Computational Physics Homework Set #1

(Due 9/24, at noon)

1) Differentiate the functions $\cos(x)$ and $\exp(x)$ at $x = 0.1, 10$ using single precision forward-, central- and extrapolated-difference algorithms.

a) Write a code that implements the three methods.

b) Print out the derivative and its relative error ε as a function of step h, reducing h until it equals machine precision ϵ_m.

c) Make a log-log plot of relative error ε versus step h and check whether the number of decimal places obtained agrees with simple estimates you can make.

d) Truncation and roundoff error manifest themselves in different regimes of the plot in part b). Can you identify the regimes and are the slopes as expected?

2) Consider the trivial integral,

$$I = \int_0^1 \exp(-t)dt, \tag{1}$$

and compare the relative error ε for the trapezoid rule, Simpson's rule and Gauss-Legendre quadrature for single precision.

a) Write a code that implements the three methods.

b) Make a log-log plot of ε as a function of the number of intervals N (choose reasonable values of N, e.g. $N = 2, 10, 20, 40, 80$, etc) up to N "large enough" so you see the effects of roundoff error. Please *think* before doing extra work, for each method you will need different range in N.

c) Explain what you see in the plot.

3) Consider a *random walk* in one dimension (1D) that starts at $x_0 = 0$ and at each step of the walk one can make a step to the right or left of size $\ell = \pm 1$ with equal probability.

a) Write a code for a 1D random walk, using the linear congruential generator with values $a = 9301$, $c = 49297$ and $m = 233280$. Your code should give the sequence of x_n's for a given initialization `iseed` and sequence length $n_{\max}$. You will calculate expectation values at a fixed n by averaging over sequences of different `iseed`.

b) Using random walks of size $n_{\max} = 500$ and averaging over $N_{\mathrm{R}} = 1000$ realizations (corresponding to different values of $\texttt{iseed} = 1, \ldots, 1000$), construct plots of $\sigma_n^2 = \langle x_n^2 \rangle$, $s_3 = \langle x_n^3 \rangle / \sigma_n^3$, and $s_4 = (\langle x_n^4 \rangle / \sigma_n^4 - 3)$ as a function of n.

c) Can you explain the behavior you see in the plots? *Hint:* Set up a recursion relation, i.e. $x_n = x_{n-1} + \ell$, and calculate analytically the expectation values in the large n limit. We will see later that the behavior in this limit is due to x_n becoming a Gaussian random variable: this is a consequence of the famous *central limit theorem.*