

Physical Chemistry Unit, Departament de Química

User Guide of Computational Facilities

An User Guide for the standard user of the computer facilities in the "Unitat de Química Física"
in the Universitat Autònoma de Barcelona

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Table Of Contents

1 Introduction.....	4
2 Computer resources.....	4
3 Some Linux tools	5
4 The Cluster	6
4.1 Frontend servers	6
4.2 Filesystems	6
4.3 Computational nodes.....	7
4.4 User's environment.....	9
4.5 Disk space quota	9
4.6 Data Backup	9
4.7 Generation of SSH keys for automatic SSH login	10
4.8 Submitting jobs to the cluster	11
4.8.1 Typical queue system commands	11
4.8.2 HomeMade scripts	13
4.8.3 Create your own submit script.....	14
4.8.4 Submitting Parallel Calculations.....	15
4.8.5 Compiling Parallel applications with OpenMPI/MPICH/MVAPICH	17
5 Available Software.....	17
5.1 Chemisty/scientific software.....	17
5.2 Development Software	20
5.3 How to use the software	20
5.4 Scott and spock software	21
5.5 Non-default environments.....	21
6 Your Linux Workstation	22
6.1 Disk space on your workstation	23
6.2 Workstation Data Backup	23
6.3 Running virtual Windows XP	24
6.3.1 The Windows XP Environment.....	25
6.4 Submitting calculations to your desktop.....	25
6.5 Network dependent structure	26
7 Your Windows Workstation	26
7.1 Windows software	27
8 klingon.uab.cat server	28

8.1. The web	28
8.2. The mail	29
8.3 The printers	30
9 Frequently asked questions	30

1 Introduction

This User Guide is aimed to the standard user of the computer facilities in the "Unitat de Química Física" in the Universitat Autònoma de Barcelona. It is not assumed that you have knowledge of UNIX/Linux. However, you are encouraged to take a close look to the Linux guides that will be pointed out. In the case you can't find what you need in this guide, please address your questions or technical problems to admin@klingson.uab.cat or to an experienced user nearby.

Moreover, you can find several manuals at <http://harry.qf.uab.es/manuals/manuals.php> (access only allowed from IPs of Physical Chemistry Unit).

Checking <http://klingson.uab.es> web is important to have extended and updated information about our cluster. Nowadays, the updated information is only in Catalan.

2 Computer resources

The "Unitat de Química Física" provides researchers with several computational facilities. The Computational cluster consists of 62 active nodes and three mainservers: quanta.uab.es is the central server and it serves the disk, the user login accounts and the batch queue system, the other two servers are scott.uab.cat and spock.uab.cat, the frontend servers. The nodes configuration varies from one to another and comprises old Pentium 4 machines for testing and simple calculations purpose, dual socket Opteron and the Nehalem Intel processors with different memory and disk configurations. All these nodes are interconnected using a Gigabit network and some of them using Infiniband network. The nodes are placed in "Unitat de Química Física" and, temporally, in SI (Servei d'Informàtica of UAB).

Moreover, a standard user working in the Physical Chemistry unit is assigned to a desktop PC which normally is configured in a particular and standard way. So, there are some things a standard user also needs to know about his/her desktop PC.

On the other hand, we have klingson.uab.cat, which serves web, mail, and printers.

The next figure shows our cluster network scheme.

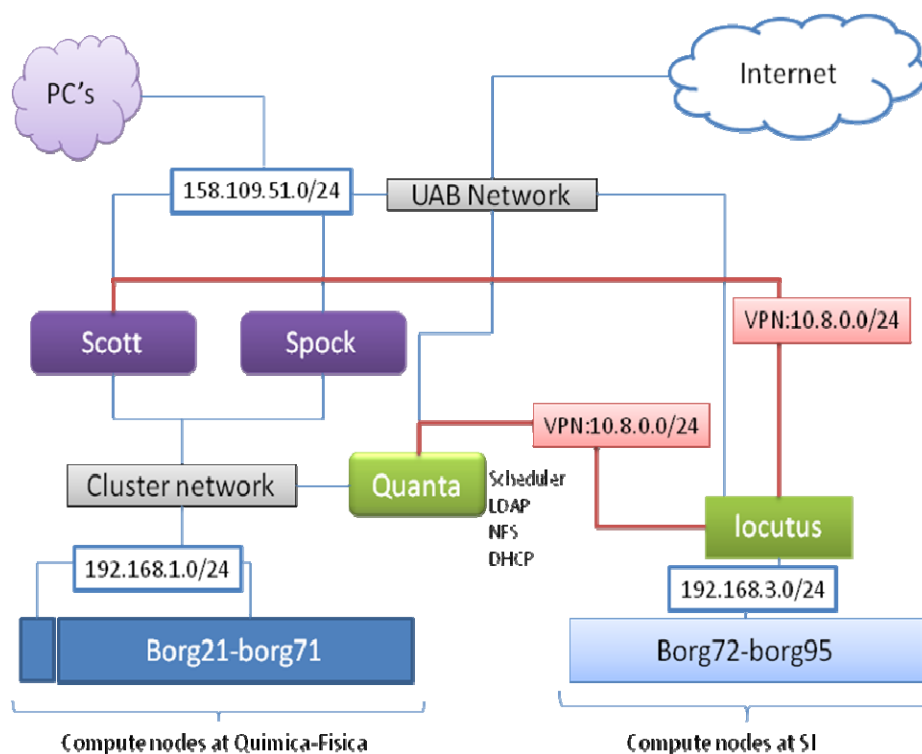


Figure 1 - Network Scheme for HPC

3 Some Linux tools

Most of the computational facilities and scientific software that you will be using in your research at Química Física is under Linux. This does not exclude the possibility of use a Windows OS in your personal desktop computer. It is therefore advised to take a look at some quick Linux one-sheet guides in order to be able to use a shell, edit a text or feel comfortable when in a Linux session. What follows is some interesting documentation to look at:

- Vim Quick Reference Card. <http://www.cheat-sheets.org/saved-copy/vimqrc1.pdf>
- Linux Quick Reference. http://solar.physics.montana.edu/sol_phys/help/LinuxQuickRef.pdf
- BASH Quick Reference.

<http://www.digilife.be/quickreferences/QRC/Bash%20Quick%20Reference.pdf>

- Harry repository manuals (<http://harry.qf.uab.cat/manuals/manuals.php>).
- Modules HomeSite and documentation. <http://modules.sourceforge.net/>
- Help yourself using man pages (i.e.: "man qsub" in a Unix session)

On the other hand there are some particular Computational Chemistry applications

that can only be used under the Windows SO. ChemOffice, Chemcraft or Scifinder are examples of such applications.

4 The Cluster

4.1 Frontend servers

The only way to use the computational resources is by connecting to spock.uab.cat or scott.uab.cat machines or by using one of the Linux workstation which is physically in the "Unitat de Química Física". The first one, spock, is a 64 bit Linux machine while scott is a 32 bit Linux machine.

