About using computers

Jean-Christophe SOETENS

Department of Chemistry
University of Bordeaux

jean-christophe.soetens@u-bordeaux.fr

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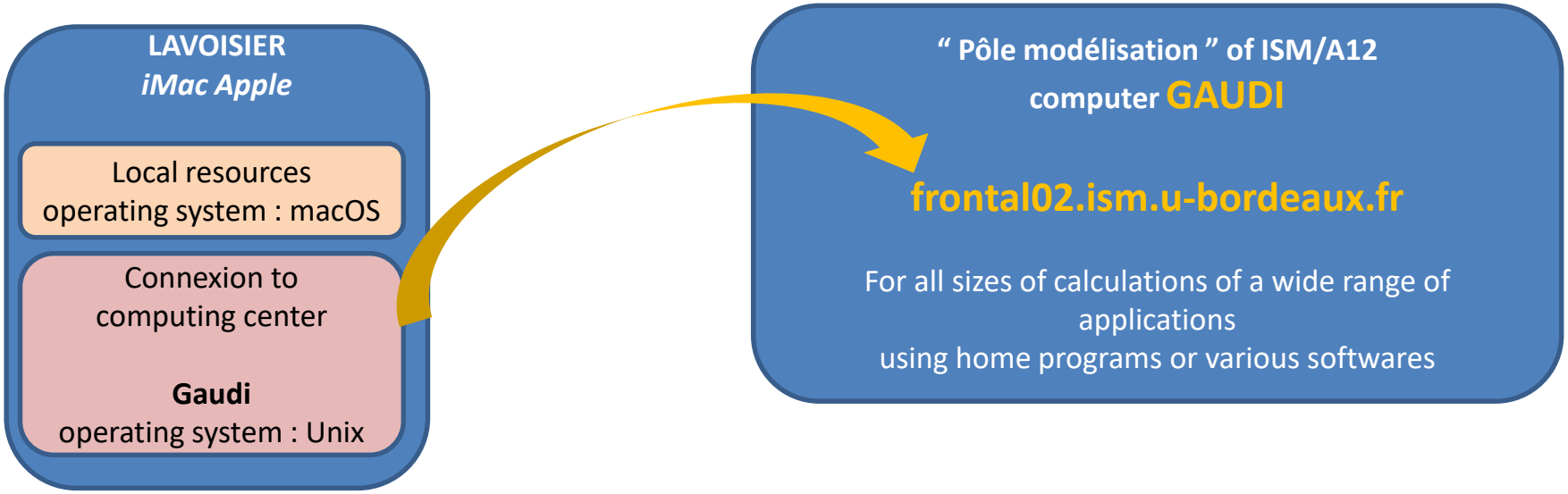
Connexion to GAUDI using IMAC at Lavoisier



