ICIQ COMPUTER-ROOM STARTER MANUAL

WELCOME

Welcome to ICIQ HPC (High Performance Computing) service. Our cluster consists of rack computing nodes interconnected by ethernet and infiniband networks. There are nodes of different generations that form isolated computational queues, and the hardware is divided into computer cells, each one associated with one research group.

Specifications:

- 6,020 CPU CPUs
- 91,008 GPU processors
- 21,212 GB of RAM
- gigabit ethernet network for data / computing
- infiniband network in some cells by computer

Access to the computer cluster is private and in order to use it, official access must be requested by e-mail to the group leader or researcher in charge of the cell to be accessed.

CEL·LA	OWNER	CPUs
iciqaeg	Prof. Antonio Echavarren	624
iciqallg	Prof. Antoni Llobet	176
iciqasg	Prof. Alexandr Shafir	96
iciqavg	Prof. Anton Vidal	176
iciqcbg	Prof. Carles Bo	5.120
iciqfmg	Prof. Feliu Maseras	5.872
iciqjllg	Prof. Julio Lloret	640
iciqmpg	Prof. Ruben Martín	144

RESOURCES

CALCULATIONS

kimik2 allows you to run calculations on the nodes of each of the queues that make it up. This means that once the calculation has been submitted, it will enter the chosen queue and, depending on the resources requested, it will either have to wait for it to start running or it will run immediately.

The queue manager used is SGE (Sun Grid Engine) v6.2 and each of the cells is governed by a different priority policy.

The codes that can be executed are: Gaussian, ADF, VASP, ORCA, TERACHEM, TURBOMOLE, ...

DISK USAGE

Because disk space is finite, each group (cell) is assigned one space per user that will limit the amount of information a user can store. The users will be able to transfer the finished calculations to their personal computer. The system will notify you by email if space is running low.

CONNECTING TO THE HPC MACHINE

The connection to the cluster will be made through a remote access terminal. The terminal uses a bash shell.
The 'sftp' connection is also allowed for file transfer.

- CONNECTING FROM LINUX
- CONNECTING FROM MAC OSX
- CONNECTING FROM MS WINDOWS

QUEUE SYSTEM USAGE

Kimik2 offers an SGE queuing system that allow users to manage their calculations. You can find the basic commands below. Anyone who wants to learn more can read the following SGE user manual.

- Available queues → qconf -sql
- Summarized queues state: → qstat -g c

- Queues/Jobs state:
  → qstat (general state)
  → qstat -q queue_name (specific queue state)
  → qstat -l -q queue_name
  (specific queue state in long-form)
  → qstat -u username (show only 'username' jobs)
  → qstat –help (more options)

- Send jobs:
  → qsub myjob.in.sub (to send job to the queue)
  → qs app_name.queue myjob.in (generate the submit script and send to the queue)
  where:
  app_name – application to use (g09 | g16 | adf9| ...)
  queue – selected queue (c8m24 | c12m48 | ...)
  myjob.in – input script (.in extension is mandatory)

NOTE-1: If you want to change the submit script, you must put a zero (0) between the queue and myjob.in. This only generates the submission script, but it will not be sent to the queue

→ qs app_name.queue 0 myjob.in
example:
qs g09.c12m24 0 myfirstjob.in

CONNECTING FROM LINUX

TERMINAL

The connection string to run from a Linux terminal is as follow:

```
ssh -p2004 username@betelgeuse.iciq.es -t ssh kimik2.iciq.es
```

you will be asked for the password twice. The first time it is requested by betelgeuse (access portal), the second by kimik2 (SGE queuing system).
If all goes well, you will be inside a terminal in kimik2 and you will be able to manage the calculations and information generated.

TRANSFER OF FILES TO / FROM KIMIK2

To transfer the information you will have to mount a tunnel to kimik2 via betelgeuse and then mount the remote ‘home’ directory of the user in a local folder.

- MAKE A TUNNEL

In a terminal run the following command:

```
ssh -p2004 username@betelgeuse.iciq.es -L 7777:kimik2.iciq.es:22
```

leave the terminal minimized, if we close it, the tunnel breaks.