If you want to access to spock or scott you MUST use a SSH connection and have previously obtained a login name and a password for that login. Typical SSH clients are Starnet's OpenSSH and putty among many others. You can obtain putty for free from the internet. Putty can be used to login to scott or spock through an encrypted connection. Windows computers within the unit normally have OpenSSH installed for connection. Linux OS typical distributions include ssh clients. Be aware that if you intend to remotely use graphical applications through a SSH connection you will need to use X11 tunnelling through SSH channel. Please refer to the FAQ section in this same guide for instructions.

- Putty download page. <http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html>
- OpenSSH manual. <http://www.ssh.com/support/documentation/online/ssh/winhelp/32/>

4.2 Filesystems

There are some filesystems of which a standard user should be aware. These contain the user data space, application data space, scratch space and user scripts space. All of these filesystems are accessed from the nodes and from authorized desktop PCs.

- *User disk space.* User data is always located under the **/users** directory. This directory is shared within the cluster and can be accessed using the same path from all the nodes and from allowed desktop PCs. The common quota is 10GB/user.
- *Environment and useful scripts.* Under the **/QFcomm** directory you can find some scripts, which are useful for submitting typical calculations. Moreover, this is the place where environment loading scripts are found (petit.profile, info.profile and modules.profile).

- *Application space.* Application software is found under the **/QFsoft** directory. All computational software is found in this directory and can be used by your user account. You can find a detailed list further in this document or in the "Química Física" website (<http://klingon.uab.es>).

- *Scratch space.* Scratch space is locally found on each of the nodes of the cluster and on the frontend servers under the **/scratch** or **/tmp** directory (usually **/scratch** is a link to **/tmp**). These directories are used by the OS and application to store the temporary data which they use for calculations. Contents of the scratch space are automatically deleted when files become old in order not to fill up the disk. Scratch space has no quotas so you can use it if you need to, taking into account its ephemeral existence. There is the possibility to permanently use this node disk space for particular jobs. Please ask to admin@klingon.uab.es.

Moreover, spock and scott have extra disks for scratch purpose called **spockscratch** and **quifiscratch** respectively. Spockscratch is a 1.5TB disk placed in spock and quifiscratch is a 0.5TB disk in scott. The two disks are shared for the entire cluster. There is no quota of the data stored in these disks and there is no backup, they are only to store heavy data temporarily. It is not advised to calculate on spockscratch and quifiscratch directories since the read/write process will be slower through the network than on the local **/scratch** directory of the nodes.

4.3 Computational nodes

Right now (February, 2011), there are 62 computational nodes active in the cluster. Due to traditional restrictions all nodes have been named as "borgs" due to a specific race in the Star Trek World.

Borgs from 21 to 71 (borg21.uab.es-borg71.uab.es) are online at this time and they are found physically at the "Unitat de Química Física". Borgs from 72 to 95 are in SI (Servei d'Informàtica of UAB) and [borg72](http://borg72.uab.cat) (also called locutus.uab.cat) routes all traffic between [borg73-95](http://borg73-95.uab.cat) and quanta through a Virtual Private Network connection. Technical detailed information about the configuration of each node (memory, disk, CPU) can be obtained through the "*pbsnodes -a name of the node*" command (see "submitting jobs section" section). Configuration of a node can change due to hardware failure or node substitution. Recheck using `pbsnodes` command if in doubt. Nodes are associated to queues, which, in general, belong to different research groups.

The nodes are administrated by a TORQUE/PBS server with MAUI scheduler. There are different queues, two queues are shared between the different groups and the other queues are exclusive of a particular group. The next tables show a summary of our queues and computational nodes (February 2011).

Table 1. Queues in our cluster.

Queue	Nodes	CPU (time)	Jobs/user	Group	Architecture	Procs	Net*
qdynamics6	borg[45,53,54,63,64]	-	-	Dynamics	EM64T/AMD64	20	GB
qdynamics7	borg[73-79,82-89]	-	-	Dynamics	EM64T	120	GB/IB
qstruct2	borg[43, 50]	-	4	Struct + serq	EM64T/AMD64	10	GB
qgetab1	borg[44,55-58,65,66]						
qgetab2	borg[80,81,90-93]	-	-	Struct	EM64T	48	GB/IB
qserq1	borg[59,60]	-	2	Serq	AMD64	4	GB
qserq2	Borg67	-	-	Serq	AMD64	4	GB
transmet2	borg[52,61,62]	60	2	Transmet	AMD64	4	GB
transmet3	borg[48,51]	100	1	Transmet	AMD64	10	GB
transmet4	Borg[46,47]	500	2	Transmet	EM64T	16	GB
transmet5	borg[94,95]	-	-	Transmet	EM64T	16	GB/IB
parallel	borg[68-71]	-	-	All	AMD64	16	GB/IB
qproves	Borg[21-32]	-	-	All	i386	12	GB

*GB (gigabit) / IB (infiniband)

Tables 2. Nodes in our cluster.

Node	Queue	Procs/node	Disk (/scratch)*	Mem*	Architecture
borg[21-32]	qproves	1	22GB	0.5GB	i386
borg43	qstruct2	8	885GB	16GB	EM64T
borg44	qgetab1	8	3.7TB	16GB	EM64T
borg45	qdynamics6	8	885GB	16GB	EM64T
borg[46-47]	transmet4	8	885GB	16GB	EM64T
borg48	transmet3	2	165GB	4GB	AMD64
borg50	qstruct2	2	165GB	4GB	AMD64
borg51	transmet3	2	132GB	4GB	AMD64
borg52	transmet2	2	132GB	4GB	AMD64
borg[53,54]	qdynamics6	2	132GB	4GB	AMD64
borg[55-58]	qgetab1	2	132GB	4GB	AMD64
borg[59-60]	qserq1	2	132GB	4GB	AMD64
borg[61,62]	transmet2	4	436GB	8GB	AMD64
borg[63,64]	qdynamics6	4	436GB	8GB	AMD64
borg[65,66]	qgetab1	4	436GB	8GB	AMD64

borg67	qserq2	4	436GB	8GB	AMD64
borg[68-71]	parallel	4	436GB	8GB	AMD64
borg[73-79]	qynamics77	8	780GB	16GB	EM64T
borg[80,81]	qgetab2	8	780GB	16GB	EM64T
borg[82-89]	qynamics7	8	780GB	16GB	EM64T
borg[90-93]	qgetab2	8	780GB	16GB	EM64T
borg[94-95]	transmet5	8	780GB	16GB	EM64T

**Maximum disk and RAM memory (you should take into account that the disk and memory are distributed between the different jobs running in a node and the system requirements)*

You can also check this information at: <http://klingon.uab.cat/catala/cluster/cues-nodes.php>

4.4 User's environment

Whenever you login into spock.uab.cat, scott.uab.cat or you login into a Linux network workstation within the unit a default environment is loaded. This environment consists of transparent access to batch queues, some visualization software, modules environment loading, disk quota and Message of the Day (MOTD) display.