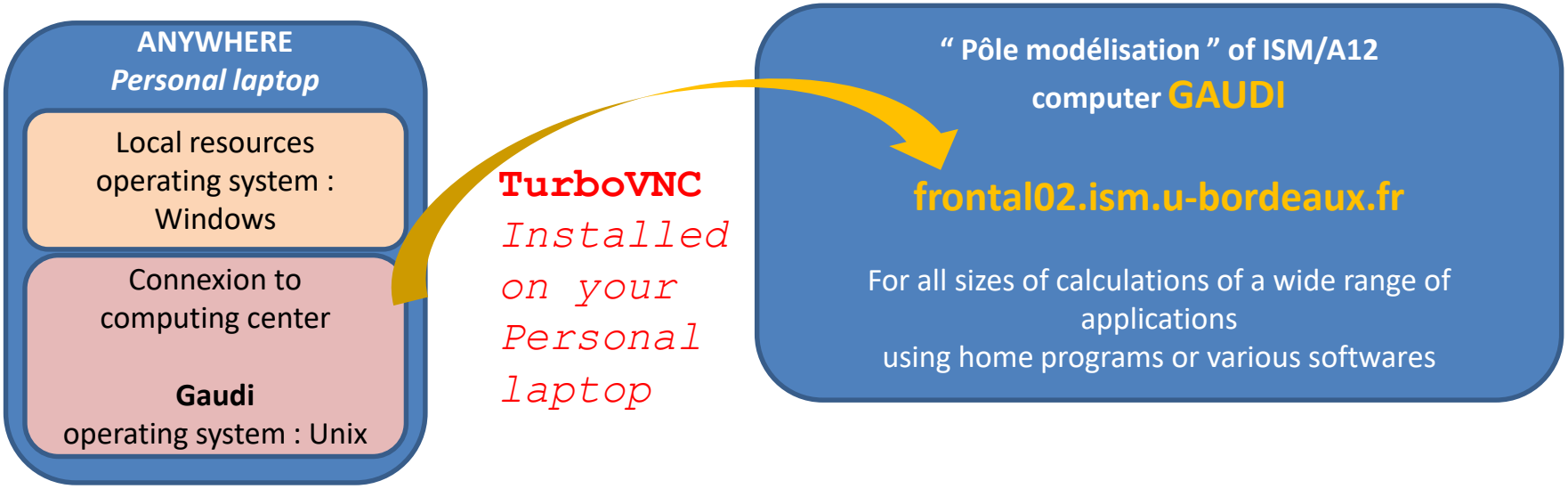
Use one of these two softwares on the IMac: terminal or X11

And the command :

```
$ ssh -Y ENT_login@frontal02.ism.u-bordeaux.fr
```

← opening a session
on Gaudi for user ENT_login

Connexion to GAUDI using your personal windows laptop with *TurboVNC*



Dowload *and* ***install*** *TurboVNC on your* ***windows laptop*** *:*

https://sourceforge.net/projects/turbovnc/files/3.0.3/

Configuration and use of TurboVNC on next slides…

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Configuration and use of TurboVNC on next slides…

PC windows

Apple

Processor INTEL

Processor ARM

turbovnc-3.0.3.i386.rpm	2023-02-27	3.3 MB	3	
TurboVNC-3.0.3-x86_64.dmg	2023-02-27	38.8 MB	7	
TurboVNC-3.0.3-x86.exe	2023-02-27	39.0 MB	7	
TurboVNC-3.0.3-x64.exe	2023-02-27	41.3 MB	63	
TurboVNC-3.0.3-arm64.dmg	2023-02-27	38.0 MB	5	
Totals: 16 Items		**356.8 MB**	**345**	

Configuration

Step 1 : you must connect to frontal02 to start the VNC server

Step 2 : install and start TurboVNC on your laptop and configure it

Use

Step 3: Now you can lunch TurboVNC on our laptop to connect on frontal02 and work within a graphical environnement

How to configure and use TurboVNC

Step 1 : you must connect to frontal02 to start the VNC server
this step only needs to be done once

Open the command interface on your windows laptop ( + r)

$ ssh -Y ENT_login@frontal02.ism.u-bordeaux.fr ← connexion to frontal02 with **ENT_password**

$ vncserver ← start vncserver on frontal02. Define a **VNC password** if this is requested (simple and different of the ENT one)

$ vncserver –list ← to get the **display number**

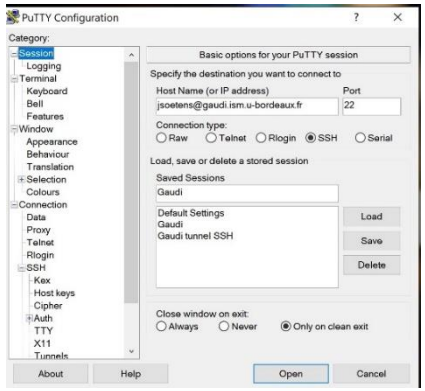
Example :

```
[jsoetens@frontal02 ~]$ vncserver -list

TurboVNC sessions:

X DISPLAY #     PROCESS ID
:3              9168
[jsoetens@frontal02 ~]$
```

