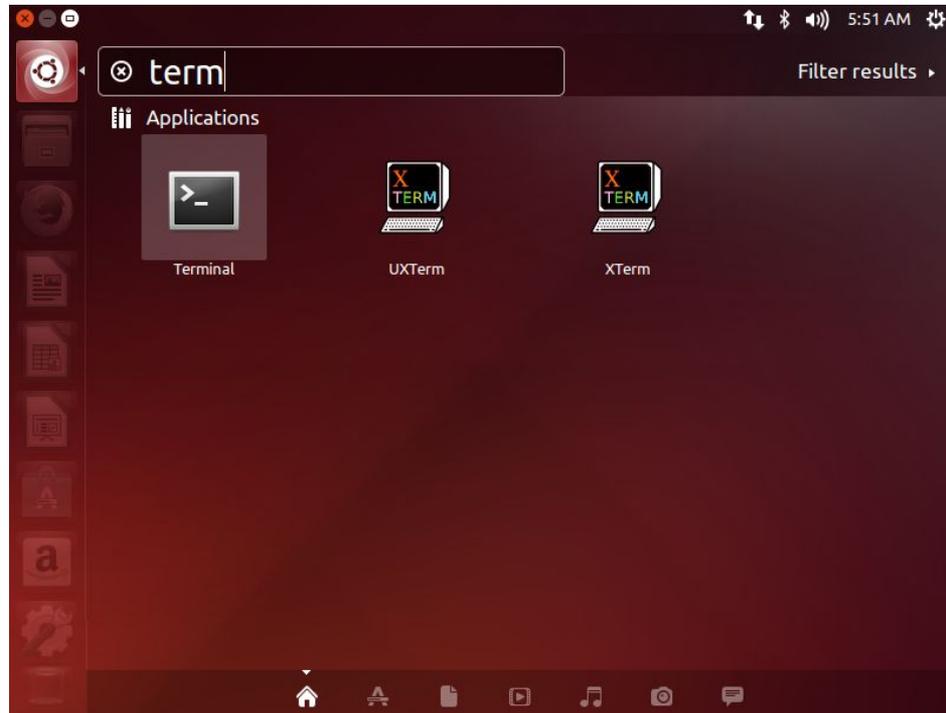
For macOS and various Linux distributions you can use the native terminal program.

macOS

A) Mac OS



B) Linux (Ubuntu, Debian, CentOS, Fedora, Red Hat,..)