4.5 Disk space quota

Every user on the Physical Chemistry computational cluster can use up to 10.0GB. This quota can be changed under particular conditions. Quota usage can be shown at anytime on your Unix session using the "quota" command.

Group quotas are also enabled for the /QFsoft application space. That is, each research group can compile, develop or modify its own software under the /QFsoft/soft(groupname) directory. Quotas for this space depend on the need of each research group.

4.6 Data Backup

Daily Backup is carried out each night (23.45h) for all data contained on /users directory. Access to each user's own data is only allowed with the intervention of the sysadmin due to security reasons. After asking to the sysadmin, each user can access his/her own data by changing directory to the "/auto/backup/users/username" directory only when logged through scott or spock servers. This is very useful if a file or group of files is accidentally deleted.

4.7 Generation of SSH keys for automatic SSH login

In the Physical Chemistry Unit SSH channels are used for connection among all the machines. SSH provides an encrypted channel where information is not visible to a potential hacker and therefore makes it difficult to sniff password or other information from the network.

One drawback of SSH, and many other login channels, is that, by default, the user is asked to type in a password every time that he/she logs in or whenever he/she tries to execute a command via SSH. This can be resolved easily by the user using SSH keys. SSH keys are stored under the user homedir/.ssh directory. They are called id_dsa and id_dsa.pub or id_rsa and id_rsa.pub depending on the method used to generate these keys.

Note that SSH keys consists of two components, the first is a private file which can only be read by the user and is never transmitted through the network. The pub file is the one that is transmitted over the network in order to verify our identity. If the destination server recognizes this pub identity file, then the server will allow the connection without any password prompting. The steps to configure SSH keys are:

1. Generate SSH keys on the "from" machine. The desktop from where you want to connect. To do this, type:

```
Spock:/users/testuser/.ssh>ssh-keygen -t dsa -b 1024
```

```
Generating public/private dsa key pair.
```

```
Enter file in which to save the key (/users/testuser/.ssh/id_dsa):
```

```
Enter passphrase (empty for no passphrase):
```

```
Enter same passphrase again:
```

```
Your identification has been saved in /users/testuser/.ssh/id_dsa.
```

```
Your public key has been saved in /users/testuser/.ssh/id_dsa.pub.
```

```
The key fingerprint is:
```

```
5c:48:14:06:16:2c:10:69:84:13:43:d1:2e:09:35:3a testuser@spock
```

```
Spock:/users/testuser/.ssh>
```

2. Use the newly created id_dsa.pub file contents to authorize automatic login on the remote machine. That is, copy the contents of this file (the one with pub) to a file name "authorized_keys" in the \$HOME.ssh/ directory on the remote machine. Take into account that the home dir of any user in physical chemistry Linux computers is

shared. In this way, all users will have the same homedir (which is /users/testuser/ in our example) on all the computers that the named user is authorized to login.

3. Test the automatic connection by using the ssh. If everything has been correctly done, no password will be prompted for.

4.8 Submitting jobs to the cluster

Typically, if you use the cluster you will want to carry out calculations using any of the available software. For short time CPU use, you can use your shell interactively for up to 10 minutes (scott and spock). However for longer CPU use time you must use a batch queue system. The batch queue system takes care, once the calculation is submitted, of the allocation of the computational demands of your calculation, control of the execution of the job and its output and of the cleanup of the node in order to make the node available to other jobs. The cluster's queue system is based on OpenPBS/Torque software. Torque controls job queuing and execution through the cluster and allows for non-attended execution and resource control. Torque needs submit scripts where needed resources and job commands are specified. Each user can create his scripts from scratch or by taking a reference script and modifying it. You can find a complete manual at <http://www.clusterresources.com>

4.8.1 Typical queue system commands

Here there are some of the commands you will want to use to interact with the batch queue system. Please check the manpage of each command ("*man command*") for a full list of available options for each command.

- *qstat*. Check use of the queues
- *qsub*. Submit a calculation using a previously created script
- *qdel*. Delete a calculation
- *pbsnodes*. Checks the state of the computational nodes.

On the other hand, there are *infocues* and *infnodes* scripts. These commands print complete information about the queues or nodes. For example:

```
Scott:/users/testuser>infocues transmet5
```

```
#####
```

```
CUA transmet5
```

#####

Grup: Transmet

Borgs: 94, 95

Arquitectura: 64 bits (em64t)

Numero processadors: 16

Numero proc/borg: 8

Maxim hores: no

Maxim calculs(processadors)/usuari: 4

#####

Estat actual de la cua

#####

Calculs corrent: 7

Calculs en cua: 1

Processadors usats: 16

Processadors lliures: 0

quanta.uab.es:

Req'd Req'd Elap

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Memory	Time	S	Time
--------	----------	-------	---------	--------	-----	-----	--------	------	---	------

99509.quanta.uab user1 transmet job-name1 971 1 -- -- -- R 240:0

borg95+borg95+borg95+borg95

100500.quanta.ua user2 transmet job-name2 3599 1 -- -- -- R 27:49 borg94+borg94

100501.quanta.ua user2 transmet job-name3 3625 1 -- -- -- R 27:49 borg94+borg94

100555.quanta.ua user1 transmet job-name4 15406 1 -- -- -- R 16:09 borg94+borg94

100660.quanta.ua user4 transmet job-name5 25395 1 -- -- -- R 06:03 borg94+borg94

100664.quanta.ua user4 transmet job-name6 17794 1 -- -- -- R 05:11 borg95+borg95

100665.quanta.ua user5 transmet job-name7 17882 1 -- -- -- R 05:09 borg95+borg95

Furthermore, *infnodes* prints the free procs/node of a particular queue.

Scott:/users/testuser>infnodes transmet5

#####

CUA transmet5

(node: procs totals // procs lliures)

#####

borg94: 8 // 0

borg95: 8 // 0

```
#####
```

```
Scott:/users/testuser>
```

You can also check the information for all the queues of a group executing “*infocues groupname*”.

4.8.2 HomeMade scripts

For heavily used applications some scripts have been created. You can use these scripts if you do not want to create your own scripts by hand. Homemade scripts are:

- *adf.pl* To submit ADF calculations.
- *charmm.pl* To submit Charmm calculations.
- *cpmd.pl* To submit CPMD calculations.
- *crystal.pl* To submit CRYSTAL09 calculations.
- *g03.pl* To submit Gaussian 03 calculations.
- *g09.pl* To submit Gaussian 09 calculations.
- *g98.pl* To submit Gaussian 98 calculations.
- *gamess.pl* To submit Gamess calculations.
- *jaguar.pl* To submit Jaguar calculations.
- *modeller.pl* To submit Modeller calculations.
- *molpro.pl* To submit Molpro calculations.
- *nwchem.pl* To submit NWchem 5.1.1 calculations.
- *nwchem6.pl* To submit NWchem 6.0 calculations.
- *orca.pl* To submit ORCA 2.8.0 calculations.
- *qchem64.pl* To submit QCHEM calculations.
- *vasp.pl* To submit VASP4.6 calculations.
- *vasp5.pl* To submit VASP5.2 calculations.