display number : 3 for the present case

Alternative method for a ssh connection to frontal02 : software Putty

PuTTY

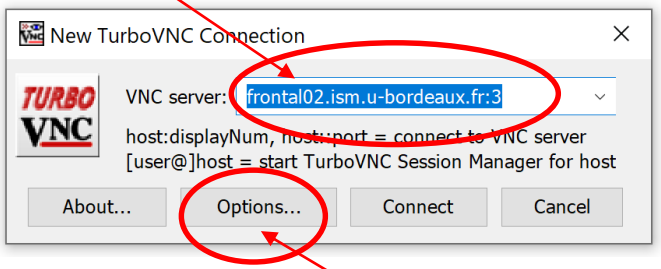


How to configure and use TurboVNC on your personal laptop

Step 2 : start TurboVNC on your PC or Mac and do the following steps

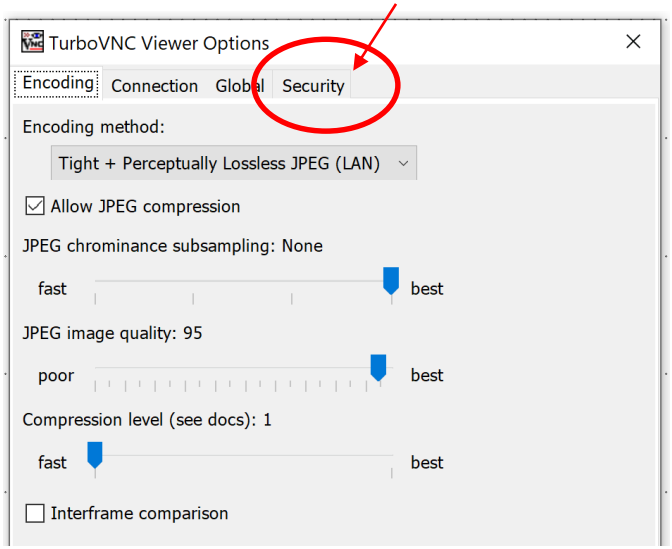
these steps also needs to be done only once

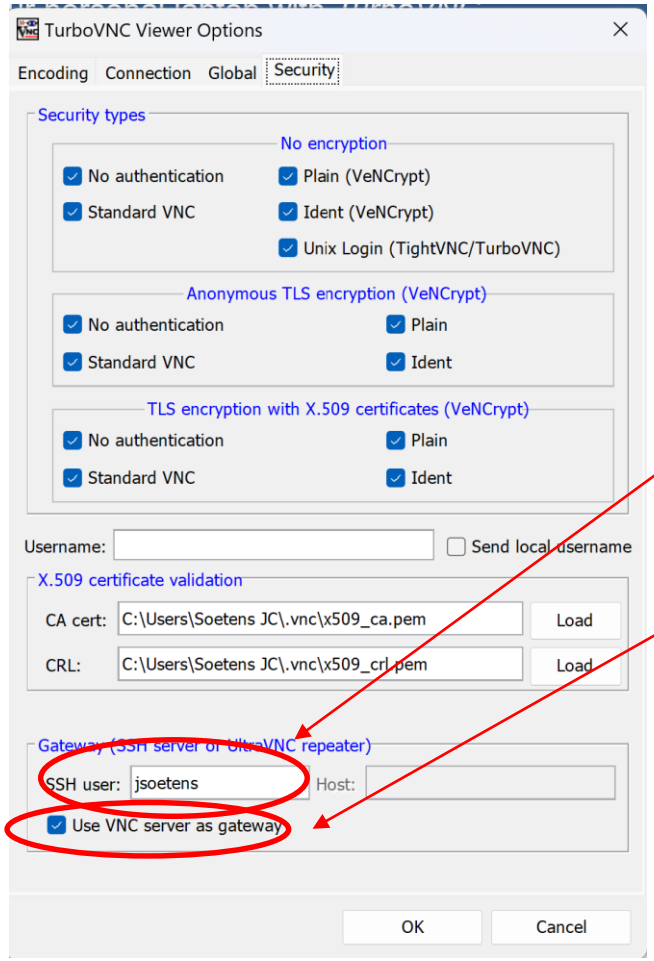
1) frontal02.ism.u-bordeaux.fr:**your vnc display number**