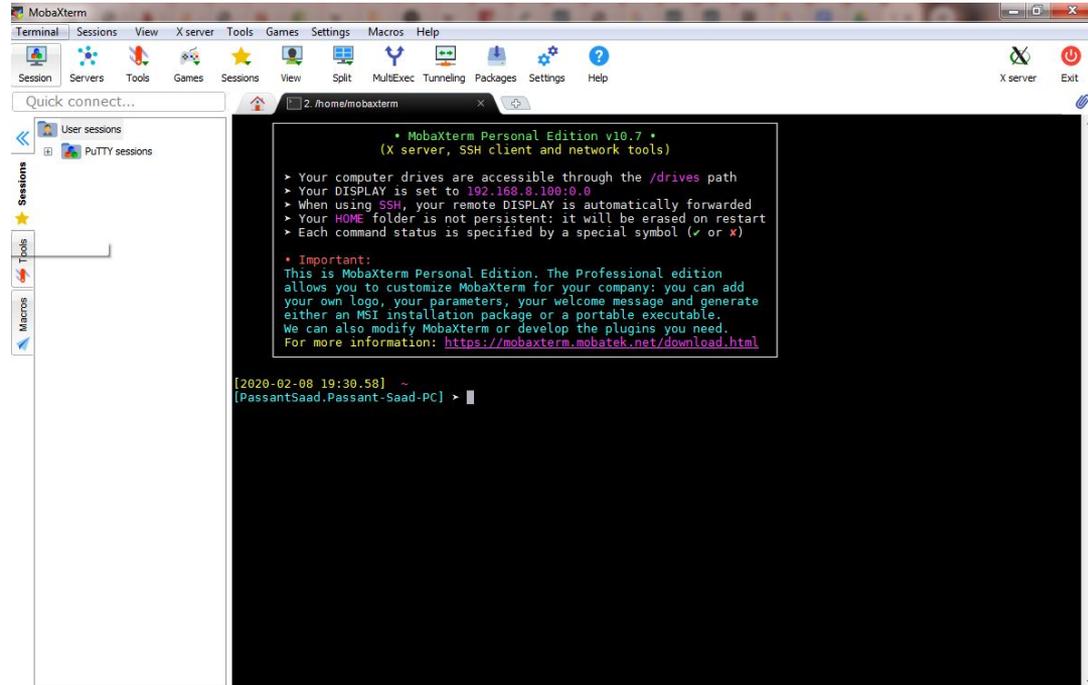
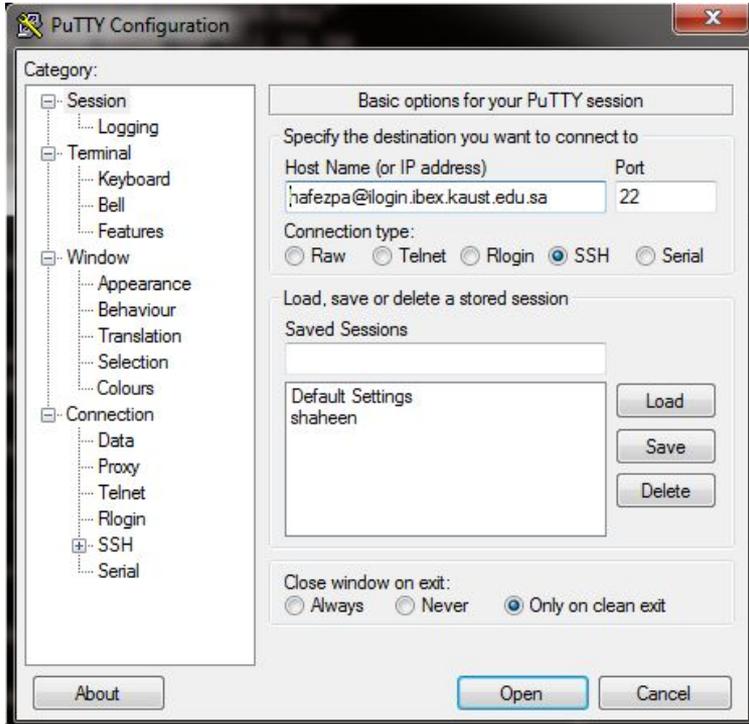


For MS Windows users you'll need to use third party SSH client tool like [PuTTY](#) or [MobaXterm](#).

Note:

MobaXterm is an enhanced terminal for Windows which includes an X11 server, if you're using PuTTY you'll need to install and run an X11 server like Xming.

C) Windows



MOTD (Message Of The Day)

Upon successful login to Ibex, you'll see a message with any updates the team wants to share with you.

```
Using username "hafezpa".
Authenticating with public key "imported-openssh-key"
Last login: Tue Feb  4 17:11:05 2020 from 10.152.29.41
/-----** IBEX Announcements **-----\

In order to accommodate the new hardware upgrades KSL is
undertaking to IBEX, as of September 25, 2019 - the "amd" SLURM
partition will be decommissioned and access will be blocked.

Please make sure your job submission scripts do not include any
references to this partition.

IBEX cluster will still contain nodes with AMD CPUs, therefore
SLURM constrains related to AMD CPUs will be still working.

In case of any question please contact us at ibex@hpc.kaust.edu.sa
+-----*** Maintenance Session ***-----+

Due to data centre preventative maintenance, the next Ibex
maintenance session will be:

Start: Sunday 15th March @ 07:00
Finish: Thursday 19th March @ 08:00
+-----*** Support ***-----+

For help with Ibex use either:

http://hpc.kaust.edu.sa/ibex - Wiki containing ibex information

http://kaust-ibex.slack.com - use #general for simple queries

ibex@hpc.kaust.edu.sa - to create a request ticket
/-----\
```

Welcome Email

A welcome email is also sent to you upon your first login to Ibex providing different information about your storage spaces (home, scratch), modes of support, attaching useful documents.

2 attachments



Download all

Welcome to Ibex!

Your account has been configured in slurm but can take up to **60 minutes** before being available.

