Jacobs University Bremen

Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)
www.clamv.jacobs-university.de

CLAMV Primer

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Contents

1 Introduction - What is CLAMV ?

CLAMV (Computational Laboratory for Analysis, Modeling and Visualization) is the center for scientific computing at Jacobs University. It serves as support initiative for computationally oriented disciplines and provides the platform for exchange and cooperation in applied computing. CLAMV services cover the following topics:

Software for courses and projects in computationally oriented disciplines
Computer Teaching Labs
High Performance Computing (HPC)
Data Storage
Visualization
WWW-Presentations and Data Bases
Research Group Computer Integration

CLAMV was founded in April 2002 by 12 faculty members and is now used by more than 750 users (150 faculty/staff, 600 students). It is used for (advanced undergraduate and graduate) teaching as well as for research.

2 Software

CLAMV provides access to a huge pool of software for teaching and research in computationally oriented disciplines including the necessary license management. The software pool includes applications for the following topics:

Mathematics
Data Analysis
Visualization
Molecular Science
Life Science
Earth and Space Science
Software Development

More information about installed software can be found on the CLAMV webpage. Most software is for the Linux operating system. Some frequently requested software packages are also available for other operating systems like MS Windows or MAC OS.

2.1 Software for Linux

The easiest way to get access to the software pool is through the computers in the CLAMV Teaching Lab. With a valid CLAMV account the CLAMV Teaching Lab computers can be used from anywhere on campus by remote access. See next section for more information about CLAMV Teaching Lab and CLAMV account.
Linux software on the CLAMV server can be mounted on campus to local Linux computers (laptops or PCs). Some software packages on the CLAMV server are configured in such a way that they must be mounted at /usr/local on the Linux client. Execute the following command to mount the software:

```
tcsh% mount clabfs2.clamv.jacobs-university.de:/disk/software/Linux /usr/local
```

resp.

```
tcsh% mount 10.72.1.12:/disk/software/Linux /usr/local
```

If the mount point /usr/local is not empty you can use another mount point and create links to /usr/local.

2.2 Software for MS Windows

Software installation files of frequently requested applications for MS Windows can be found on the network share:

clabfs2.clamv.jacobs-university.de**windows**

resp.

10.72.1.12**windows**

Several useful tools for Windows can also be downloaded from the CLAMV download webpage.[1]

2.3 Software for MAC OS

A few software installation files for MAC OS can be found on the network share

clabfs2.clamv.jacobs-university.de**mac**

resp.

10.72.1.12**mac**

3 Computer Teaching Labs - CLAMV Account

3.1 CLAMV Teaching Lab

The CLAMV Teaching Lab is located in the Westhall basement and is used for computer courses and workshops at all levels. There are five class rooms with a total of 50 computers (Dell Optiplex, IBM IntelliStation resp.). The rooms are of different size; the operating systems (OS) Linux and MS Windows are available.

[1] http://www.clamv.jacobs-university.de/CLAMV/downloads.html

Room	Nickname	Nickname	Seats	OS	Hardware
Room 1	Teaching Lab I	Large Teaching Lab	21	Linux	Dell Optiplex
Room 2	Project Room 1		5	Linux	Dell Optiplex
Room 3	Project Room 2		4	Linux	IBM IntelliStation
Room 5	Teaching Lab II	Windows Lab	11	Windows	Dell Optiplex
Room 6	Teaching Lab III		9	Linux	Dell Optiplex

The Linux computers are permanently online and are also used for student projects and small simulation projects. The workload of the CLAMV Linux computers can be monitored via the CLAMV Teaching Lab webpage.[2]

3.2 CLAMV Account Linux

In order to work with the Linux computers users must have a valid CLAMV account. CLAMV accounts are created upon request. Usually the course instructor or group leader sends a request to the CLAMV Office (see section 5) if new accounts are required. Nevertheless individual requests are also possible.
Per default CLAMV aacounts for students have a harddisk quota of 256 MBytes. CLAMV aacounts for nonstudents have a default quota of 2 GBytes. Upon request the harddisk quota can be increased. The harddisk quota can be monitored by users with the command *quota*.
Users can change their password with the command *passwd*. Password change requires to type the current password, then the new password and to repeat the new password for confirmation. If users have forgotten their CLAMV password and if there are other login problems they should contact the CLAMV Office (see section 5) for assistance.
Currently the tcsh and bash login shells are supported and environment definitions for both shells are regularly updated. The default shell for a CLAMV account is the tcsh. With the command

```
tcsh% chsh -s /bin/bash
```

the bash can be set to login shell. New CLAMV accounts get default files for the shell definition files .cshrc (for tcsh) and .bash_profile, .bashrc resp. (both for bash). Users can copy the default shell definition files anytime from `/usr/local/etc/skel`.

