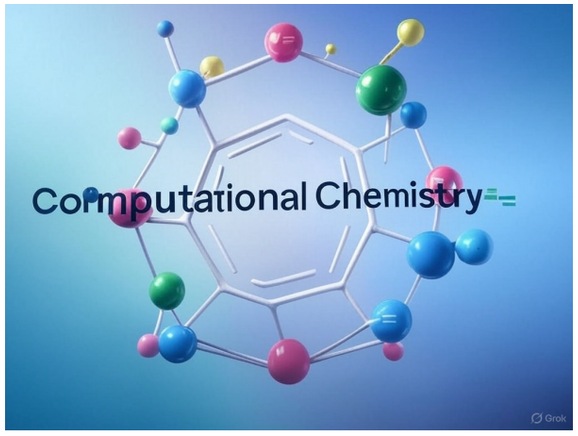
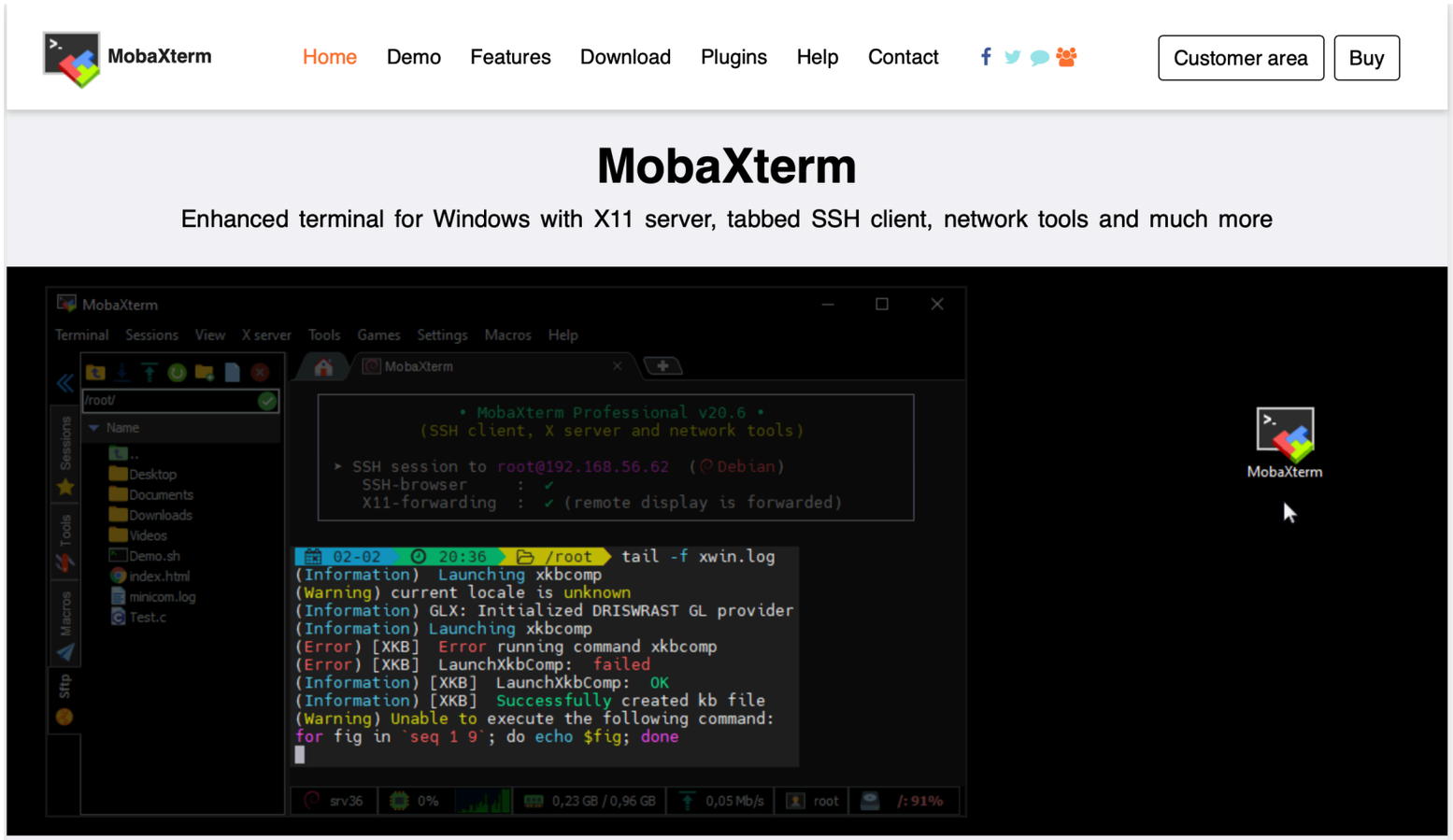


Getting started, practical session

March 21st 2025

Remote access to computers

https://mobaxterm.mobatek.net



MobaXterm X server and SSH client

MobaXterm is your **ultimate toolbox for remote computing**. In a single Windows application, it provides loads of functions that are tailored for programmers, webmasters, IT administrators and pretty much all users who need to handle their remote jobs in a more simple fashion.