- MOUNT THE ‘home’ ON THE PERSONAL COMPUTER

Open a new terminal.
Create a directory with the name of the cluster and then do the assembly.

```
cd $HOME
mkdir kimik2
sshfs -p7777 username@localhost:/home/username/ ./kimik2
```

the remote ‘home’ directory is now mounted in the local ‘kimik2’ directory.
This allows us to access remote files as if they were on our own personal computer.

CONNECTING FROM MAC OSX

TERMINAL

The connection string to run from a mac-osx terminal is as follows:

```
ssh -p2004 user@betelgeuse.iciq.es -t ssh kimik2.iciq.es
```

you will be will asked for the password twice. The first time it is requested by betelgeuse (access portal) the second kimik2 (SGE queue system).
If all goes well, you will be inside a terminal in kimik2 and you will be able to manage the calculations and information generated.

TRANSFERING FILES FROM/TO KIMIK2

To transmit the information we will have to mount a tunnel through the portal betelgeuse to kimik2 and then mount the remote 'home' directory of the user in a local folder.

- MAKE A TUNNEL

In a terminal the following command must be executed:

```
ssh -p2004 username@betelgeuse.iciq.es -L 7777:kimik2.iciq.es:22
```

leave the terminal minimized, if we close it the tunnel breaks.

- MOUNT THE REMOTE 'home' ON YOUR PERSONAL COMPUTER

Open a new terminal.
Create a directory with the name of the cluster and then do the assembly.

```
cd
mkdir kimik2
sshfs -p7777 username@localhost:/home/user/ ./kimik2
```

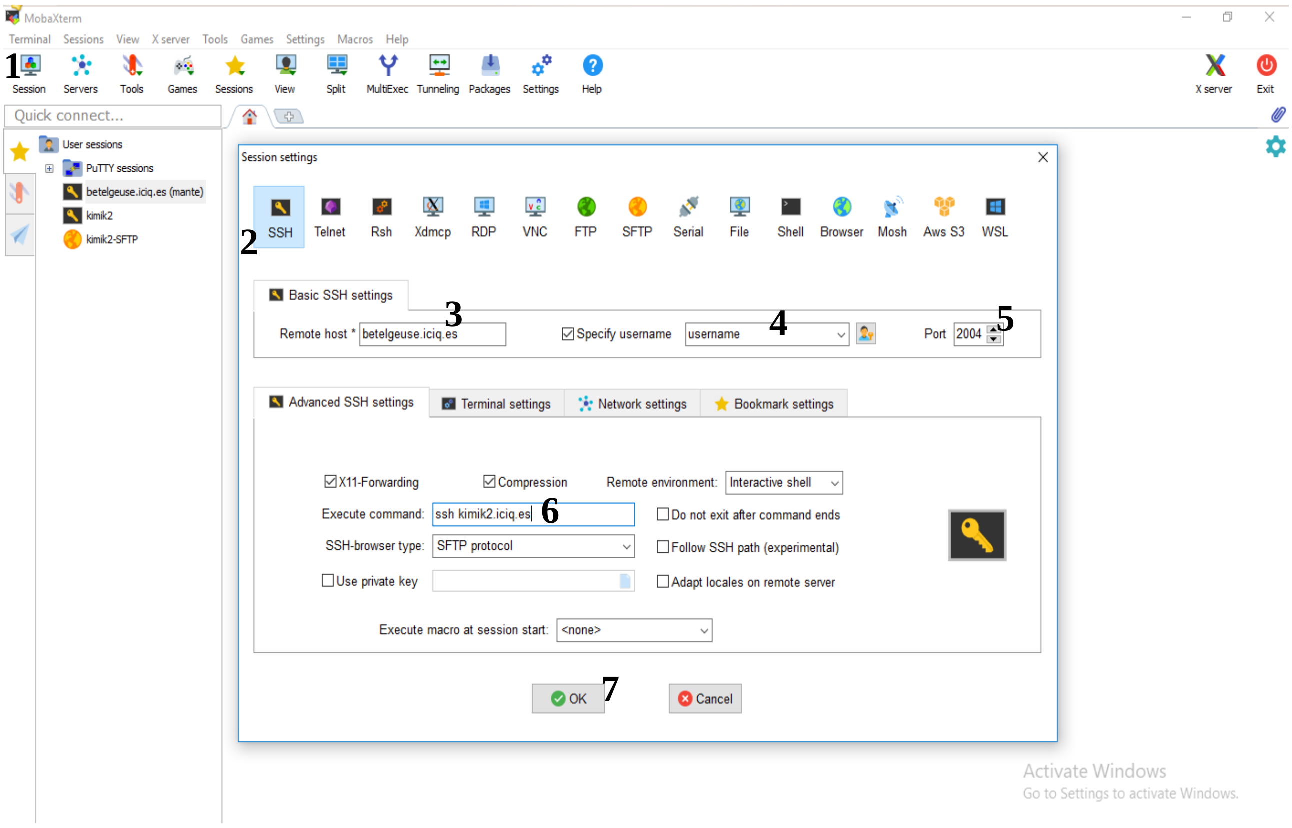
the remote 'home' directory is now mounted in the local 'kimik2' directory.
This allows us to access remote files as if they were on our own personal computer.