2) Click on « Options »

3) Click on « Security »





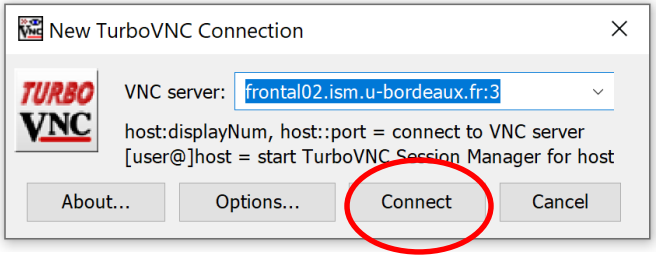
4) Your **ENT_login**

5) click

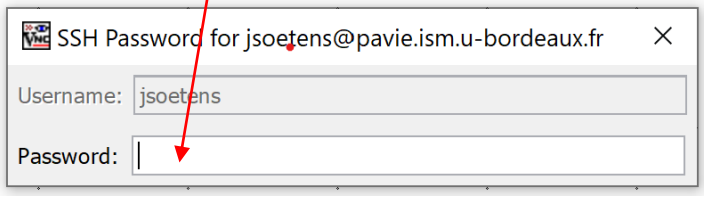
How to configure and use TurboVNC

Step 3: Now, each time you want to use TurboVNC on your PC

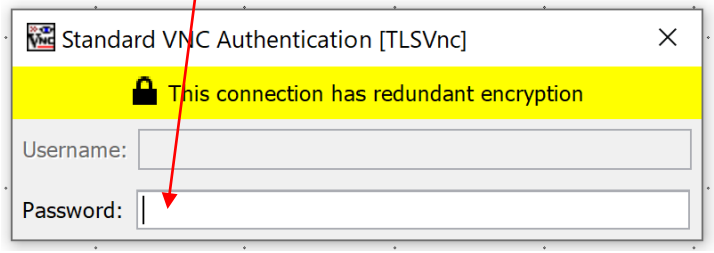
1) Start TurboVNC and click on « Connect »



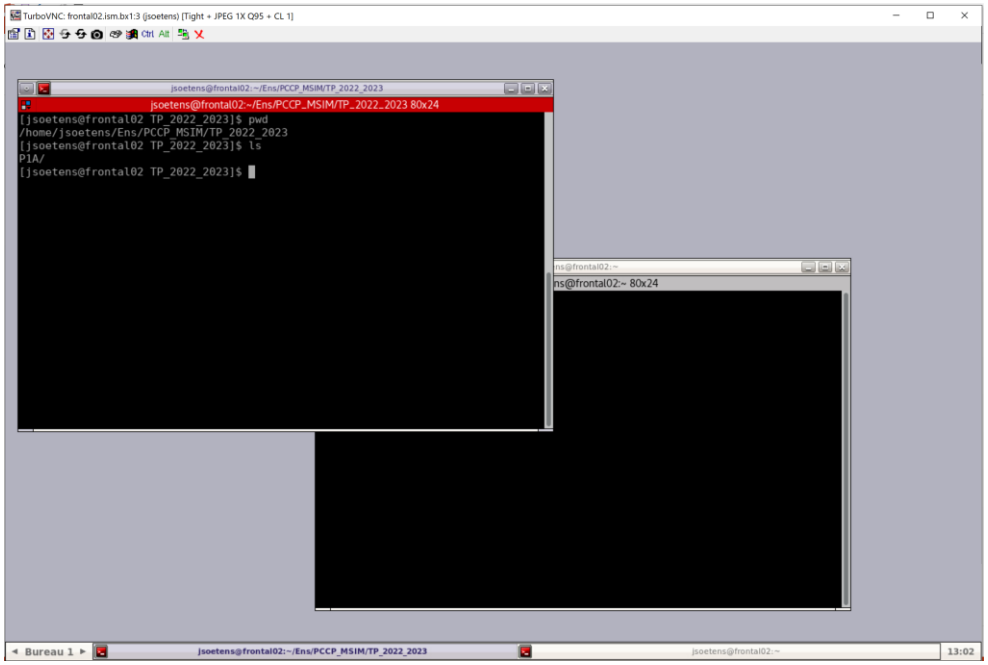
2) Your **ENT password** to be identified by the gateway pavie



