University of Cambridge

Department of Materials Science and Metallurgy

MPhil Computing Projects 2000

Computing Examples Class 1

Objectives

The aim of this first examples class is to give you practice in using some of the basic UNIX commands described in the lectures. In particular it will introduce you to the following concepts and procedures:

* gaining access to the system (logging in)
* file and directory structure (moving around the system; creating new files and directories)
* file manipulation (listing, printing, copying, renaming and removing files)
* file editing (data input and modification)
* file processing and execution (the `make` command)
* data visualisation (x-y plots)

The Coffee Cooling Problem

You are asked to use your knowledge of UNIX to investigate a problem in heat flow known as the Coffee Cooling Problem. This problem involves the numerical solution of a first-order differential equation describing the rate of change of temperature of a liquid (coffee) as it loses heat to the surrounding air. This equation is given by:

$$\frac{dT}{dt} = -r(T - T_s),$$

where T is the temperature of the coffee, T_s is the temperature of the surroundings and r is the "cooling constant." A graph of the function $T(t)$ produces a simple cooling curve. You are provided with a FORTRAN program called `coffee` which solves this equation numerically using the Euler method. This method converts the differential equation to a finite difference equation by assuming that dT/dt is constant over a small time interval dt. The accuracy of the method depends on the size of the time step dt. Thus the following four parameters control the solution of the equation:

* the cooling constant r

* the time step dt
* the surrounding temperature T_s
* the initial coffee temperature T_0

In the exercises that follow you will be asked to vary these parameters to see how they affect the solution. In addition you will need to compare your solution to a set of $T(t)$ measurements for a real cup of coffee. A final problem you will be given is the following: if you are in a hurry and want the coffee to cool as soon as possible, is it better to add some milk immediately after the coffee is made, or should you wait for a while before adding the milk?

The above differential equation can, of course, be solved analytically and in Examples Class 2 you will be asked to write a short FORTRAN code to do this and compare your results with those that you obtain today.

Exercises

(a) Login to a Silicon Graphics workstation or a PC running Linux, as you prefer.

(b) Using the following commands (or using the point-and-click interface if you prefer), make a new directory called `exercise` and copy the sources of the coffee and plotxy programs and the makefile into it from the `/mphil/examples` directory:

```
mkdir exercise
cd exercise
cp  /mphil/examples/coffee.f    coffee.f
cp  /mphil/examples/plotxy.f    plotxy.f
cp  /mphil/examples/makefile   makefile
```

(c) List the files in your new directory and display their contents with the `more` command.

(d) Compile the plotxy program using the command:

```
make plotxy
```

(e) Use `nedit` to create a data file (`plotxy.txt`, say) containing the following experimental measurements of $T(t)$ recorded with the surrounding temperature at 22.8°C:

time (min)   T (°C)   time (min)   T(°C)

0	83.0	8.0	64.7
1.0	77.7	9.0	63.4
2.0	75.1	10.0	62.1
3.0	73.0	11.0	61.0
4.0	71.1	12.0	59.9
5.0	69.4	13.0	58.7
6.0	67.8	14.0	57.8
7.0	66.4	15.0	56.6

Write the data in two unformatted columns.

(f) Run the plotxy program using the command:

```
plotxy   plotxy.txt
```

`plotxy` will prompt:

```
Graphics device/type  (? to see list, default  /XWINDOW):
```

By default output will go to the screen (and this should be done). To write the output to a file, say `xyout.ps`, reply `xyout.ps/ps` to the prompt above, which will create a file `xyout.ps`. To print this file, use

```
lpr xyout.ps
```

(g) Compile and run the coffee cooling program using:

```
make coffee

coffee
```

`coffee` asks for values of the four parameters r, dt, T_s and T_0. Start with the following:

$$r = 0.1$$

$$dt = 1.0$$

$$T_s = 22$$

$$T_0 = 83$$

The `coffee` program will automatically plot your numerical results (as lines extrapolated between calculated t values) together with the experimental data (plotted as circles).

(h) How accurate is your solution? Repeat part (g) systematically varying the time step dt. Do the results change significantly?

(i) How well does the solution compare to the cooling curve of real coffee? Choose the best fit dt and repeat part (g) systematically varying the cooling constant r so as to get the best match to the experimental data.

(j) Suppose the initial temperature of the coffee is 90°C, but the coffee can only be sipped comfortably when its temperature is below 65°C. Assume that at 90°C, the addition of milk cools the coffee by 5°C. If you are in a hurry and want to wait the shortest possible time, should the milk be added first and the coffee allowed to cool, or should you wait until the coffee has cooled to 70°C before adding the milk? Use your best value of r and “simulate” the two cases using the coffee program.