Type “*software.pl*” at your command prompt to learn how to use these scripts. The general form is:

```
software.pl -q name_queue -n procs input ./output
```

You can also specify the net using “*-net GB or IB*” option. Moreover, you can specify the x86_64 architecture with “*-64*” option, however this is not necessary for *g09.pl*, *molpro.pl*, *orca.pl*, *nwchem6.pl*, *crystal.pl*, *adf.pl*, *qchem64.pl* and *vasp5.pl*.

You will find more information at: <http://klignon.uab.cat/catala/faqs/faq14-pbs.php>

4.8.3 Create your own submit script

In order to submit jobs that don't have any homemade script, you must edit your own submit script. The general structure of such a script should be:

```
---Begin Contents---  
#PBS -q name of the queue  
#PBS -l nodes=number of procs  
#PBS -k oe  
#PBS -M mail address  
#PBS -N Name to identify the job  
<Commands of the job>  
---End contents---
```

To understand "nodes=" specification some examples are useful. Let's imagine you only need 1 processor, then this particular line will be: "#PBS -l nodes=1". If you need 4 processors and it is not important if they are allocated in different nodes within the same queue then: "#PBS -l nodes=4". On the other hand, if you need 4 processors and you need them in the same node, then you MUST use the ppn directive: "#PBS -l nodes=1:ppn=4". Some other combinations are possible, like, for instance: "#PBS -l nodes=1:ppn=4+1:ppn=2+2". In this case we are asking for four processors within one node plus two other processors within one node plus 2 other processors that may or may not be in the same node.

Naturally, <Commands of the job> is heavily dependent on the application choice. However, you can use Modules software to load the appropriate environment for your application and directly execute the desired binary. For instance:

```
---Begin Contents---  
./QFcomm/modules.profile  
module load software  
export SCRATCH=/tmp/scratch  
mkdir $SCRATCH  
cd $SCRATCH  
exe <input> output  
---End Contents---
```

The first line makes "Modules" software available to the running job, the second line loads the needed environment for X software and the final lines run the calculation on a

scratch directory. There are modules available for the most common applications. You can check it using *"module avail"* or *"module av"* at your prompt.

Use *"module help"* to learn more. If you can find no module for your application, ask the system administrator. Remember that using *"module list"* you can check the loaded modules.

Notice that a SCRATCH directory is created and the job runs on it. The /scratch is a local directory, not shared by the network. It is recommended to prepare jobs that run on /scratch to avoid slow calculations that run over the network, especially for the borgs placed in the Servei d'Informàtica.

You will find more information about the script.pbs file at <http://klignon.uab.cat/catala/faqs/faq14-pbs.php>

4.8.4 Submitting Parallel Calculations

Parallel jobs are somewhat more complex to run. Most of the available codes that can run parallelly are compiled using an MPI layer.

In particular, in the quanta cluster, there are different implementations of MPI layers. For instance, **MVAPICH2** implementation of MPICH is used as nodes that are advised to use for parallel calculations have Infiniband interconnects installed. MVAPICH2 is an implementation of **MPICH2** which is optimized in order to obtain the maximum efficiency for such networks. To know more about MPICH2 basic usage and specific MVAPICH2 options, please take a look at:

- MPICH2 <http://www.mcs.anl.gov/research/projects/mpich2/documentation/files/mpich2-1.3.2-userguide.pdf>
- MVAPICH2 http://mvapich.cse.ohio-state.edu/support/mvapich_user_guide-1.2rc1.html

However, for Intel 64bits architectures, the most used parallel implementation is **OpenMPI**. The major part of the parallel software installed for Intel 64 bits and Infiniband is compiled with OpenMPI. You can find more information at :

- OPENMPI <http://www.open-mpi.org/>

Historically, MPICH2 and MVAPICH2 layers are used with PGI compilers which are considered better for AMD64 architectures while OpenMPI layer is used with Intel Fortran Compiler which, obviously, is the best compiler for Intel architectures.

For typical jobs there is a set of scripts available. These are *g03.pl*, *g98.pl*, *nwchem.pl*, *cpmd.pl*, *vasp.pl*, *molcas.pl*, *molpro.pl*, *crystal.pl*, *charm.pl* and can submit parallel calculations using 2,4,6,8 processors. These scripts can be used also for standard parallel (that is, non optimized software with "slow" interconnects). One or the other are automatically detected depending on the queue that the job is submitted to.

Moreover, when one of these scripts is used a file named "script.pbs" is created. This file contains all the definitions that are needed for a parallel job. You can also manually edit this script and adapt it to your needs if the predefined ones are not suitable to your job. Parallel jobs prerequisites OpenMPI, MPICH2 and MVAPICH2 implementations need some things to be set up for parallel execution. These are explained in the corresponding manuals which have been just indicated.

Although the script.pbs file is made to facilitate the user work and all the information is correctly placed in this file, it might be useful to indicate the important points to use parallel applications over OpenMPI, MPICH2 or MVAPICH2 layers.

- For MPICH2 and MVAPICH2 layers, create a file called ".mpd.conf" in your homedir. contents of this file must be, at least: "MPD SECRETWORD=your secret word here" Once the file has been created you must set its read/write permissions. Set permissions in order that only your user account can read or write this file and no one else can. This can be done using "cd chmod 600 .mpd.conf"
- Set up your ssh pub keys to be authorized in all nodes. You can check if the sysadmin has done this work for you trying to access by ssh protocol to any node of the cluster without introducing your password. If not, issue the following command:

```
Spock:/users/testuser/.ssh>ssh-keygen -t dsa -b 1024
Generating public/private dsa key pair.
Enter file in which to save the key (/users/testuser/.ssh/id_dsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /users/testuser/.ssh/id_dsa.
Your public key has been saved in /users/testuser/.ssh/id_dsa.pub.
The key fingerprint is:
5c:48:14:06:16:2c:10:69:84:13:43:d1:2e:09:35:3a testuser@spock
Spock:/users/testuser/.ssh>
```

This will create the files "id_dsa" and "id_dsa.pub" in the \$HOME/.ssh/ directory. Check it. Now copy or add the id_dsa.pub file to the "authorized_keys" file under the same

directory. If done correctly, this will allow you to login on every node of the cluster without the need to type the password but, otherwise, checking the identity key.

4.8.5 Compiling Parallel applications with OpenMPI/MPICH/MVAPICH

Most typical chemical software is compiled, configured and prepared by the system administrator. However, in some cases, computational code undergoes heavy development by end users. In these cases, you may need to compile software quite often. In the case you need your software to be run in parallel you will need some parallel implementation layer. In quanta cluster there are OpenMPI, MPICH2 and MVAPICH2 available for such purposes. OpenMPI, MPICH and MVAPICH are open implementations on MPI (Message Passing Interface) standards. It is advised to take a look at the user guides of these implementations before going further. MVAPICH is an MPICH implementation which is optimized for Infiniband hardware and takes advantage of high transmission data rate and low latency. Our OpenMPI compilation is also optimised to be used with Infiniband efficiently.

