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Theoretical and Computational Biophysics Group

Hands-on Sessions

University of Western Australia, Perth
Workshop on Theoretical and Computational Biophysics
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Introduction

The hands-on sessions are a fundamental part of our school. In them, you will go through several tutorials that will introduce you to topics and tools in Theoretical and Computational Biophysics. You will learn how to use programs like VMD, NAMD, xmgrace, Matlab and others. The instructions we provide in this section are designed for the user of a summer school laptop, like the one you have been assigned today.

The laptops are 15" G4 Powerbooks, running the Mac OS X operating system. If you are not familiar with this operating system, we encourage you to take a look at the OS X primer. The tutorials require some knowledge of Unix. You can get familiar with Unix commands by looking at the UNIX primer.

Getting started

Dock

The Dock is where you'll go most of the time to open the applications you use on your computer. It is located on the bottom of your screen (Fig. 1) and contains links to applications. We have customized the Dock with the applications you will be using during this workshop.
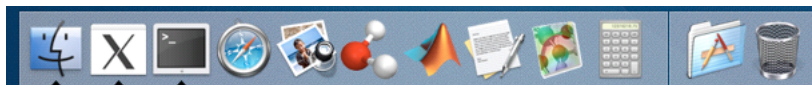

Figure 1: The icons for different applications appear in the Dock. You can open the applications by clicking on their icons. When an application is open, a black triangle appears under its icon. The default icons in the Dock are, from left to right: Finder, X11, Terminal, Safari, Preview, VMD, Matlab, TextEdit, Spartan, Calculator, Applications and Trash.

X11

X11 is an X Windows System implementation for Mac OS X. The X Windows System is the standard for graphical user interfaces on UNIX systems. Most tutorials use applications developed in X11.

You need to make sure X11 is running (X11 will launch by default when you sign in as `laptopuser`).

1 You can verify that X11 is running by looking in the Dock, located at the bottom of your screen. You should see the X11 icon with a small black arrow under it. This means an application is running (Fig. 1).

Terminal

The application Terminal must also be open. This is a UNIX terminal, that you will use throughout the tutorials.

2 Make sure Terminal is running by checking on its icon in the Dock. To start Terminal, click on the Terminal Icon in the Dock (Fig. 1).

Figure 2: The menus for an application appear on the top of your screen. The bold text next to the apple is the name of the application currently active.

Summer School directory

All the tutorial material is located in a directory called `tbss`, that you can find in your home directory.

3 To get a new Terminal Window, click on the Terminal icon in the Dock. On the top of your screen, the menus should correspond to the Terminal menus (Fig. 2).

4 Type ⌘-N to get a new terminal. When a new terminal opens, you are located in your home directory (If you are not familiar with UNIX commands, we strongly recommend that you look at the UNIX primer now!).

5 In the terminal, type:

```
cd tbss
```

This will place you in the summer school directory, where all the tutorial files are located.

6 Now, look at the contents of this directory by typing:

```
ls
```

This command shows the list of all files and subdirectories in your current directory (tbss), i.e., the list of the available tutorials.

Working on a tutorial

To start working on a tutorial, you need to be located in the right directory.

7 Inside the `tbss` directory, go to the directory of the tutorial you want to work on, e.g., the VMD tutorial:

```
cd vmd-tutorial
```

8 The tutorial directory will contain a PDF file with the tutorial itself, and a directory with the necessary files for the tutorial. In the case of the VMD tutorial, type `ls` to get a list of the contents ofthe directory:

```
vmd-tutorial-files/          vmd-tutorial.pdf
```

9 Open the PDF file by typing:

```
open vmd-tutorial.pdf
```

This will open the tutorial's PDF file in the program Preview (You can do the same by double-clicking on the icon of the tutorial using the Finder).

10 Now, go to the tutorial files directory:

```
cd vmd-tutorial-files
```

You are ready to start using the tutorial by following the instructions on the PDF file. Good luck!

Using the Software

The tutorials require use of a number of software programs. As mentioned above, some of thiese programs run in the X11 environment, while others run in the native Mac OS X environment (AQUA).