MobaXterm provides all the important **remote network tools** (SSH, X11, RDP, VNC, FTP, MOSH, ...) and **Unix commands** (bash, ls, cat, sed, grep, awk, rsync, ...) to Windows desktop, in a **single portable exe file** which works out of the box. More info on supported network protocols

Key features

Embedded X server
Fully configured Xserver based on X.org

Easy DISPLAY exportation
DISPLAY is exported from remote Unix to local Windows

X11-Forwarding capability
Your remote display uses SSH for secure transport

Tabbed terminal with SSH
Based on PuTTY with antialiased fonts and macro support

Cloud computing

https://cloud.garr.it

https://youtu.be/gqdDyEEn92Y

https://twitter.com/ReteGARR

http://hscw.herla.unipg.it

FrontEnd Cluster Report at Fri, 04 Oct 2019 13:54:54 +0200

Get Fresh Data

Last | hour | 2hr | 4hr | day | week | month | year | job | or from [ ] to [ ] Go Clear

Physical View

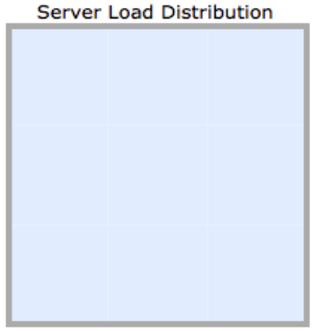
VHERLA Grid > FrontEnd > --Choose a Node

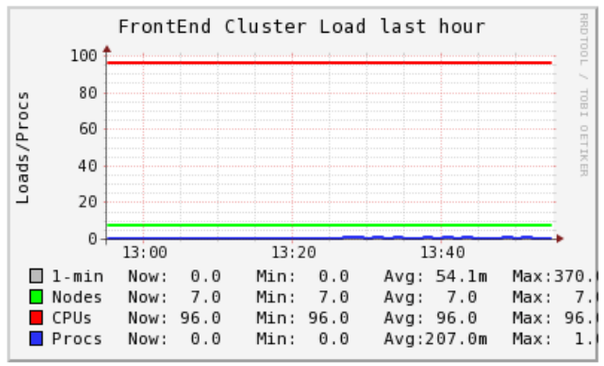
Overview of FrontEnd @ 2019-10-04 13:54

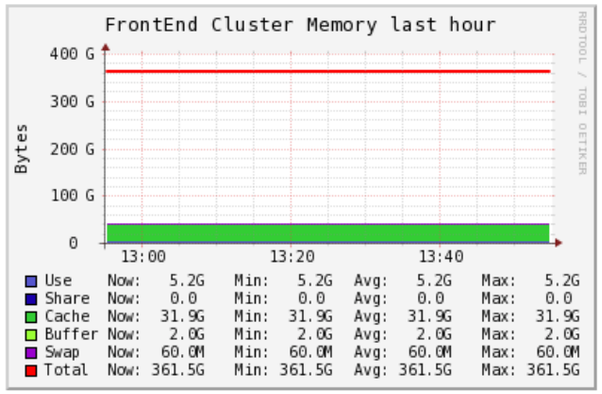
CPUs Total: **96**
Hosts up: **7**
Hosts down: **0**

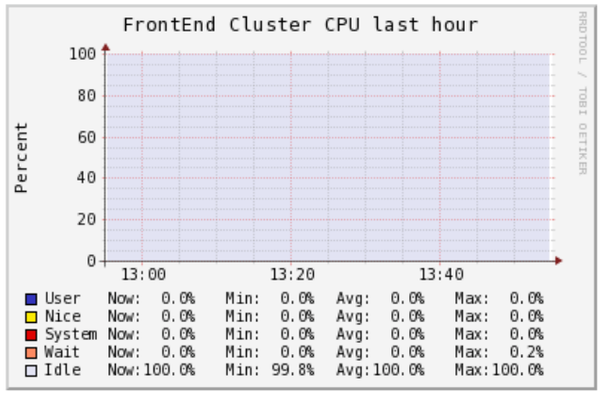
Current Load Avg (15, 5, 1m):
0%, 0%, 0%
Avg Utilization (last hour):
0%