Ibex online documentation is available at:

<http://hpc.kaust.edu.sa/ibex>

Important storage tips:

/home/hafezpa - this is your personal home directory and is limited to 200GB of data. Do not run HPC jobs in your home directory - just use it for keeping configurations, scripts etc.

/ibex/scratch/hafezpa - this is your HPC storage. Use this storage for saving the output of, and input to compute jobs. This is much faster than your home directory so your jobs will run quicker. This directory has a limit of **1.5TB**. If you need more storage contact the Ibex support team.

/tmp - for job specific temporary files specify this directory. Once your job finishes all files in this directory will be deleted. Placing job temporary data in this directory will be result in higher performance than storing it in your scratch area; won't contribute towards your used quota; and will automatically be deleted when your job finishes.

Assistance / Support

Ibex support operates Sunday to Thursday from 8am thru to 5pm. Requests for support will be responded to within 24 hours.

ibex@hpc.kaust.edu.sa - email this address to create a service request

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

Attached are two quick reference guides:

- o [Ibex_cheat_sheet_Jan_17_2019.pdf](#)
- o [Slurm_cheat_sheet.pdf](#)

Welcome to the Ibex Community.

We are here to help you, whether you are a novice at HPC or experienced.

- The Ibex Team.

Passwordless Authentication

You can login to Ibex without the need to type your password every time

(and watching out for typos..)

Contact us ibex@hpc.kaust.edu.sa and we'll provide information based on your OS

Software on Ibex

Software on Ibex:

Two options:

- 1) Local Installation: customizable, Ibex team will provide help if needed, just watch your storage quota ;)
- 2) Public Installation: the most common/general mode of installation is available as shared module for multiple users.

For help with either case, as always, email ibex@hpc.kaust.edu.sa

Software on Ibex:

Environment Modules:

- Are used to manage public installations on Ibex.
- Rich AppStack of >400 modules.

Software on Ibox:

The most common subcommands you'll find useful would be:

module av/avail → With no arguments, lists all the modules available for use.

module av/avail <string> → Used to check the availability of a module that starts with *string*.

module load/add <module> → adding that module to your environment.

module unload/rm <module> → removing that module from your environment.

module swap/switch <module1> <module2> → switches between module1 and module2

module purge → removes ALL loaded modules

module list → lists the currently loaded modules

module show <module> → views what this module is supposed to change in your environment.

To list ALL available modules:

```

[hafezpa@dbn503-35-r ~]$ module avail
----- /sw/csi/modulefiles/applications -----
abaqus/2017                               lumpysv/0.3.0/anaconda3env
abricate/0.9.8                             macs/1.4.2-anaconda2-2.5.0
abyss/2.0.2                                macs2/2.1.1.2/anaconda2-2.5.0
abyss/2.1.4                                madagascar/2.0/gnu-6.4.0
adf/2016.102/precompiled                   maestro/1.6
adf/2016.106/precompiled                   maestro/1.7.1
adf/2019.103/precompiled                   mafft/7.407-with-extensions
aescrypt/3.14                              mafft/7.407-without-extensions
amber/18/gnu-6.4.0                         maker/2.31.10
amber/18/openmpi-3.0.0                     maker/3.10.02
ambertools/18/anaconda3env                manta/1.6
ambertools/18/openmpi_3.0.0               marvel/6d68df1/e17.5_gnu6.4.0_python3.6
amos/3.1.0                                  mash/2.2/gnu-6.4.0
amphora2/8742a1                             mashtree/0.33/gnu6.4.0_perl5.26.1
annotsv/2019                               masurca/3.2.4
annotsv/2.2                                materialstudio/2017R2
ansys/18.1                                 materialstudio/2019
ansys/19.1                                 mathematica/11.2.0
antismash/4.1/anaconda2-2.5.0              matlab/R2016b
antismash/5.0/gnu6.4.0_python3.5.3        matlab/R2017b
anvio/3.0.0                                matlab/R2018a
anvio/5.2                                  matlab/R2019a
any2fasta/0.4.2                            mcce/3.0
  