- **Programs native to OS X** will have menus on the top of the screen (Fig. 2), and their icons can be seen in the Dock (Fig. 1) which will have a black triangle under them when they are running (Fig. 1). Programs in this category that you will be using are:

    - VMD
    - Terminal
    - Matlab
    - Spartan
    - TextEdit
    - Preview

- **Programs that run under X11** will not have menus on the top of the screen. Instead, the menus of X11 will appear on the top of the screen. These programs will have their menus in the window(s) they create when they launch. They will not have an icon in the Dock, and will not start if X11 is not open. Programs that you will be using in this category include:

  - xmgrace
  - Moe
  - nedit

- **Programs launched from the UNIX command line** will not have a graphical environment at all. You run them from the command line in a Terminal window. These programs will sometimes produce output you can see in the terminal itself, or will produce files that you can later look at. These programs include all the UNIX commands, such as `ls and cd` and many others, explained in the UNIX primer, as well as shell scripts and other programs, such as:

  - NAMD
  - vmdtext (a text version of VMD)
  - psfgen

Editing Text Files

There are several ways to edit text files. Here, we introduce two of them: one that runs natively in OS X and another that comes from the UNIX environment.

TextEdit is native to OS X. You can start it by clicking on its icon in the Dock or by finding it in the Applications directory. The way it works is intuitive. You can copy and paste with the ⌘-C and ⌘-V shortcuts, etc.

nedit is a UNIX graphical text editor that resembles TextEdit. It has some advantages, like line numbering, syntax highlighting for several programming and scripting languages, etc. **nedit** exists in X11. To copy and paste in **nedit**, you need to use Ctrl-C and Ctrl-V.

Other UNIX text editors such as **vi** and **emacs** are very useful and powerful. If you don't know these programs, we encourage you to take a look at them in the future. For the present users, we provide the Quick Reference Cards in the Reference section of the webpage.

VMD

In Mac OS X, VMD is launched by clicking on its icon, in the Dock or in the Applications directory (Fig. 1).

For this workshop, we have created an alias that allows you to start VMD like you would in UNIX. Type:

```
vmd
```

in the terminal window and hit enter. This launches VMD in the current directory and will use the current Terminal window as the VMD console. Once you quit VMD, you can continue working on this Terminal window as normal.

Sometimes, it is useful to run VMD in text mode. These situations arise when you are using VMD for analysis, to generate psf files, etc. The command line version of VMD is called by `vmd -dispdev text` in UNIX and Linux versions of VMD. For this summer school, we have created an alias

```
vmdtext
```

that allows you to run vmd in text mode.

Note that these aliases may not work in new releases of VMD. [1]

NAMD

Whenever a tutorial asks you to run NAMD, follow these steps:

11 In the Terminal window use the `ls` command to check if the configuration file needed to run NAMD is located in your current directory. If it is not there, you have probably missed a previous step in the tutorial. Hence, make sure you have followed the specific instructions of the tutorial and use the `cd` and `ls` commands to locate the appropriate directory.

12 In order to run a NAMD job type in the Terminal window:

> `namd2` *configurationfile.conf* `>` *outputfile.log* `&`

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[1] In UNIX and Linux environments, VMD is launched from the command line (terminal window) by simply typing `vmd` in a UNIX terminal. The present release of VMD for Mac OS X can not be launched from the command line (terminal window).

Launching from the command line presents some advantages. The principal one is that when VMD is launched from the command line, VMD will open setting the working directory to the one the terminal is in, i.e., if you are in the `/tbss/vmd-tutorial/vmd-tutorial-files/` directory, vmd will start with that directory as the working directory. Running from the icon will set the current directory of VMD to your home directory, and forces you to change into the right directory. This is done by typing in the VMD console, for the above example:

```
cd  /tbss/vmd-tutorial/vmd-tutorial-files/  .
```

Here you should replace *configurationfile.conf* and *outputfile.log* by the actual names of your configuration file and your output file. After typing this and hitting enter, NAMD will start running on your computer. In order to check it type `ps` in the terminal window and look at the list of running processes that should appear.

13 To see the progress of your simulation, you can use the `tail` command. For example, to see continuous updates of the output file (*outputfile.log*), type the following:

   `tail -f` *outputfile.log*

where, again, you should replace *outputfile.log* by the actual name of your output file. In the screen you will see how the last part of the output file is displayed as it is being updated. When you want to stop monitoring, press `Control-C`. Tail will not interfere with your simulation in any way. Once the simulation is done, tail will not report any more updates, so if tail is still running you will need to press `Control-C` to stop it.

Matlab

Matlab can be started by clicking on its icon (Fig. 1) in the Dock or in the Applications directory. It can also be launched simply by typing in a Terminal window

   `matlab`

Safari

Safari is the OS X Web Browser (similar to Internet Explorer, Mozilla or Netscape). You can open it by clicking on its icon (Fig. 1) in the Dock or in the Applications directory. You will find useful information related to our workshop in the homepage that Safari opens when started.