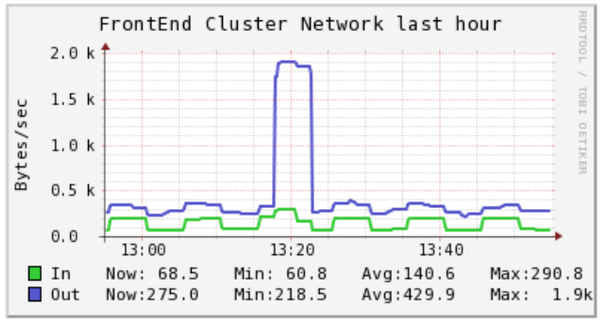
Server Load Distribution



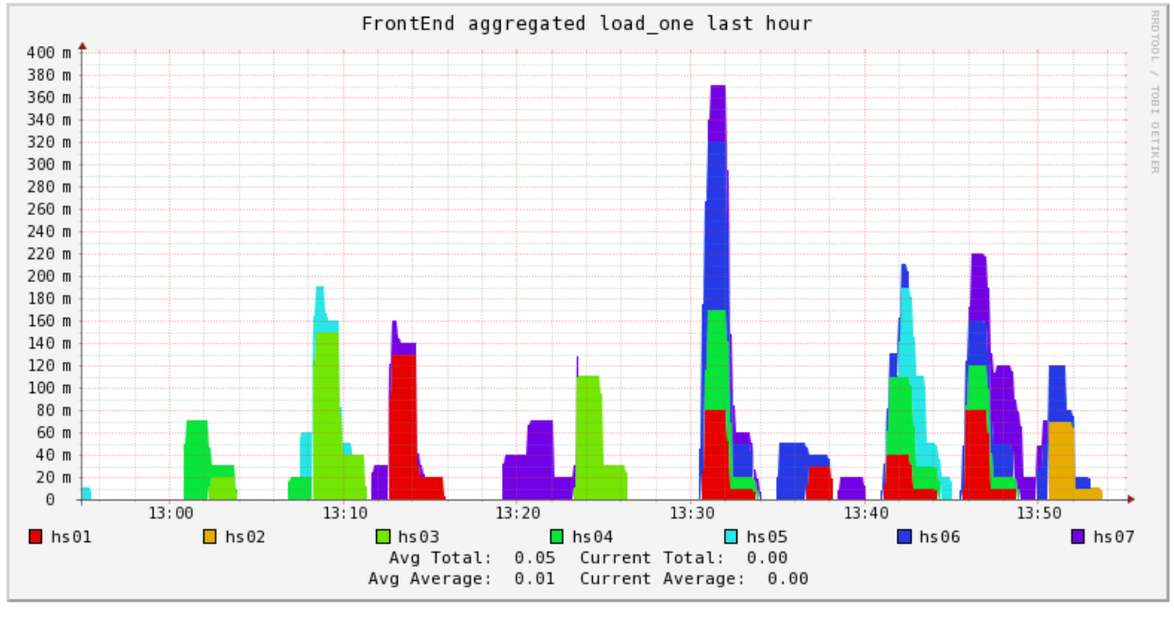








Stacked Graph - load_one



Access to computational resources

Security is an issue

Public key authentication is a way of logging into an SSH/SFTP account using a cryptographic key rather than a password

- Keys come in pairs of a **public key** and a **private key**. Each key pair is unique, and the two keys work together.
- These two keys have a very special and beautiful mathematical property: if you have the private key, you can prove you have it without showing what it is. It's like proving you know a password without having to show someone the password.
- Public key authentication works like this:
  (1) Generate a key pair.
  (2) Give someone (or a server) the public key.
  (3) Later, anytime you want to authenticate, the person (or the server) asks you to prove you have the private key that corresponds to the public key.
  (4) You prove you have the private key.

RSA algorithm

encryption is based upon factorization of integers as a product of prime numbers: a complex computational problem

Key generation

- Choose two distinct primes p and q of approximately equal size so that their product $n = pq$ is of the required bit length.
- Compute $\phi(n) = (p - 1)(q - 1)$.
- Choose a public exponent e, $1 < e < \phi(n)$, which is coprime to $\phi(n)$, that is, $\gcd(e, \phi(n)) = 1$.
- Compute a private exponent d that satisfies the congruence $ed \equiv 1 \pmod{\phi(n)}$.
- Make the public key (n, e) available to others. Keep the private values d, p, q, and $\phi(n)$ secret.

semi-prime number: product of two prime numbers

In order to break it, they would have to find the prime factorization of the large semi-prime number – that is, two or more **prime numbers** that multiplied together result in the original number.