3.3 Environment Modules Linux Computer

Some installed software packages are not included in the default CLAMV Linux environment and users have to apply software environment modules. This is helpful if several versions of the same software are installed and users would like to choose which version to work with. Software environment modules can be handled by users with the command *module*. For example, the command

```
tcsh% module load Gauss09D01
```

[2] http://www.clamv.jacobs-university.de/CLAMV/Wizard/Accounting/html/CLAMVCluster.html

initiates the environment for the quantumchemistry program Gaussian09, Rev. D01.

module avail	Show available modules
module load modulefile	Load modulefile
module list	Show loaded modules
module unload modulefile	Unload modulefile
module purge	Unload all modules
module help	Show all options for command module
module help modulefile	Show help for modulefile

3.4 Remote Access Linux Computer

The Linux computers of the CLAMV Teaching Lab are permanently online and can be used from anywhere on campus by remote access. Users are encouraged to choose a computer with low worklaod whenever remote access is used. The worklaod of the CLAMV Linux computers can be monitored via the CLAMV Teaching Lab webpage.[3]

3.4.1 Remote Access Linux Computer from Linux

The secure shell command *ssh* can be used to create a connection from a local Linux computer to the Linux computers in the CLAMV Teaching Lab. For example

```
tcsh% ssh dduck@tlab040.clamv.jacobs-university.de
```

creates a connection to the account of user dduck at computer tlab040. If you start a program with a graphical user interface (GUI) on the Linux computers you need the option *-X* to divert the display to your local Linux computer.

```
tcsh% ssh -X dduck@tlab040.clamv.jacobs-university.de
```

3.4.2 Remote Access Linux Computer from Windows

In order to connect to the Linux computers of the CLAMV Teaching Lab from a local Windows computer a few software tools have to be installed. See subsection Software for MS Windows (2.2) for help where to find these tools.
The program *putty* is a secure shell client for Windows and is used to create a terminal session. The programs *WinSCP* and *FileZilla* can be used for file transfers between the Windows computer and the Linux computer.
It is also possible to redirect the graphical display from the Linux computer to the local Windows computer with the help of Virtual Network Computing (VNC).[4] The VNC

[3] http://www.clamv.jacobs-university.de/CLAMV/Wizard/Accounting/html/CLAMVCluster.html
[4] http://www.tightvnc.com

client toolhas to be installed on the local Windows computer. A terminal seesion to the Linux computer is necessary in order to start the VNC server software there. The program *putty* can be used for that. On the Linux computer he command *vncserver* has to be executed to start the VNC server. If the *vncserver* command is used for the first time users are asked to define a VNC password which should be different from the CLAMV and CampusNet password. After the VNC server has been successfully started user see a sentence like 'New X desktop is tlab042:1' meaning that a new VNC server with session number 1 was started on Linux computer tlab042. On the Windows computer the VNC client can be started by double-clicking. Users are asked which VNC server seesion they would like to connect to - for the example the correct entry is:

`tlab042.clamv.jacobs-university.de:1`

Finally users are asked for their VNC password.

3.4.3 Remote Access Linux Computer from MAC OS

There is also a secure shell command for MAC OS. See instructions for conecctions from a local Linux computer (3.4.1).

3.5 Research 1 Lecture Hall

The computer lecture hall in building Research 1 hosts a computer pool of 40 diskless stations which can be started via network boot with Linux boot images. The computer lecture hall pool is intregrated into the CLAMV Teaching Lab environment and a valid CLAMV account is necessary to access the computers. Hardware and software environment differ from the CLAMV Teaching Lab environment.

3.6 CLAMV Terminal Server

There is also a Linux terminal server for users who use the CLAMV resources only occassionally (lab rotation students, guests, ...). The fully qualified domain name for the terminal server is:

`tlabterm.clamv.jacobs-university.de`

You need a valid CLAMV account and additional access permission for the terminal server. Contact CLAMV Office (see section 5) if you intend to use the terminal server.

4 Research Facilities

5 Contacts - Where to find?

CLAMV Office:
Dr. Achim Gelessus

Jacobs University Bremen gGmbH
CLAMV

Street address:	**Mailing address:**
Campus Ring	P.O. Box 750 561
28759 Bremen	28725 Bremen
Germany	Germany

Office: Research 3, room 156
Phone: +49-421-200-4623
Email: a.gelessus@jacobs-university.de
WWW: http://www.clamv.jacobs-university.de

CLAMV System Administrator:
Florian Neu
Office: Research 3, room 157
Phone: +49-421-200-3177
Email: f.neu@jacobs-university.de

CLAMV Teaching Lab:
Westhall Basement
Phone: +49-421-200-3610

Computer Lecture Hall:
Research 1
Room: 53
Phone: +49-421-200-4652

CLAMV 3D Visualization (Holobench):
Campus Center Basement
Room: 1-259 left, 1-259 right
Phone: +49-421-200-4649