Computational Physics

PHYS 410 2014W

Assignment #1

Due: Wednesday, September 24, 2014 at 6PM

Note: Repeat all numerical experiments using both single and double precision numbers

1. The Riemann Zeta Function can be defined through the sum

$$\zeta(s) \equiv \sum_{n=1}^{\infty} \frac{1}{n^s}$$

At $s=2$ we have the analytic result

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

Let's define the partial sum $S_N = \sum_{n=1}^{N} \frac{1}{n^2}$.

Write algorithms to compute S_N

I. By summing from $n=1$ up to $n=N$

II. By summing from $n=N$ down to $n=1$

Assignment #1 cont.

1. cont.

For each case plot the fractional error as a function of $h \equiv 1/N$, from $N=10$ to 10^7.
How does the fractional error scale as a function h in each case?
How can you explain the observed behavior?

2. One approximation to the numerical derivative of a function $f(x)$ is:

$$f'(x) \approx \frac{f(x+\frac{1}{2}h) - f(x-\frac{1}{2}h)}{h}$$

Write an algorithm to compute $f'(x)$ for $f(x) = \sin(x)$ at $x=3$.

How does the fractional error scale as a function of h between $h=10^{-1}$ and $h=10^{-17}$?
How can you explain this behaviour?

Assignment # 1 cont.

3. Richardson extrapolation improves the convergence of a given method by eliminating the leading error term.

a. Write down expressions for the first and second order Richardson extrapolation of an arbitrary algorithm that otherwise has a linear error term. Take the scale factor $K=2$ in your examples.

b. Repeat the numerical experiments above using these alternative expressions and compare the h dependence of the error term to your original algorithms.

Document and explain any behaviour you observe.