In this user guide, small information about OpenMPI, MPICH and MVAPICH on quanta cluster is provided. However for a complete user guide on how to compile on the MPI layers please take a look at the user guide pointed out above.

5 Available Software

There is much software apart from that included in a typical distribution which you will need in order to carry out research. As mentioned previously, this software is found under the **/QFsoft** directory. Notice that computational chemistry software is usually under a license. These licenses occasionally are associated to fees paid by the research groups. Some of them can be eventually tied to a unique research group. Also, note that some version of the following software may be quite old. If you need an update of some software package please contact admin@klingon.uab.es.

5.1 Chemistry/scientific software

- **ADF Suite.** Electronic structure calculations. Available version: ADF 2010.
- **Amber.** Molecular Mechanics. Available version: Amber 11.
- **AUTODOCK.** Suite of automated docking tools. Autodock4 and autogrid4.

- **Babel.** Molecular structure formatting tools. Available version: OpenBabel 2.2.3.
- **Cambridge Structure Data Base.** A repository of small molecules crystal structures. Only for scott. Last version: 2009.
- **carma.** Molecular simulation analysis.
- **CHARMM.** Molecular simulations program. Available versions: c33b1 and c35b1.
- **Chimera.** Molecular Visualization. Available versions: Chimera 1.4 and 1.5.2.
- **CPMD.** Molecular Dynamics. Available versions: CPMD 3.11 and CPMD 3.13.
- **Crystal.** Periodic systems calculations. Available Version: Crystal 06 1.0.2, Crystal 09 1.0.1.
- **ECCE.** Molecular visualization for NWchem. Available Version: 3.2.4.
- **Gabedit.** Molecular visualization. Available version: 2.0.7.
- **GAMESS.** Electronic structure calculations. Available versions: 11.1.08 and UK version.
- **Gaussian Suite.** Electronic structure calculations. Available versions: 98 A.9, 03 D.01 and E.01, 09 A.02 and B.01.
- **Gaussrate.** Interface between POLYRATE and GAUSSIAN. Available version: 9.7.
- **Gaussum.** Gaussian output treatment scripts. Available version: Gaussum 0.4.
- **GOLD.** Molecular docking software. Available versions: Gold 4.1, Gold5.0.
- **Goldmine.** Molecular docking software. Available version: Goldmine 1.0.1.
- **Gopenmol.** Molecular Visualization. Available version: gOpenmol 3.00
- **Gromacs.** Molecular Mechanics. Available version: Gromacs 4.0.4.
- **Jaguar.** Electronic Structure calculations. Available version: 7.7.
- **JCHEM suite.** Programs and toolkits for many cheminformatics tasks. Available version: 5.4.
- **jmol.** Molecular Visualization. Available version: 12.0.3.
- **Macromodel.** Molecular mechanics program. Available version: 9.8.
- **Maestro.** Molecular Visualization. Available version: 9.1.
- **Marvin.** A collection of tools for drawing, displaying and characterizing chemical structures, substructures and reactions.
- **Mathematica.** Program to compute results. Available version: 6.0.
- **MGLtools.** Molecular visualization. Available version: 1.5.4.
- **MIDAS.** Molecular Interactive display program.
- **MINRMS.** A tool for determining protein similarity.
- **MM392.** Molecular mechanics.
- **MMABIN98.** MMABIN for Gaussian98.
- **MMTK.** Molecular modelling toolkit. Available version: 2.4.10 and 2.6.1.
- **MNDO97.** Electronic structure calculations with semiempirical methods.
- **MNDO99.** Electronic structure calculations with semiempirical methods.

- **Modeller.** Program for protein structure modelling. Available version: 9.8.
- **Mogul/Quest/Mercury.** Cambridge structural database user interface.
- **Molcas.** Electronic structure calculations. Available version: Molcas 6.4.
- **Molden.** Molecular Visualization. Available versions: 3.7, 4.7 and 4.8.
- **MolecularTools5.0 suite.** APBS for solution of the Poisson-Boltzmann equation, Tinker and Force Field Explorer for molecular engineering and visualization. Available version: 5.0.
- **Molekel.** It is an open-source multi-platform molecular visualization program. Available versions: 5.2 and 5.3.
- **Molpro.** Electronic structure calculations. Available versions: Molpro 2010.1.
- **Molscript.** Visualization software. Available versions: 2.1.2.
- **MOPAC.** Semiempirical molecular orbital package. Available version: 6.
- **NAMD.** Molecular Dynamics. Available versions: NAMD 2.6 and 2.7.
- **NBO.** Molecular orbital calculations. Available version: 5.0
- **NWchem.** Electronic structure calculations. Available versions: NWchem 5.1 and NWchem6.0.
- **ORCA.** Electronic Structure calculations, DFT. Available version: Orca 2.8.0.
- **P4VASP.** Visualization software for VASP. Only in spock.
- **PDB2PQR.** Python software package that prepares structures for continuum electrostatics calculations, converting protein files in PDB format to PQR format.
- **Polyrate.** Chemical Reaction Rates calculation. Available version: 9.7.
- **QCHEM.** Electronic Structure Calculations. Available version 3.2.
- **QMPot.** Electronic Structure Calculations.
- **SAPT.** Electronic Structure Calculations. Available version: 2006.
- **Schrodinger suite.** Contains Jaguar, Macromodel and Maestro.
- **Turbomole Suite.** Electronic structure calculations. Available versions: Turbomole 5.6 and 6.0.
- **VASP.** Electronic structure calculations for surfaces. Available versions: 4.6 and 5.2.
- **Viewmol.** Molecular Visualization. Available version: Viewmol 2.4.1
- **VMD.** Molecular visualization. Available version: VMD 1.8.7
- **WORDOM.** Molecular simulation analysis and manipulation. Available version: 0.21.
- **XAIM.** Graphical user interface to compute aspects of the Atoms in Molecules theory. Available version: 1.0.
- **Xdrawchem.** Molecular visualization. Available versions: 1.8 and 1.9.9.
- **XMGRACE.** Graph plotting tool. Available version: 5.1.

