Figures Intro & Xfig & Xmgrace

1. Graphical Information:

I will start with a general introduction to graphical information and its importance in academia and beyond. I will use slides of Prof. Ibrahim Sulai, who gave a presentation on graphical information in Phys 310 (see link on our webpage). Prof. I. Sulai is summarizing in his slides the book by Edward R. Tufte, "The Visual Display of Quantitative Information," 2nd ed. (Graphics Press, Cheshire, Connecticut, 2018). Meanwhile Edward Tufte has published further books on graphical information, the newest is called "Beautiful Evidence."

2. Xfig Intro

I will guide you through the following main commands of `xfig`, which is a drawing tool:

- To get started: Type on the command line: `xfig &`
  This will open a new window.
- drawing tools: background grid, circle, line, text, picture, grouping, scaling, copying, editing. [1]
- To save an xfig session use `File` → `SaveAs` and give your xfig-file a name ending with `.fig`. You can get back to this session any time on the command line with `xfig filename.fig &` or within xfig with `File` → `Open`.
- To make an eps-file out of your figure use `File` → `Export`, make sure to choose "EPS (Encapsulated Postscript)" and choose the same filename but with the ending `.eps`. This eps-file can then be included in your latex file for the paper. (Later into the course I will also show you a variation of latex, latex beamer, which you may use to make talk-slides.)

(optional) Comment for Advanced xfig Users:

In case you would like to use latex commands within xfig use the following steps: First copy
`~kvollmay/share.dir/papertools.dir/xfig2eps`
and
`~kvollmay/share.dir/papertools.dir/xfig2pdf`
then make both executable (these are perl-scripts)
`chmod u+x xfig2*`. These `xfig2*` files will be needed for step (4) below.

[1] These commands are provding descriptions on the top right for a three button mouse. If you have a mouse with one or two buttons try the following description taken from the webpage
`http://mcj.sourceforge.net/`
"Use of a three-button mouse is recommended, but it is also possible to use a two-button mouse (if you have a two-button mouse and your X server doesn't emulate a three-button mouse, press the Meta (or Alt) key and right mouse button together to simulate mouse button 2). Normally, mouse buttons 1 to 3 are assigned to the left, middle, and right buttons respectively. "
And if that doesn't work, maybe look at
`http://jhetrick.io/IntroSciCompTools/textbook/html/ch9/ch9sec1.html`
which unfortunately recommends that you buy a mouse (or let me know, to get you one organized).

Instead of `xfig` use
(1) `xfig -specialtext -latexfonts -startlatexFont default`
(2) You can use now latex in text, so for example `$\alpha$`.
(3) first save then export to "Combined PS/LaTeX (both parts)."
This creates two files: `filename.pstex` and `filename.pstex_t` .
(4)To then make an eps-file (which you can include in your paper)
(4a) `xfig2eps filename`
or to make a pdf-file use
(4b)`xfig2pdf filename`

2. Xmgrace Intro

I will walk you through a set of tools how to use xmgrace to fullfill the following list of requirements for figures for scientific papers and talks. I will show you the main tools using the following data (of the mean squared displacement data of a simulation of a binary Lennard-Jones model [KVL, AJP 2020].)
Either download from our course webpage or copy into your working directory the following files:

```
~kvollmay/share.dir/papertools.dir/msdA.data
~kvollmay/share.dir/papertools.dir/msdB.data
```

Copy either one of your main project results or the above data into your working directory.

Mini-Intro to Xmgrace:

• To get started with xmgrace type on the command line `xmgrace &`. To pull in a dataset use `Data` → `Import` → `ASCII` and under Selection add `msdA.data` then click `OK`.
Or alternative is to type in the terminal window (on the command line) `xmgrace msdA.data`
To pull in several data sets you would list them on the commandline (separated by spaces).

• I will show to you below several commands within xmgrace. To save an xmgrace session, you use within xmgrace `File` → `Save As` (Note: When you save for the first time, it is important that you use `Save As` instead of `Save`, because the latter overwrites the datafile.) and add to the end of the Selection directory the xmgrace-file name, which should end with `.xmgr`, e.g. `msd.xmgr`
To open a previously saved xmgr-file, you either use on the command line `msd.xmgr` (or replace the according xmgrace-filename), or you use `xmgrace &` and then `File` → `Open` and edit again in the Selection section.

• To make an eps-file, use within xmgrace `File` → `Print setup` and change PostScript to `EPS` and give the filename (it should end with .eps), or if you had saved the xmgr-file before, then already the same name with the .eps ending is suggested. This only sets up the printing, to get the eps-file printed use `File` → `Print`.

• You can make a pdf-file by using `epstopdf filename.eps filename.pdf`

Requirements for Figures:

In the following I will comment on the following requirements for scientific figures and I will show you how to fullfill these requirements when using xmgrace.

- no title
- axes:
  - label axes (large enough, neat font-tools via clicks and via commands, location of axis label)
  - axis width thick enough
  - number of tick marks large enough
  - tick label size large enough
  - tick marks width and size large enough
  - choose wanted x-range and y-range (main features visible) and for these data also how to make a log-log plot
- position & size of figure (to get axis label included and white space removed)
- legend (or equivalent with labels) large enough and each set should be labeled (or clear trend of which parameter was varied and in which range) and should not cover data
- label for major parameter large enough (in talk in figure, in paper if not in figure then in figure caption)
- symbols large enough and distinguishable and lines thick enough and distiguishable (keep in mind potential color blind person in audience) and in case of error bars thick enough error bars (labeled: see legend)
- in paper figure caption for each figure

Further xmgrace-tools:

- extra cool fonts: italics, greek, boldface, superscript, shift (switch to italics with `\f{1}` ,to greek with `\x`, to boldface with `\f{2}`, back to default of roman with `\f{0}`, to get superscript `\S` and back to normal `\N` and to subscript with `\s` and to horizontally shift us `\h{0.4}` and vertically `\v{0.3}` where you adjust the amount of shifting by changing 0.4 and 0.3)
- pull in further data-set via block-data
- arrows and labels etc. (drawing objects)
- how to recycle figure via deleting data and replacing with new data or via change of xmgr-file
- symbols: filled and open symbols
- if time: insets
- (not xmgrace but useful: keep logfile for how you made data and where they are)