Installing GROMACS 4.0.5

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“Computational scientists solve tomorrow’s problems with yesterday’s computers; computer scientists seem to do it other way around.”

-anonymous

From: Landau, R. H. A first course in Scientific computing. Princeton University Press, 2005. pp-1.

Index

GROMACS

GROMACS is a program developed for computational molecular dynamics simulation of macromolecules (van der Spoel et al., 2005). It is currently in its 4.0 version (June 2009). The present tutorial describes how to install the program GROMACS 4.0.5 on Linux. Once GROMACS is installed we may run next tutorials for energy minimization and molecular dynamics simulations. This tutorial is available for download at http://azevedolab.net/md_75.html .

Files needed to install GROMACS 4.0.5

You will need 2 files described in table 1.

Table 1. Files needed to install GROMACS

File	Description
fftw-3.1.2.tar.tar	This file brings FFT libraries, which are of pivotal importance for GROMACS performance, it is expected that FFTW3 is installed previously to GROMACS installation. This FFT library is free and can be downloaded at http://www.fftw.org. This C subroutine library can be employed for computing discrete Fourier transform (DFT) in one or more dimensions, including complex data (Frigo and Johnson, 2005).
gromacs-4.0.5.tar	This file brings the gromacs-4.0.5.

Commands needed to install GROMACS 4.0.5 on Linux

To install GROMACS in Linux it is assumed that:

1) You have root privileges
2) Both files fftw-3.1.2.tar.tar and gromacs-4.0.5.tar are at directory /usr/local

All Linux commands are italics in this tutorial.
Type the following commands:

tar -xvf fftw-3.1.2.tar.tar
cd fftw-3.1.2
./configure
make
make install
cd ..

Now we have FFT libraries installed, the default installation is double precision. We will need this since the installation option for GROMACS is also double precision.

It is assumed that you are at /usr/local and gromacs-4.0.5.tar is in this directory, type the following commands:

tar -xvf gromacs-4.0.5.tar
cd gromacs-4.0.5
./configure --enable-double
make
make install
make links

If everything goes fine you will not get any error messages, and you will be able to run the following tutorials.

References

Frigo, M. and Johnson, S.G. (2005) *Proceedings of the IEEE*, **93**, 216–231.

van der Spoel, D.; Lindahl, E.; Hess, B.; Groenhof, G.; Mark, A. E. and Berendsen, H. J. C. (2005) *J. Comp. Chem.* **26**, 1701–1718.