CONNECTING FROM MS WINDOWS

TERMINAL

MS Windows has the '[mobaXterm]' tool that allows you to access a UNIX system, open a remote terminal, create an sftp connection to transfer files, ...
The [FREE] version will be enough.

- OPEN A TERMINAL

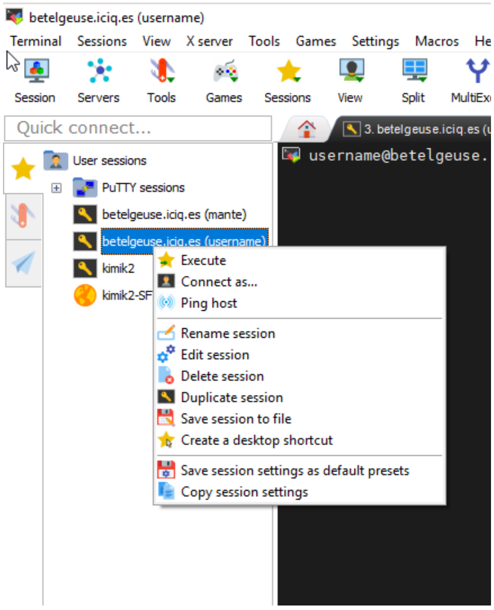


1. Tap 'Session' to create a new connection.
2. Choose 'SSH' option.
3. Type 'betelgeuse.iciq.es' in Remote host.
4. Check the 'Specify username' option and enter your 'username'.
5. Port 2004.
6. Access 'Advanced SSH settings' TAB and fill the 'Execute command' box with:

