

PY 421 - Introduction to Computational Physics

Assignment 3 howto.

This document provides some guidance for the steps needed to do the first assignment. It describes the basics of:

- using gnuplot to plot data;
- using latex to prepare a report, incorporating plots;
- using the tar command to assemble files.

The information on the tools (gnuplot, latex, and tar) that you will find here is minimal. You should strive to learn more about these and other available tools, by taking advantage of man pages, the help command, manuals, tutorials or the expertise of friends. But, if you are totally unfamiliar with the tools, these pages will get you going.

Note: **boldface font** is used to represent lines as they appear on the screen.

Gnuplot howto.

Gnuplot allows you to plot mathematical formulae or data. To use gnuplot type

gnuplot

you will get a message and then

gnuplot>

I assume that you have the data, in the format produced by `blur_pict_mod`, in three data files “blur.dt1”, “blur.dt2” and “blur.dt3”. Typing **plot “blur.dt1”** at the **gnuplot>** prompt

gnuplot> plot “blur.dt1”

will produce a plot of the data in the file. To plot the other data files in the same plot, use **replot**

gnuplot> replot “blur.dt2”

gnuplot> replot “blur.dt3”

You can also plot mathematical functions. Try (in the following lines, of course, you only type what follows the **gnuplot>** prompt):

```
gnuplot> a1=-2
```

```
gnuplot> b1=-0.0005
```

```
gnuplot> replot a1+b1*x
```

You can plot more lines on the same plot by defining more variables and continuing to use replot. If you want to start a graph anew, use the command plot.

After you have obtained a satisfactory graph, you will want to save it on an eps file for later inclusion in your report “assignment3.ps”. For the purpose, change the terminal type by typing

```
gnuplot> set term post eps
```

This sets the terminal type to postscript, file of type eps. If you like to produce a graph with color, type instead

```
gnuplot> set term post eps color
```

The image will disappear (because you changed the terminal type), but do not panic. Define now the name of the output file. Suppose you want to call the output file “graph1.eps”. Type then

```
gnuplot> set out "graph1.eps"
```

and, finally, type

```
gnuplot> replot
```

If you list the files in your directory, you will see graph1.eps. You can visualize the plot with **evince graph1.eps**.

Gnuplot provides you with some basic help. Type

```
gnuplot> help
```

and choose topics and subtopics.

To leave gnuplot type

```
gnuplot> quit
```

Latex howto.

For this assignment you must return a postscript file “assignment3.ps” or a pdf file “assignment3.pdf” which contains the calculations done for problem 3 as well as the two graphs requested in problem 2 and 5. You can use any tool you like to prepare this file, but it **must be** a postscript or pdf file viewable on the CAS cluster with the program evince. Latex is a very widely used tool for the preparation of scientific documents and I recommend that

you use it. You will find in the notes subdirectory of `~rebbi/courseware` the file “sample_asgn3.tex”. It is a simple file, that gives you the basics of a latex document. (There is much, much more in latex and I urge you to learn further about this document preparation tool by consulting a manual, or a guide, or following a tutorial etc.) In order to make a postscript file, you should copy the file “sample_asgn3.tex” as well as the two eps files “sample_fig1.eps” and “sample_fig2.eps” into your working directory.

Use then the following commands

latex sample_asgn3.tex

latex sample_asgn3.tex

(This must be typed twice, as above.)

dvips sample_asgn3.dvi -o sample_asgn3.ps

The first time you type the latex command, latex writes a `sample_asgn3.aux` file, that contains information on equation labels, figure captions etc., if you have any in your text. The second time latex is invoked, the information in that .aux file is used to insert the references in proper order. Latex produces a .dvi file, `sample_asgn3.dvi` in our case, which contains device independent information about the typesetting of the document. The dvips command converts the .dvi file into a postscript file. Latex and dvips assume that the extension of the file is .tex and .dvi, respectively, so

latex sample_asgn3

latex sample_asgn3

dvips sample_asgn3 -o sample_asgn3.ps

will also work. In the process the files “sample_fig1.eps” and “sample_fig2.eps” will be incorporated into the final postscript file.

