## Assignment III : Numerical Differentiation

Due 9/19/2016

**1.** Differentiate the functions $\cos x$, and $\sqrt{x}$ at $x = 0.1, 1.$, and 30. using single-precision forward-, central-, and extrapolated-difference algorithms. [Modify the program *diff.f90* accordingly.]

**(a)** Print out the derivative and its relative error $\varepsilon$ as a function of $h$. Reduce the step size $h$ until it equals machine precision, $h \approx \epsilon_m$,

**(b)** Plot $\log_{10}|\varepsilon|$ versus $\log_{10} h$, and check whether the number of decimal places obtained agrees with the estimates in the text.

**(c)** See if you can identify truncation errors at large $h$ and the roundoff error at small $h$ in your plot. Do the slopes agree with the predictions from the book?

**(d)** Repeat your analysis for $\cos x$ and $\sqrt{x}$ in double precision and compare to the single precision results.

**2.** For the second derivate one can derive analogously a three-point formula, Eq. (8.30) in the textbook:

$$f_c''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - \mathcal{O}(h^2). \tag{1}$$

Using two more points, $x \pm h$, one arrives at a five-point formula for the 2nd order derivative:

$$f_c''(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} - \mathcal{O}(h^4). \tag{2}$$

Derive Eqs. (1) and (2) and include a scan of the written derivation in your tarfile.

**(a)** Modify your code for the 1st order derivative to calculate the 2nd order derivative. Pay attention to the grouping of the numbers, to keep the error in adding/subtracting numbers small. Calculate the 2nd order derivate for $\cos x$ in single precision for the same x values as in **1.** Start with $h \approx \pi/10$ and keep reducing $h$ until you reach machine precision.

**(b)** Print out the derivative and its relative error $\varepsilon$ as a function of $h$. Reduce the step size $h$ until it equals machine precision, $h \approx \epsilon_m$,

**(c)** Plot $\log_{10}|\varepsilon|$ versus $\log_{10} h$, and check whether the number of decimal places obtained agrees with the estimates in the text.

**(d)** See if you can identify truncation errors at large $h$ and the roundoff error at small $h$ in your plot.

**3. Coffee Cooling using the Euler Method**

The nature of heat flow from hot water to the surrounding air is complicated and involves mechanisms like convection, radiation, evaporation, and conduction. However, if the temperature difference between the water and its surroundings is not too large, the rate of change of the temperature of the water is proportional to this temperature difference:

$$\frac{dT}{dt} = -r(T - T_s), \tag{3}$$

where $T$ is the temperature of the water, $T_s$ is the temperature of its surroundings, $t$ is the time, and $r$ is the 'cooling constant'. The cooling constant $r$ depends on the heat transfer mechanism, the contact area with the surroundings, and the thermal properties of the water. The minus sign implies that if $T > T_s$, the temperature of the water decreases in time.

**(a)** Prove to yourself that the analytic solution of Eq. (3) can be written in the form

$$T(t) = T_s - (T_s - T_0)e^{-rt}. \tag{4}$$

Note that $T(t = 0) = T_s - (T_s - T_0) = T_0$, and that $T(t \to \infty) = T_s$.

**(b)** Write a code *cool.f90* with guidance from a pseudocode to solve the differential equation using the Euler method. Use for your check e.g. r=1 $\text{min}^{-1}$ to speed up your code development time.

**(c)** By varying the time step, e.g. $\Delta t$ = 0.1, 0.05 0.025, and 0.005, determine the error accumulating in your calculation. Choose $t$ = 5 min, and make a table showing the difference between the exact solution and your numerical solution as function of $\Delta t$. If $\Delta t$ is decreased by a factor of two, how does the difference change? Plot the difference as function of $\Delta t$ .

**(d)** Because time is measured in minutes, the unit of the cooling constant $r$ is $min^{-1}$. You may notice, that the value $r = 0.1min^{-1}$ yields a cooling curve $T(t)$ that does not correspond to the experimental values given in the data file *coffee.dat* included in the tarfile of this week. Find an approximate value of $r$ that describes the experimental results given in that dataset. What is your implicit criterion for determining the best value of $r$? Can you fit the empirical data for all $t$?

**(e)** Use the value of $r$ found in (c) and make a graph showing the dependence of temperature on time. Plot the empirical data on the same graph and compare your results.

**(f)** Is the value of $r$ the same for black coffee as it is for coffee with cream? Determine both values. Based on what you know about coffee and cream, do you expect $r$ to be greater or smaller for black coffee?