    ssh kimik2.iciq.es

7. Click 'OK' to finish/save

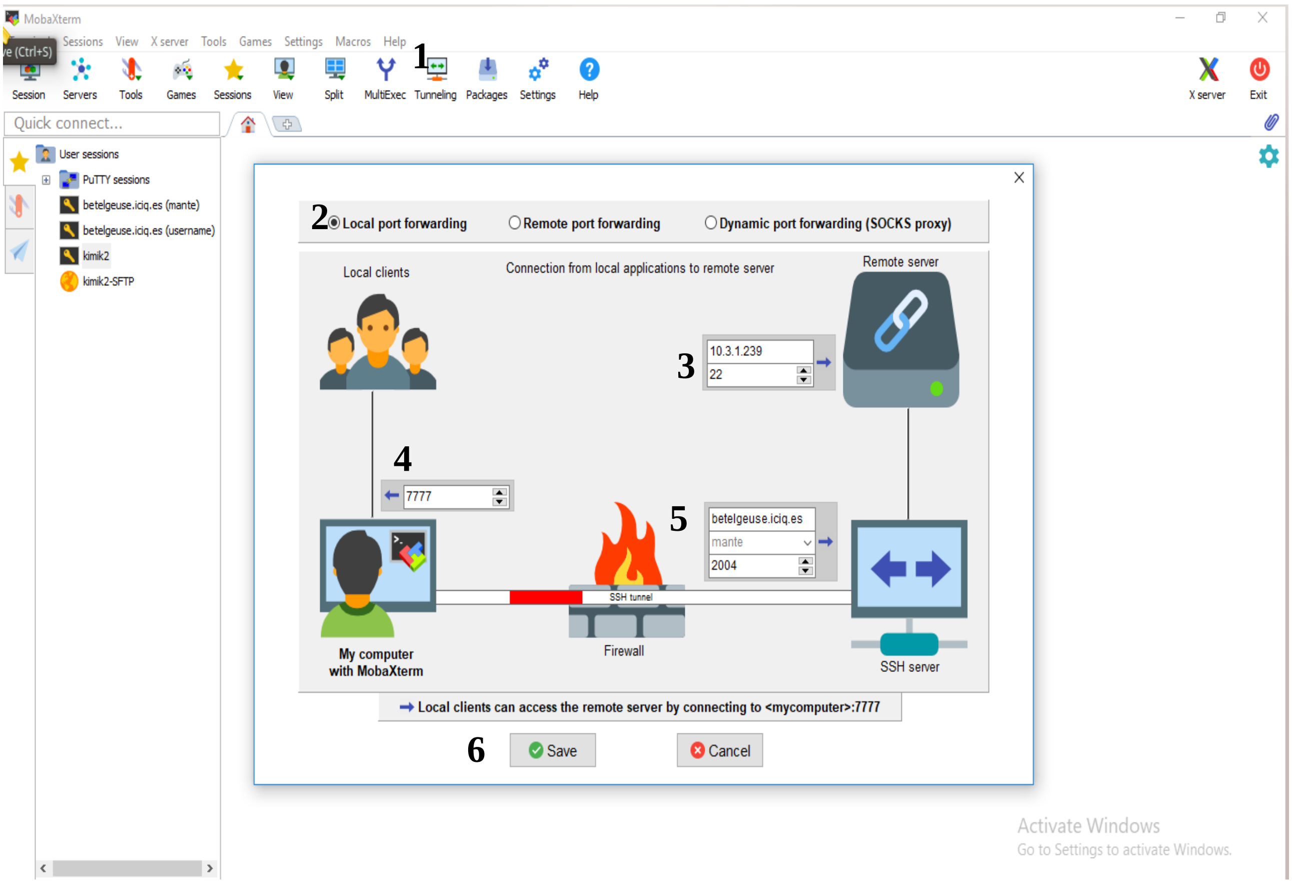
Rename the session to recognize it and double-click to run the terminal.



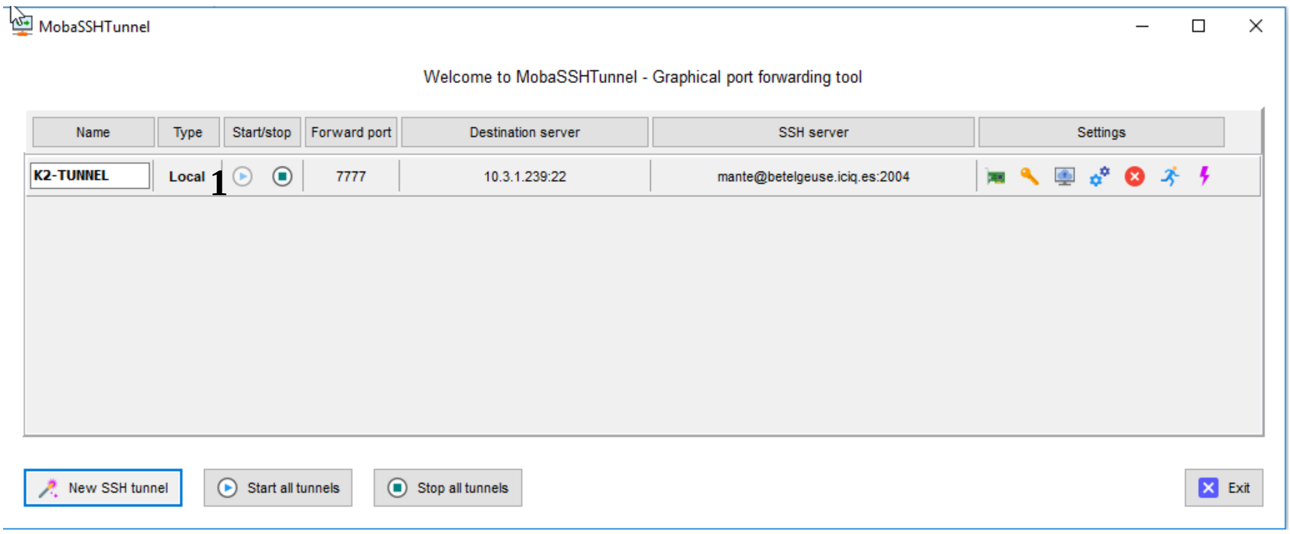
It will be necessary to enter the password twice.