5.2 Development Software

- **ATLAS.** Atlas libraries. Available version: 3.6.0.
- **BLAS.** Blas libraries from GNU and MPICH2 compilers.
- **FFTW.** Fourier transform libraries. Last Version: fftw 3.1.2
- **GA.** Global Arrays Toolkit, a "shared-memory" programming interface for distributed-memory computers. Version: 4.1 for mvapich2/pgi7.0.
- **GNU-comp.** GNU compilers. 32 bits. Version: 4.5.
- **IFC.** Intel Fortran and C/C++ Compilers, plus MKL libraries. Last Version: 11.1.072.
- **MKL.** MKL BLAS and LAPACK libraries from IFC. Last version: 11.1.072.
- **Modules.** Unix environment loader. Last version: Modules 3.2.3
- **MPICH.** Parallel computation layer, gigabit interfaces. Available versions: 1.2.7 (for GNU and PGI compilers).
- **MPICH2.** Parallel computation layer, gigabit interfaces. Available versions: 1.0.6 (for PGI, GNU and IFC compilers).
- **MVAPICH.** Parallel computation layer, Infiniband interfaces. Available version: Mvapich 0.9.9 (for PGI compilers).
- **MVAPICH2.** Parallel computation layer, Infiniband interfaces. Available versions: 1.0, 1.2 and 1.4 (for PGI and IFC compilers).
- **NAG Fortran 95 Compiler.** Last Version: NAGF95 5.0
- **OpenMPI.** Parallel computation layer, Infiniband interfaces. Available versions: 1.2.4 and 1.4.2 (for PGI and IFC compilers).
- **PGIWKST.** Portland Fortran and C/C++ Compilers. Available versions: 7.0 and 8.0. Only for SCOTT and borg70.

Please note that software versions change constantly and that some listed version may be out of date.

5.3 How to use the software

For most of the typical computational chemistry and compilers you can find a modules that, when loaded with *"module load XXXX"*, load the appropriate environment to easily run that particular software. Remember to use *"module av"* to see all the modules installed. Some others are found in the default user PATH.

5.4 Scott and spock software

Some software is installed locally and spock and scott and it is not in /QFsoft directory. This is not Chemistry software but it is important for other task. You have to take into account spock is a 64 bits and scott a 32 bits especially with the compilers.

- **acroread**. Acrobat Reader in scott and spock.
- **display** (imagemagick). To display images. In scott and spock.
- **firefox**. Web browser. In scott and spock.
- **Gnu compilers**. gfortran and gcc compilers. In scott and spock.
- **gnuplot**. To plot graph. In scott and spock.
- **GIMP**. To display and modify images. Only in spock.
- **lynx**. Web browser in text format. In scott and spock.

5.5 Non-default environments

It is expected that at some stage standard environment will not be enough for your needs. You can modify the default environment to suit them in different ways. The first and most direct is to edit and modify some user environment files such as: .bashrc and .bash profile, .alias, .vimrc and some others.

“.bashrc” and *“.bash_profile”* are located in every user’s home directory if the users uses the BASH shell, which is the default at Química Física. *“.bash profile”* is parsed every time a user logs in and *“.bashrc”* is executed if you’ve already logged into your machine and open a new terminal or a new bash instance typing /bin/bash. Therefore, every modification on your shell environment that you define in *“.bash_profile”* will have effect at every new login in scott or spock, so you do not have to bother again modifying you environment by hand. Note that KDE or GNOME login does not execute *“.bash_profile”* in your PC Desktop, while when you execute a terminal in your Desktop session, *“.bashrc”* is always executed. Moreover, to avoid problems due to SSH bugs, do not introduce commands which print information in *“.bashrc”* file, always use *“.bash_profile”* for these commands. You can alter these files either by loading a non system-wide default module which you use, altering your PATH variable, or forcing the shell to parse an *“.alias”* file, for instance. The *“.alias”* file is usually used to define aliases for long or uncomfortable commands, however it is not used as default because you can define alias into the *“.bashrc”* and *“.bash_profile”* files. For instance, an alias definition can be: *“alias ls=“ls -lahRts””*, which, by the way, list in format all files, ordered by size, which are ordered

by date of modification. You can define as many aliases as you need. A common alias is the one which allows ssh access to spock and scott only using "scott" or "spock" as commands and without asking the password. These aliases are necessary since the Linux SO of your PC Desktop confuses the local and the network user of your system (in fact, both users have the same uid) and it always recognize you as user.local, although you are logged as network user. For instance:

```
alias scott='ssh -X -i /users/testuser/.ssh/id_rsa testuser@scott.uab.es'  
alias spock='ssh -X -i /users/tesuser/.ssh/id_rsa testuser@spock.uab.es'
```

The ".vimrc", on the other hand, defines how the different features of the vim editor are loaded or used when a particular user edits a file. Please refer to the vim editor homepage for a manual, or simply type "man vim" or "vimtutor".

6 Your Linux Workstation

The general policy in the Physical Chemistry Unit, at least in the computational part, is to have one computer per user. This means that when arriving at the unit you will be able to use one computer exclusively. Typically, user desktop computers can run WindowsXP or Linux(SuSE) Operative Systems.

OpenSuse is the recommended Linux distribution due to its user-friendly configuration interface and its hardware detection engine. In general normal users are not expected to have administrator privileges and any modification to be carried out on the system need sysadmin intervention. Moreover, Windows XP SP2 or SP3 SO is running on a virtual machine within Linux. This Virtual machine is accessible for all users working on a particular workstation. Windows XP virtual machine is stored under the Linux tree while the machine is configured in such a way that the user can save documents in a folder shared between Windows guest and the /home partition on the Linux host. This scheme is designed to maximize easiness at backup time and/or system reinstallation.

When booting the PC OpenSuse Linux S.O. will be booted. If everything proceeds correctly you will be prompted for a login and a password. These will be the same that you use to log in spock or scott, as passwords and users information is centrally managed. However,

you will also have a “*user.local*” user, this user is located in your computer and it is not controlled by our central server.

6.1 Disk space on your workstation

The basic idea is that software structure and user data will be the same either you login on your desktop or on scott/spock. In fact user and group management is centralized. This means that your username and password will be the same for scott, spock, or your workstation and the same for disk space. That is:

- Application Software. Application will be imported to each machine from the **/QFsoft** Directory. You will be able to use as if logged in spock or scott. Moreover, the most common visualization software: **Gaussview**, **Molden** and **VMD** are installed locally in your machines (/opt directory). You can call these programs using: *gview.local*, *molden.local* and *vmd.local* commands.
- Scratch Space. Similarly, scratch space will be locate under the **/scratch** or **/tmp** directories. Take into consideration that contents on these directories are volatile.
- Environment Scripts. Also **/QFcomm** directory will allocate environment related scripts.
- Home Directories. Home Directories will be under the **/users** directory. However, in user desktop PC, the corresponding user also has access to a personal directory under **/home** which has larger disk space and is local. This space is meant to hold data which is not often used or is too large to be kept under the /users due to quota restrictions.

6.2 Workstation Data Backup

There is a backup system installed with a total capacity of 1.5TB in order to store important data located on your workstation just in case the workstation dies. All connections used for the backups are encrypted and SSH keys must be setup in the workstation users homedir in order for the backup system to work properly. To configure the backup, follow the next steps:

- 1) Create .backup directory in /users (*mkdir .backup*).
- 2) Create “*files*” and “*host*” files into *.backup/* directory. In “*host*” file, there is the name of your machine (execute “*hostname -f*” if you are not sure). In “*files*” file, you have to specify the path of the directories you want to backup. For instance:

/home/user/Documents

/home/user/Doctorate

Please, do not specify the entire home directory. We do not have enough backup for all the PC Desktops, so, choose only the important information in your machine.

