



SEVENTH FRAMEWORK
PROGRAMME

Research Infrastructures

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WeNMR virtual machine prototype



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Section 1: Summary of Deliverable

Background

Computational Structural Biology relies on computational programs that are neither easy to install nor to maintain. Many the tools available cannot be used on different platforms (Windows, OS X or Linux); some may require additional libraries or third-party software for a correct execution; even when installed, their optimal performance usually requires a subtle set up based on the hardware and the working environment. Because software installation is time demanding and often requires expertise that is not always at hand, WeNMR intended to develop a generic tool that could be easily installed anywhere, with minimal hardware requirements and does not require *a priori* knowledge for the installation. To this end, a virtual machine was developed that was used both for educational purpose (cloud computing) and for various HADDOCK tutorials.

Goal

The advantages of the virtual machine are many: we can provide the application beforehand to users and attendees of trainings and workshops, which makes the installation and maintenance easier; we have a complete control on the working environment and on all the dependencies between the programs; we can easily update the virtual machine (operating system, software, virtualization programs) and test it before deployment; we can share it upon demand, which allows one to continue working on his/her project after the end of the workshop. The developed tool has been successfully used for a number of international workshops and always received many positive feedbacks.

For now the virtual machine has been used especially for workshops, but in the near future, the virtual machine might also be made available through the WeNMR VRC, , although its size (>4 GB) might be a limitation. We expect that such virtual appliances will greatly lower the barrier that typically prevents interested users from entering the Computational Structural Biology field and in particular the usage of high-end applications such as those implemented on the WeNMR grid.

Section 2: Technical details

Specifications of the virtual machine

Virtual hardware

The virtual hardware configuration of the virtual machine in its most recent setup consists of 1 CPU with 32bit architecture, 1024 MB of RAM memory (can be configured by the user) and a maximum storage capacity of 8GB which is configured for dynamic resizing to ensure that the virtual machine does not take up unnecessary space on the host environment

Virtualization software

Installation required by user

The virtualization software that is required to be able to run the developed virtual machine is VirtualBox, in at least version 4.2.16 (the latest version at the moment of preparation of this document). VirtualBox 4.2.16 can be freely downloaded from the VirtualBox website (<https://www.virtualbox.org/wiki/Downloads>), and is available for Windows, OS X, Linux and Solaris. In addition to VirtualBox, the Oracle VM VirtualBox Extension Pack (<https://www.virtualbox.org/wiki/Downloads>) is also required.

Pre-installed components

In the virtual machine, VirtualBox Guest Additions have been installed to allow us to optimize the guest operating system for better performance and usability, without requiring user intervention.

Virtual machine

Operating system

The operating system installed on the virtual machine is Scientific Linux, version SL6.1 - i386.

Software pre-installed

The following software is all pre-installed on the virtual machine as it is provided:

- Default applications of SL6.1
- Pymol v1.3
- Grace3.01
- Rasmol 2.7.4.2
- Gromacs 4.5.5
- Crysol 2.8

Tutorial data provided on the machine

As the virtual machine is currently especially used for educational purposes for the HADDOCK tools, the following tutorial data sets are pre-installed on the virtual machine, so that they are easily available to all participants in a workshop:

- protein-protein tutorial
- protein-DNA tutorial
- multi-body docking tutorial
- protein-ligand tutorial
- free energy calculations tutorial
- special topics: SAXS scoring & crosslink data-driven docking tutorials
- grid use cases: Gromacs tutorial & CNS examples

Grid functionalities

To ensure Grid functionality for the virtual machine, Milu-1.0.2 is provided. By using the Milu distribution, a user with a valid certificate and properly registered with the enmr.eu VO can have direct access to the WeNMR grid resources, which brings the power of the grid as part of the easy to use package that the Virtual Machine is. The two use cases listed above (CNS and Gromacs) provide examples and instruction for directly interacting with the grid.

Section 3: Usage of the virtual machine in workshops

In 2013 and 2012, the virtual machine has been used in the following workshops to teach grid based usage of computational structural biology tools, in particular the HADDOCK tool:

Usage in 2013

- ISMAR Rio de Janeiro (Brazil, May)
- ISGC Taipei (Taiwan, March)
- Lisbon (Portugal, February)
- INSTRUCT course Florence (Italy, January)
- Education in the Clouds (B.Sc. Chemistry course Utrecht University, SURF SARA, November 2012 – February 2013)

Usage in 2012

- WeNMR workshop Vilnius (Lithuania, May)
- ISGC Taipei (Taiwan, March)
- Education in the Clouds (B.Sc. Chemistry course Utrecht University, SURF SARA, November 2011 – February 2012)