TRANSFERING FILES FROM/TO KIMIK2

- CREATE AND CONNECT A TUNNEL



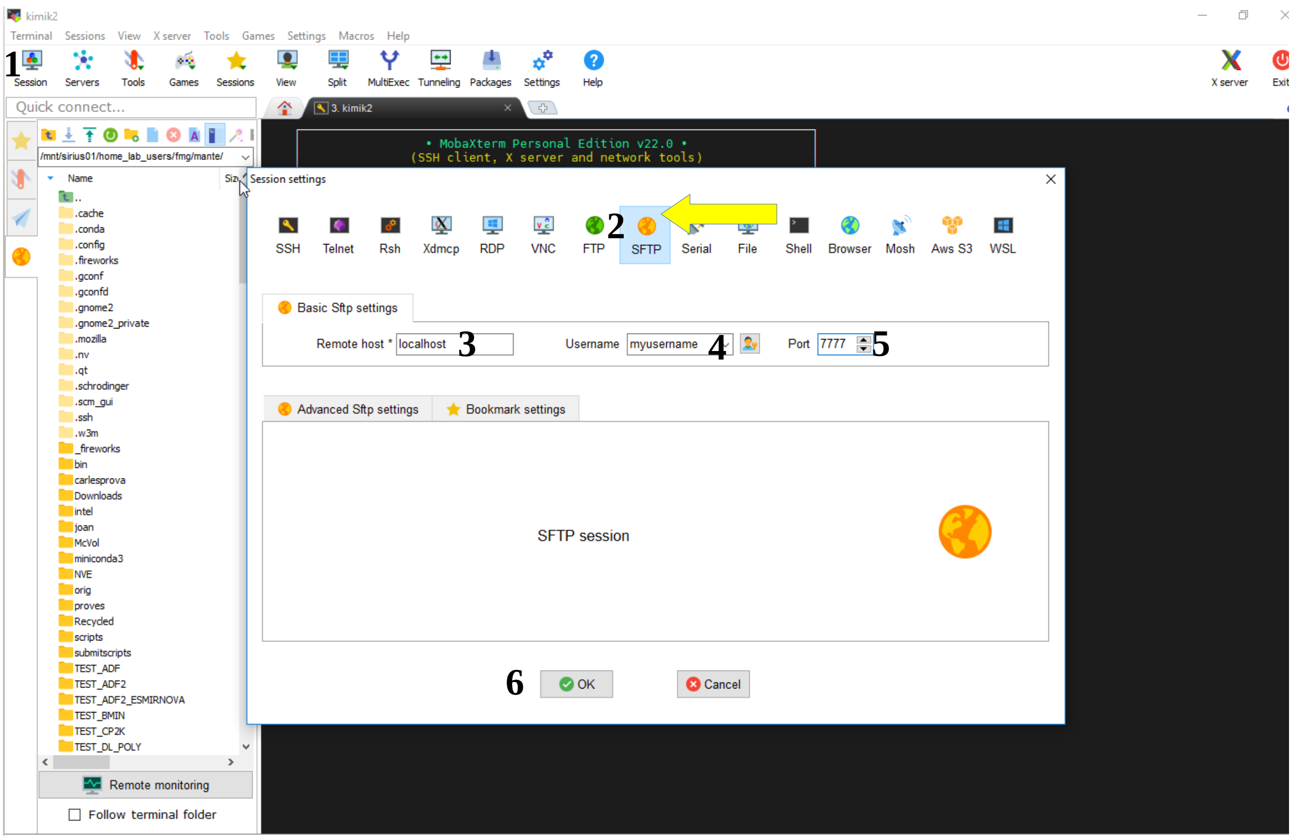
1. New tunnel connection.
2. Select ‘Local port forwarding’.
3. Configure kimik2 IP: 10.3.1.239 PORT: 22
4. Select a free port on your local computer, PORT: 7777 is a good choice.
5. betelgeuse URL/username/port: SERVER: betelgeuse.iciq.es USER: PORT user: 2004
6. ‘Save’