You can now call evince to visualize the file `sample_asgn3.ps`.

Copy the `sample_asgn3.tex` file to `assignment3.tex` and bring this file into your emacs editor. You should be able to understand the meaning of the various commands and change the text and reference to figures (i.e. the names of the .eps files) in order to convert that example into the file that you must return for your assignment. Produce the postscript file. Of course, you will have to use now the name `assignment3`:

latex assignment3

latex assignment3

dvips assignment3 -o assignment3.ps

A very good suggestion is that you do the changes in small steps, saving in emacs the modified file and running latex on it. The command $\hat{\text{Ctrl}} \hat{\text{S}}$, where $\hat{\text{}}$ stands for the ctrl button that must be pressed together with the key, saves the emacs file in the current buffer. (You should invoke emacs in background: **emacs assignment3.tex &**. This will allow to execute the commands **latex assignment3** and **dvips assignment3 -o assignment3.ps** without having to leave emacs. Also you should be running evince in background: **evince assignment3.ps &**. Remember to click on the reload button under the “View” option of evince after you have run the dvips command, to make evince display the new version of the file.) By proceeding in small steps, if you make a change that produces an error in the latex file, you should be able to retrace your steps back and correct the error.

If you would like to produce a pdf file instead, you should insert two extra terms in the dvips command

dvips assignment3 -Ppdf -G0 -o assignment3.ps

and then

ps2pdf assignment3.ps

This will generate a pdf file. The flags -Ppdf and -G0 may not be crucial. In general they help to produce a clearer font.

tar howto.

In your working directory make a subdirectory called tmp and copy the files you want to assemble together to this directory (this is just for safety, so that if something goes wrong you will still have the original files). Change directory to tmp.

Say that the files you want to return are “blur_pict_mod.f90”, “make_pict.c”, and “assignment3.ps”. Then, always in the tmp directory, execute the command

tar cvf asgn3.tar blur_pict_mod.f90 make_pict.c assignment3.ps
(all in one line)

tar will assemble together (c flag) the three files into the file asgn3.tar (f flag followed by the target file name). You can use any name you like, instead of “asgn3.tar”. I have called the tar file asgn3.tar for sake of definiteness. The v flag (for verify) will cause tar to echo the names of the files that are put together.

You can check the content of a tar file with

tar tf asgn3.tar

This will display the list of the files which have been assembled together in asgn3.tar.

For your information, the command

tar xvf asgn3.tar

will extract the files contained in asgn3.tar (notice the x flag, rather than the c flag).

In order to return the assignment, all that remains to be done is to copy the tar file to the asgn3.xxyyyy file. I assume that you are working on the CAS cluster. If not, transfer the asgn3.tar file to the the CAS cluster then log in to the CAS cluster. For this you should run the command **scp asgn3.tar yourusername@327lfs:.** You will be prompted for your password on the CAS cluster and scp will generate a remote copy. Login then to the CAS cluster and execute the command

cp asgn3.tar ~rebbi/courseware/asgn/asgn3.xxyyyy

Alternatively it should be possible to scp the file directly to the courseware/asgn directory. Try the following

scp asgn3.tar yourusername@327lfs:~rebbi/courseware/asgn/asgn3.xxyyyy

Again, you should be prompted for your password on the CAS cluster and scp will copy your file directly to the file asgn3.xxyyyy in my courseware/asgn directory.

Of course, do not use the extension xxyyyy, but replace this with your personal code. The asgn subdirectory does not have read permission. So you cannot list the files it contains nor use the tab command to complete the asgn3.xxyyyy file name. Enter its name in full. But you can copy your work to the asgn3.xxyyyy file as many times as you like, overwriting the previous copy. In particular, if you realize you made a mistake and want to submit another version of your assignment, just repeat the above copy command. You will be able to do so until the write permission on the files asgn3.xxyyyy is revoked, after the deadline for submission of the assignment has passed.