- 3) Create the `id_dsa.backup` keys. When “*Enter file in which to save the key*” appears, answer “*/user/XXX/.backup/id_dsa.backup*”. Example:

```
Spock:/users/testuser/ssh-keygen -t dsa
```

```
Generating public/private dsa key pair.
```

```
Enter file in which to save the key (/users/testuser/.ssh/id_dsa): /user/testuser/.backup/id_dsa.backup
```

```
Enter passphrase (empty for no passphrase):
```

```
Enter same passphrase again:
```

```
Your identification has been saved in /users/testuser/.backup/id_dsa.backup
```

```
Your public key has been saved in /users/testuser/.backup/id_dsa.backup.pub.
```

```
The key fingerprint is:
```

```
5c:48:14:06:16:2c:10:69:84:13:43:d1:2e:09:35:3a testuser@spock
```

- 4) Add “*/users/XXX/.backup/id_dsa.backup.pub*” file into “*/users/XXX/.ssh/authorized_keys*”. Be careful, it is important that you add the new key but you don’t have to delete your other keys stored in `authorized_keys` file.

Please follow these instructions carefully and ask to the sysadmin when you finish the backup configuration. Backup will take place automatically every night.

Access to this data is allowed without the intervention of the sysadmin as the data is the one stored locally in your PC. When logged in `spock` or `scott`, each user can access to his/her data by changing to “*/auto/desktop_backup/home/name_of_the_machine/*” directory.

Check this information in Catalan also at <http://klignon.uab.cat/catala/fags/faq12-backup.php>

6.3 Running virtual Windows XP

You will be able to run Windows XP Virtual machine only if you are the main user of the workstation. That is, while you can eventually log in any of the Linux machines using remote authentication, Windows XP use needs a local disk space on the machine which any user will be able to access only after a local user has been created on that machine.

6.3.1 The Windows XP Environment

As Windows XP runs on a virtual machine there are some particularities that must be pointed out:

- User data must be saved under the shared network disk unit between Windows and Linux if you want to access to this information by your Linux host. This disk unit corresponds to a folder which is shared between the guest Windows OS and the host Linux OS. If this network unit does not appear please ask the sysadmin. The common name of this directory is **windata**.
- Documents and Settings folder is stored under the D: network drive. This drive is a virtual one and it should only contain the user windows configuration data and the user information.
- Guest-Host Interaction allows for some interaction modes. For instance, Ctrl-F switches to Full Screen mode for the Guest, while Ctrl-L switches to/From Seamless Mode. Just give it a try and choose that on which you feel more comfortable.
- You will not be able to burn a CD under the windows XP virtual system. Use Linux CD burning tools for that purpose (i.e. K3B, cdrecord)
- It is advised to use OpenOffice Offimatic Suite as the main text processor, spread sheet, and presentation application. OpenOffice Suite exists for Linux and Windows, is open source, and can open the same documents under both OSes.

6.4 Submitting calculations to your desktop

If you ask to the sysadmin, you can also submit a calculation to your PC as the structure of a desktop PC is similar to that of a computational node. It is not advised to submit a job in your PC when you are working on it because all the other computer functions will be slowed down if a job is running on it.

To avoid the proliferation of queues, the default is that the PC desktops cannot be used as calculation nodes and only the sysadmin can activate the possibility to submit calculations to your desktop if you really need it.

To submit a job, you just need to substitute the queue name for your desktop short name (this can be obtained through the *"hostname -s"* command). Moreover, you are not the only user who can submit calculations to your desktop but other users can submit calculations to your PC with your permission.

6.5 Network dependent structure

All the previously explained structure obviously means that when logged in you are working through the network and that the network is needed in order to work. This means local dependency. At the login time you will see that a (username).local account exists. This account is to be used in case network fails, or servers have to be stopped for maintenance tasks. This local user account can work with no dependency from the network. Please see *"Should the network go down"* and *"There is a scheduled maintenance stop, what must I do?"* sections for detailed instructions. The local username has the shape of username.local and will log in the /home dir as the \$HOME directory. Although the local user account is to be used only when network or servers fail or are scheduled to be disconnected and, in principle, it is not intended for everyday use, you can also access to the Windows XP virtual Machine with your local user. However, some users may prefer to use the local user because the storage capacity is larger in /home than the quota in /users and they develop and execute local programs installed in their computers.

7 Your Windows Workstation

It is possible, to have WindowsXP or Windows7 OS as the sole Operative System running on your personal desktop computer, for those who are not, nor want to be, familiar with the Linux environment. This user guide is mostly aimed toward Linux users.

All the new PC Desktops have a Windows configuration from UAB Servei d'Informàtica. In principle, Windows operative system is only recommended for those users that have to do more offimatic tasks with Office environment than computational work. Windows users have also administrative permissions and can install, erase and change the software in their machines.

Windows computers configured by Servei d'Informàtica of UAB have connection to the UAB network which provides net disks where you can store and backup data (see <http://www.uab.es/si> for more information). On the other hand, nowadays, there is not an automatic Data Backup for Windows users in "Unitat de Química Física". It is strongly recommended to backup your relevant windows data once per week in an external device such as an USB disk.

7.1 Windows software

UAB has licenses of several Windows software. To simplify the access to this software, we have different Windows licensed and free software in klingon.uab.cat server through samba protocol. This means that any Windows machine with an IP from Química Física can connect to klingon and download and install the software. Next, there is a list of the Windows software saved in klingon (February 2011):

- **7Zip.** Data compressor program.
- **Adobe Acrobat Professional.** Available versions: 7.0 and 9.0.
- **Antivirus.** Trend Micro PC-Cillin free and licensed. Malware-byte's Antimalware. CC-cleaner.
- **CDBurnerXP.** Free CD and DVD burning software. Available version: 4.3.8.
- **ChemBioOffice Suite.** Chemistry and offimatic suite. Available versions: 6.0, 7.0 and 12.0.
- **ChemCraft.** Molecular Visualization. Available versions: 3.22.
- **DaemonTools.** To mount iso images.
- **DataRecovery.** Data Recovery Software. Softonic.
- **DiVX.**
- **End Note.** Tool for publishing and managing bibliographies. Available version: 9.0.
- **GIMP.** Free image editing program. Available version: 2.6 and 2.8.
- **GoogleEarth.** Explore the world in 3D. Version: 6.
- **Hijackthis.** Trend Micro HijackThis is a free utility that generates an in depth report of registry and file settings from your computer. Available version: 2.0.4.
- **Integrat3.** Programs need by Laboratory Integrat III (teaching).
- **MOLDEN.** Version for Windows.
- **MolDraw.** Molecular visualization program. Available version: 10335.
- **Mozilla-Firefox_cat.** Mozilla browser in Catalan. Available version: 2.0 and 3.6.
- **Mozilla-Thunderbird_cat.** Thunderbird email application in Catalan. Available version: 1.0.7 and 3.1.7.
- **Office Suite.** Available versions: 2003, 2007 and 2010. 2010 has as minimum requirements Windows XP SP3 SO and an IP from UAB. The other versions require Windows XP SO and the serial number provided by the sysadmin.
- **OpenOffice.** OpenOffice Suite for Windows. Available version: 3.2.
- **Paintshop Pro.** Image editing program. Available version: 7.0. Only in French.
- **Povray.** Program to render images. Available version: 3.6.
- **Reference Manager.** Tool for publishing and managing bibliographies. Available version: 11.0.