1. Click the 'play' button to connect the tunnel

The tunnel is now connected

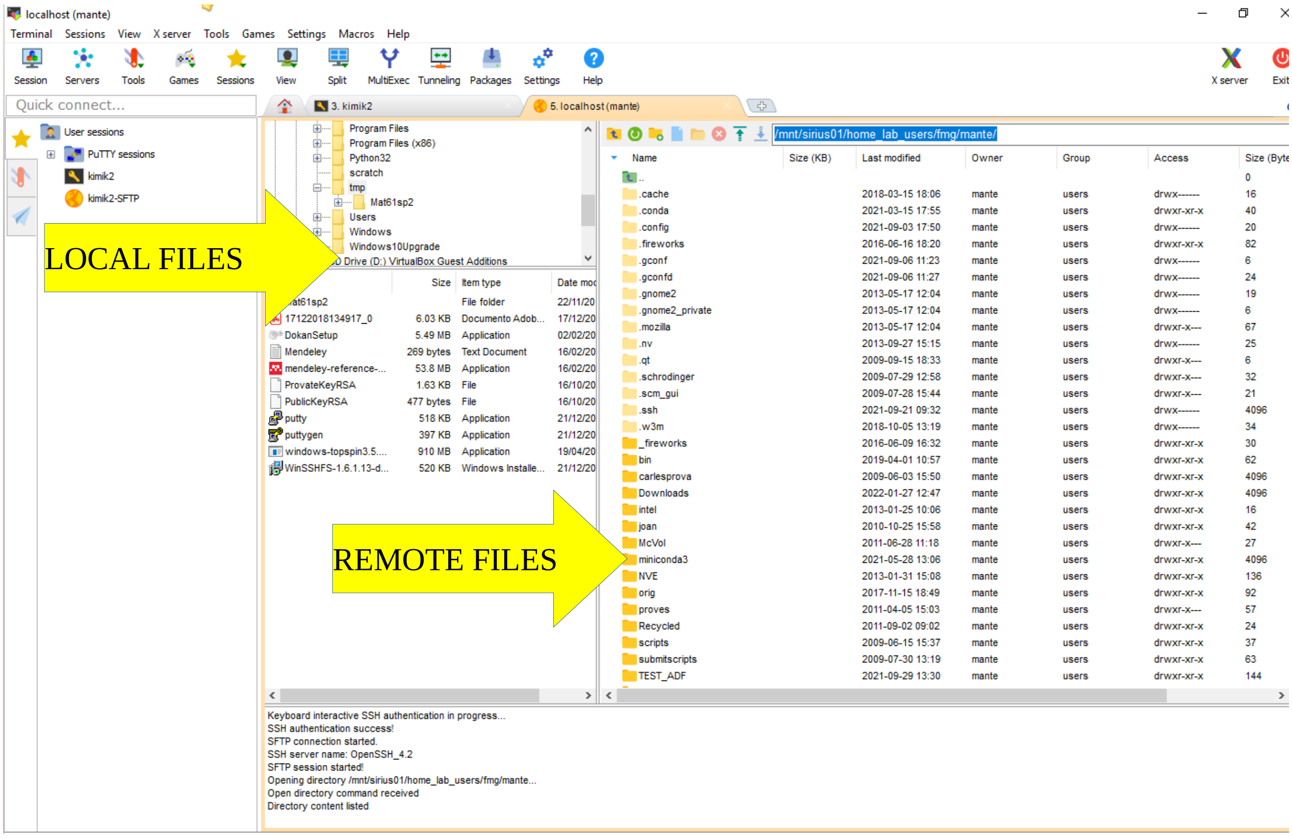
- CREATE A SFTP SESSION BETWEEN LOCAL COMPUTER AND KIMIK2



It will allow you to open a session in which to transfer bi-directionally files.

1. New tunnel connection.
2. Select ‘SFTP’ service.
3. Fill ‘Remote host’ with ‘localhost’.
4. Insert your ‘username’.
5. Use 7777 port (same as the tunnel).
6. Click on the ‘OK’ button..

When the session will be executed and connected, a window similar to this one should appear.



Questions: Martín Gumbau (mgumbau@iciq.cat)