Simulation issues for Dummies - (VMD)

I. Sticco* and F. Cornes†

*Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires,
Pabellón I, Ciudad Universitaria, 1428 Buenos Aires, Argentina.*

G.A. Frank‡

*Universidad Tecnológica Nacional, Facultad Regional Buenos Aires,
Av. Medrano 951, 1179 Buenos Aires, Argentina.*
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This article is intended as a starting point in the art of simulation. We will try to make it easy...

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I. HOW TO INSTALL VMD ON LINUX

First of all: what is VMD? what we are talking about? VMD stands for Visual Molecular Dynamics. It's a software running on Linux and Windows that lets you *see* your Molecular Dynamic (MD) simulations. It has very cool features. One of these features is that it can handle the `dump` outputs from LAMMPS. And... the most important: it is free!

How do I install `VMD` on Linux? The easy way is to run `VMD` on Ubuntu (or other Debian-like distributions). You only need to follow a few steps

1. Go to the `VMD` homepage:

   http://www.ks.uiuc.edu/Research/vmd/

   and download any of the current versions. Perhaps, you will begin to doubt on which one fits best in your computer. To get to a decision, we recommend choose between those versions that are in the list where it says *We recommend that all users upgrade to VMD xxx*. Within that list you can download the one that reads

   `LINUX_64 OpenGL, CUDA, TachyonL-OptiX`

   Notice that this is a 64-bit version. If you are not sure whether your computer supports 64 bits, you can open a "terminal" and type `lscpu`. You will get a small report on your CPU characteristics. Take a look to the specified "operation mode".

   You will be invited to register before downloading the sowtware. That's fine, you will not be charged for that. The file source file that will be downloaded is

   `vmd-x.x.x.bin.LINUXAMD64-RHEL5.opengl.tar.gz`

   where x.x.x will appear as the number of the current version. Drop this file into `/home/you/Documents`, where `you` is your username.

2. Open a "terminal" and move to the directory where the downloaded file is. Uncompress the file by typing

   `tar -zxvf vmd-x.x.x.bin.LINUXAMD64.opengl.tar.gz`

   A new directory will be created called `vmd-x.x.x` (remember that `x.x.x` is the current version number).

3. Configure and build the binaries. Type the following

   ```
   cd vmd-x.x.x
   ./configure LINUXAMD64
   cd src
   sudo make install
   ```

   The `sudo` command before the `make install` is required to avoid *permission* problems. Of course, you will be asked for your password, and for your permission to install the software. Answer with a huge YES, and wait...until the installation is complete.

4. Try if everything is fine by typing `vmd`. The program will open. Shut it down by typing `exit`.

Enjoy!

* ignaciosticco@gmail.com
† fercornes@gmail.com
‡ guillermo.frank@gmail.com