3) Your **VNC password** to be identified by the vncserver on frontal02



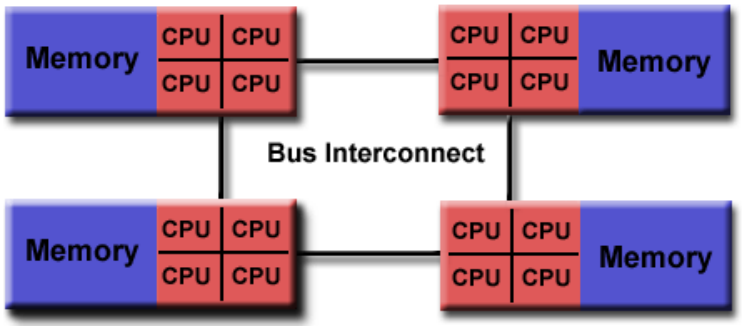
⇒ *If everything is well configured, you access to a friendly environment like this :*



In case of problems :

- *Check if only one vncserver is running on frontal02 (vncserver –list)*
- *If necessary delete the multiple vncserver (vncserver –kill process_ID)*
- *Start a new vncserver (vncserver)*
- *Check the display number (vncserver –list) and the* consistency with the display number of TurboVNC (frontal02.ism.u-bordeaux.fr:display_number)

front *behind*



“ Pôle modélisation ” of ISM/A12
Computer GAUDI

For all sizes of calculations of a wide range of applications using home programs or various softwares

The **gaudi** cluster comprises about 700 CPU-cores spread across 40 compute nodes with 32 to 256 GB of RAM and GPU. All the nodes are **interconnected** by Infiniband (scratch space of 6 To). The storage capacity is about 20 To (RAID5) and an incremental backup (30 To) is performed daily.

Software Packages

Quantum Mechanics & Dynamics

- Ampac : Semiempirical quantum mechanical program
- CP2K : Hybrid Gaussian and plane wave density functional scheme
- CPMD : Parallelized plane wave/pseudopotential implementation of DFT for ab initio molecular dynamics
- Dalton : Molecular electronic structure program
- DFTB+ : Density Functional based Tight Binding program
- Gaussian : Popular and widely-used electronic structure program
- Jaguar : Rapid ab initio electronic structure package
- Molpro : Complete system of ab initio programs for molecular electronic structure calculations
- Siesta : Electronic structure calculations and ab initio molecular dynamics simulations
- VASP : Ab initio quantum-mechanical molecular dynamics using pseudopotentials and a plane wave basis set
- WIEN2k : Electronic structure calculations of solids using DFT
- NWChem : Ab initio computational chemistry software package
- Mopac : Semiempirical quantum mechanical program

Molecular Mechanics & Dynamics

- Amber : Package of molecular simulation programs
- Gromacs : Versatile package to perform molecular dynamics
- NAMD : Parallel molecular dynamics code for large biomolecular systems
- Tinker : Complete and general package for molecular mechanics and dynamics
- GULP : General Utility Lattice Program

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