```

To list available modules for CUDA:

```
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$ module av cuda  
  
----- /sw/csgv/modulefiles/compilers -----  
cuda/10.0.130      cuda/10.1.105(default)  cuda/9.0.176      cuda/9.2.148.1  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$ module load cuda/10.0.130  
Loading module for CUDA 10.0.130  
CUDA 10.0.130 is now loaded  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$ module list  
Currently Loaded Modulefiles:  
  1) cuda/10.0.130  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$ module purge  
Unloading module for Tensorflow CUDA 10.0.130  
CUDA 10.0.130 is now unloaded  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$ module list  
No Modulefiles Currently Loaded.  
[hafezpa@login104-09 ~]$  
[hafezpa@login104-09 ~]$
```

To check what will the module python/3.7.0 change in your environment:

```
[hafezpa@dbn503-33-r ~]$  
[hafezpa@dbn503-33-r ~]$ module show python/3.7.0  
-----  
/sw/csi/modulefiles/compilers/python/3.7.0:  
  
module-whatis      Python Programming Language  
module             load gcc/6.4.0  
prepend-path      PATH /sw/csi/python/3.7.0/el7.6_gnu6.4.0/bin  
prepend-path      MANPATH /sw/csi/python/3.7.0/el7.6_gnu6.4.0/share/man  
prepend-path      LD_LIBRARY_PATH /sw/csi/python/3.7.0/el7.6_gnu6.4.0/lib  
prepend-path      INCLUDE /sw/csi/python/3.7.0/el7.6_gnu6.4.0/include/python3.7m  
prepend-path      PKG_CONFIG_PATH /sw/csi/python/3.7.0/el7.6_gnu6.4.0/lib/pkgconfig  
setenv            PYTHON_LIBS /home/hafezpa/local/python3.7.0_gnu6.4.0_libs  
prepend-path      PYTHONPATH /sw/csi/python/3.7.0/el7.6_gnu6.4.0/lib/python3.7:/sw/csi/python/3.7.0/el7.6_gnu6.4.0/lib/python3.7/si  
te-packages:/home/hafezpa/local/python3.7.0_gnu6.4.0_libs/lib/python3.7/site-packages/  
-----  
[hafezpa@dbn503-33-r ~]$  
[hafezpa@dbn503-33-r ~]$
```

Software on Ibex:

There are multiple ways to categorize the Software Stack by, for example:

- By Processor Type.
- By Science Domain.
- By Role.

Software on Ibex:

Note: Some tools are available on the system by default, for example Python and GCC, so to make sure you're using the loaded module for example check:

```
which python
```

That'll print the full path to the Python binary you'll use when you type `python` in your terminal.

Software on Ibex:

Software Stacks by Processor:

- Ibex is hybrid cluster of different processors, Intel (new and old) AMD and GPUs. The software stack varies accordingly*.
- For each type there is a dedicated login node, the ones of concern are:

`ilogin.ibex.kaust.edu.sa` (Intel Software Stack)

`glogin.ibex.kaust.edu.sa`

& `vlogin.ibex.kaust.edu.sa` (GPU-related Software Stack, for example CUDA Toolkit and Machine Learning modules)

*There is no fine line that separates both, sometimes it depends on the applications requests made by users to be used with which processor type.

Software on Ibex:

Software Stacks by Science Domain:

Bioinformatics/Genomics/Biosciences: Environmental Microbiology, Analyzing 16S Amplicon Data, Metagenomics, Differential Transcription Data, Sequencing Data Analysis, Transcriptomics, Plants Sciences...

Chemistry, DFT: Quantum Espresso, Gaussian, Gaussrate, Polyrate, ORCA.

CFD: OpenFoam, Gerris.

Deep Learning for Computing Vision and Bioinformatics: PyTorch, TensorFlow, Python.

Electrical Engineering/Statistics: Magnetic Field Simulation, Matlab, Python, R.

Cryo Electron Microscopy: 3D reconstruction with Relion, IMOD.

Software on Ibex:

Software Stacks by Role:

Software Development (Compilers & Programming Languages): GCC, Intel, PGI, Julia, Python, Perl, Java, R, CUDA,..

Libraries: OpenMPI, Boost, FFTW, GMP, MPFR,..

Applications: Matlab, Relion, OpenFoam, Gaussian,..

Containers: Singularity.

Thank You!