*To make factoring harder, p and q should be chosen at random, be both large and have a large difference

Credit: https://www.di-mgt.com.au/rsa_theory.html

SSH troubles

—I had a problem connecting to older devices, and I made it work in Ubuntu 22.04 with OpenSSH 8.9 / OpenSSL 3.0.2 by adding the following lines in the Host section of /etc/ssh/ssh_config on the client side:

HostKeyAlgorithms +ssh-rsa
PubkeyAcceptedKeyTypes +ssh-rsa

Basic Rotation matrices

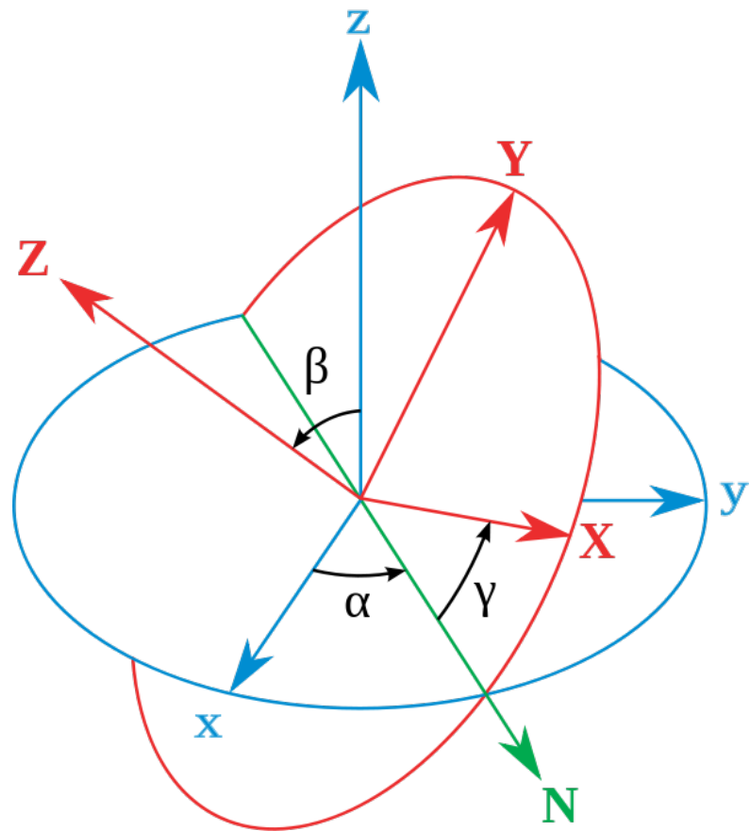
$$R_{z,\theta} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$R_{x,\theta} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$

$$R_{y,\theta} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$

Complex rotations, *Euler representation*, right-multiply vectors, the order matters

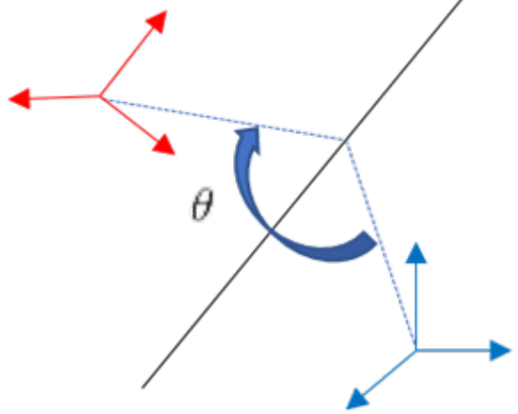
$$Rz(\gamma) * Ry * (\beta) * Rx(\alpha)$$



Axis-angle representation

Every rotation in three dimensions is defined by its axis (a vector along this axis is unchanged by the rotation), and its angle — the amount of rotation about that axis

$$u_{vector} = \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix}$$



$$R = \begin{bmatrix} \cos\theta + u_x^2\,(1-\cos\theta) & u_x u_y\,(1-\cos\theta) - u_z \sin\theta & u_x u_z\,(1-\cos\theta) + u_y \sin\theta \\ u_y u_x\,(1-\cos\theta) + u_z \sin\theta & \cos\theta + u_y^2\,(1-\cos\theta) & u_y u_z\,(1-\cos\theta) - u_x \sin\theta \\ u_z u_x\,(1-\cos\theta) - u_y \sin\theta & u_z u_y\,(1-\cos\theta) + u_x \sin\theta & \cos\theta + u_z^2\,(1-\cos\theta) \end{bmatrix}$$

Water molecule structure

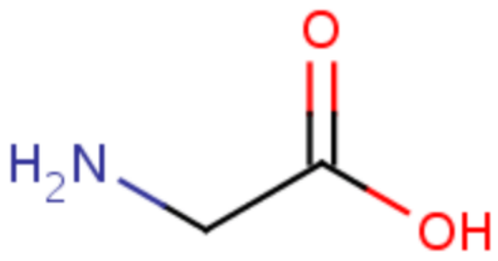
```
O  0.000000  0.000000  0.000000
H  0.758602  0.000000  0.504284
H  0.758602  0.000000  -0.504284
```

1) find the molecule plane

2) rotate molecule w.r.t. y axis

3) compare structures

Glycine structure



1) find the C_α-C=0

2) find perpendicular axis

3) rotate and compare structures

https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:15428