- **SciFinder.** Available versions: 2006, 2007 and an explanation to use the SciFinder web on-line.
- **Skype.** Available version: 5.1.
- **SSH Secure Shell.** An Open SSH client for Windows. Available version: 3.2.9.
- **Spybot.** Searches whole computer or just a certain file for malicious software commonly missed by anti-virus programs. Available version: 1.6.2.
- **Tunnelier.** An SSH client for Windows.
- **VIM.** Vim for Windows. Available version: 5.3.
- **VMD.** VMD for Windows, molecular visualization program. Available version: 1.8.7.
- **VirtualBox.** Virtualbox tool to create a Virtual Machine in a Windows host. Available version: 4.0.2.
- **WinZip.** Windows data compressor. Available version: 8.0.
- **Windows XP Catalan Patch.** Patch to translate Windows XP to Catalan language.
- **Winrar.** Windows data compressor. Available version: 3.0.
- **X-Win Pro.** Old licensed X11 Emulator for Windows. Available version: 5.3.
- **XMING.** Free and stable X11 Emulator for Windows. Available version: 6.9.

8 Klingon.uab.cat server

Klingon.uab.cat or qf.uab.cat is our web, email, printers and Windows software server. All the users of “Unitat de Química Física” are entitled to have an email address while temporal visitors can have an alias to a klingon.uab.cat email address.

Note that klingon is also running in Linux and you can access to it by SSH protocol as to the other servers, but only with IPs from the Unitat.

8.1. The web

Nowadays, our web is wrote in HTML//PHP. You can find there an updated directory of the Unitat members, teaching information, details about the seminars that are organized by the Unitat, links to the Research group’s website, etc. There are news about the new programs installed, the cluster configuration, the printers shared in the Unitat and a FAQs section. Moreover, you can find relevant information about the Administrative part of our Unitat. Finally, there is a link to openwebmail to check the mail.

All the members of the Unitat are also entitled to have a personal webpage in klingon. You can create your webpage with html or php codes in the public_html directory of the \$HOME directory of klingon. Ask to the sysadmin to publish your webpage.

8.2. The mail

As an Unitat member you will have an user@klingon.uab.cat (or .es) email address. Remember that you need also an user@uab.cat email address but for acquire this address you have to be in contact with Servei d'Informàtica or CAS (Centre d'Assistència i Suport: 2100) of UAB.

The recommended way to check the mail is to have a Thunderbird program in your computer and to download the mail using a POP3 protocol. There is also the possibility of check the mail using openwebmail (the link is located in klingon.uab.cat web), in the web browser, but the system will be slowed down if many users access to openwebmail at the same time.

To configure Thunderbird email application, check the information in klingon.uab.cat or ask to the sysadmin (<http://klingon.uab.cat/catala/faqs/faq2.php>).

It is worth mentioned that we receive huge quantities of SPAM mail. Spamassassin filter is running and identifying the spam mails but this means an extra work for the computer and it is never possible to mark all the spam. Please be careful with spam mails and never answer to any email asking for your user and password.

Remember the next alias addresses (also at <http://klingon.uab.cat/catala/directori.php>):

Table 3. Shared addresses.

Address (@klingon.uab.cat)	Description
grup_GROUP*	All the group
matxaques_GROUP*	PhD students and postdocs
permanents_GROUP*	Professors
insiders_GROUP*	RyC, JdC, lectors and professors
visitants_GROUP*	Visitors
tot_qf	All the "Unitat de Química Física"
docents_qf	Everybody but the visitors
matxaques_qf	All the PhD students and postdocs
permanents_qf	All the professors
insiders_qf	All the professors, lectors, RyC and JdC

visistants_qf	All the visitors
exp_qf	All the experimental groups
teorics_qf	All the theoretical groups

**GROUP=domenech, dynamics, igg, struct, transmet, serq.*

8.3 The printers

Klingon serves all the printers of the Unitat with LPD protocol and using a SAMBA server to share the printers to Windows and Linux systems without compatibility problems. There are three printers directly connected to the computer: HP Laserjet 2100, HP Laserjet 2430 and HP Laserjet P4015. You can find more information about the printers and how to install them at: <http://klingon.uab.cat/catala/faqs/faq1.php>

9 Frequently asked questions

- *What is X11 tunnelling and how can I use it?*

X11 tunnelling is a secure way to display a graphical application output on a remote connected SSH client. That is, you are connecting from computer "A" to spock or scott and you happen to use Molden application. Molden has a graphical user interface which the user must interact with. This display must not be shown on spock screen but on the computer "A" screen which is the one that has the user in front of it. Therefore you must redirect graphical output to computer "A". This is done by tunnelling X11 connection, which uses the same SSH channel that is being used for SSH connection to take the graphical display from spock to computer "A", in our case. X11 tunnelling can be easily activated through "putty" or Starnet openssh settings menu.

- *Should the network go down?*

Network and servers can go down unexpectedly. This may happen, either due to a failure of the electrical supply or to a malfunction of any of the hardware implied in the computer services. If that is the case, the Linux session will just hang as it need the data to be read and written over the network. If the network/service return in short time (in the order of seconds) you will be able to retake the session. If the failure is serious (ask the sysadmin) then you will have to use the local user login in order to be able to work. You can go to the login screen at anytime using the (ctrl-alt-backspace) combination or rebooting your computer.

- *There is a scheduled maintenance stop, what must I do?*

If you receive a mail announcing a scheduled maintenance stop for whatever reasons in which affect only the network or computer services and not the electrical supply you will be only able to work using the local user. Make sure not to have any open session at the scheduled time and to have your computer either at the login stage or shutdown. After the maintenance stop has taken place you can work with the local user with normality. Once the network/services are up again you will only have to login again using the normal user.

- *Where is my data?*

Data physical location is structured in order to minimize data recovery time. There are some suggestions to be taken into account:

1) *Linux Local Data*. Linux Local Data is stored under the `/home` directory. This directory is the default `HOMEDIR` for a user.local account.

2) *Linux Network Data*. Linux Network data is stored under the `/users` directory. This directory is the default `HOMEDIR` for the standard user account. Diskspace in this directory is under quota management. Quotas are defined to a standard 10GB space although this can be modified in case of particular user needs.

3) *Windows Virtual Machine User Data*. Windows User Data is stored also locally. The directory `/home/$user/windata` is used for data shared between Linux and windows operating systems. It can be accessed by any of the operative systems. However, you must AVOID accessing the same file at the same time as this can cause data CORRUPTION.

You will find more FAQs at <http://klingon.uab.cat/catala/informacio.php>