Brief Introduction to xmgrace

1. Invoking xmgrace

"xmgrace" is a useful plotting package available with the linux operating system. To invoke xmgrace, open a terminal window (click on "Applications" → "Accessories" → "Terminal" in the menu bar at upper left of your screen). Then type

```
xmgrace
```

(In past years, xmgrace was only installed on the server "line" and you needed to use instead "ssh -X line xmgrace". But xmgrace seems to be installed on all the individual nodes this year.)

2. Plotting data

If in your directory you have a data file "george.dat" which consists of two columns of numbers, you can plot it by selecting the **Data** icon at the top of the window with your left mouse button, and then selecting **Import** and **ASCII**. You should get a list of all the files in your directory which end with .dat. Highlight the desired filename with the left mouse button, and then select the **OK** icon from the bottom of the box. xmgrace will plot the data. You can import additional data sets in the same way.

3. Saving your work

Before discussing how to make your plot fancier, let's describe how to save your xmgrace file, and also how to export a postscript file.

To save your work click on the **File** icon and then choose "Save As". Type your desired name in the "Selection" box, and then hit "OK". If you make more changes and then want to save again, you just need to hit choose "Save" instead of "Save As". Xmgrace will remember what you are calling the plot. It is conventional to use the suffix ".agr" to denote an xmgrace file, e.g. "rajiv.agr".

Of course you may want to go back to your xmgrace file some other day, and you can now do that by appending the name of the saved file to the xmgrace call:

```
 xmgrace rajiv.agr
```

You can create a postcript version of your plot by clicking on the **File** icon and then choosing "Print". This will create a postscript file with the same name as your .agr file, e.g. rajiv.ps. To print a hardcopy of your file

```
lpr rajiv.ps
```

The plot should come on the printer by the wall. (Again, in past years, there was an extra step: the math lab computers would not print these postscript files. To print them we needed to convert to pdf first:

```
convert rajiv.ps rajiv.pdf
```

"convert" is a generally useful linux command to change formats, e.g. you can use it to convert from .ps to .gif, .ps to .jpg, etc. etc. Another way to convert from .ps to .pdf is with ps2pdf. This sometimes produces better resolution plots. After you have the .pdf, printing is then accomplished with

```
lpr rajiv.pdf
```

(It is also useful to know how to convert to pdf because almost anyone can open a pdf but ps is not used by some people.)

4. Refining your plot- Data Sets

xmgrace makes certain choices automatically, like the numerical ranges of the horizontal and vertical axes, the color of the line segments connecting the data points, etc. These can all be changed by you to more desirable values. To change the way the data is presented, double click with your left mouse button in the plot window. This calls up a window which lists, at the top, your various data sets (in the order you imported them). Highlight the desired data set. You can then select a symbol type under "Symbol properties". The default is None. You can change the format (color, thickness, style) of the line connecting the data points using "Line properties." You can add a "legend" (highly recommended!) in the appropriate box to explain what you are plotting. By selecting the "Symbols" submenu, you can further change the symbols, eg filling them with colors etc. Choosing "Apply" will make all the changes you have selected. "Close" exits the menu for changing the appearance of the data sets.

5. Refining your plot- Axis Properties

If you click on the **Plot** icon at the top of the xmgrace window, and then select **Axis Properties**, you will get a menu which allows you to control the range of the data shown (the values in the "Start" and "Stop" boxes). The very top box allows you to choose whether to work with the X- or Y- axis. You can also control the frequency with which numbers are listed along the axes ("Major spacing") and the number of tick marks between the labeled ticks ("Minor ticks"). Most importantly, you can label the axes with "Label string". The sizes of the labels can be controlled by choosing "Axis label & bar", "Tick labels".

I am leaving out a lot of details. For example, you can use Greek letters, subscripts and superscripts, etc in the axis labels in addition to the default roman lettering. See one of the full xmgrace guides to learn how to do this.

6. Refining your plot- Titles, Legends, etc

Just as you should *always* use legends for your data and label your axes, you should also put detailed titles (and subtitles) to say what you are doing. You can do this by selecting **Plot** and then "Set Appearance" which will then call up a box where you can enter the Title and Subtitle. You can also control the size and placement of the graph on the page with the "Viewport" numbers. The placement and size of the legends can be controlled with the items under the "Leg. box" and "Legends" screens.