1 Mathematics 406, Assignment 2'18 Due Oct 5 th

1. **Numerical Integration:**

   Write routines to perform numerical integration of a user-defined function $f(x)$ over an interval $[a,b]$: $I = \int_a^b f(x)dx$ by means of : the Midpoint rule with N cells, the Trapezium rule with N cells, Simpson's rule with $2N$ cells and three point Gauss-Legendre quadrature in each of N cells. Use these routines to evaluate the integrals (a)-(e) below. In each case complete a table of the form:

h	Midpoint	Trapezium	Simpson	Gauss-Legendre
$(b-a)/2$				
$(b-a)/4$				
$(b-a)/8$				
$(b-a)/16$				
$(b-a)/32$				

   and determine the rate of convergence of the algorithms by calculating the error for different values of N. Compare the performance of the different algorithms for each of the given integrals by establishing the order of the error term. Using the error estimate derived in class try to explain the different error behaviour for each of integrands.

   (a) $I = \int_0^1 \sin(5x)\,dx = \frac{1}{5}(1-\cos 5)$

   (b) $I = \int_0^\pi \sin^2 2x dx = \frac{1}{2}\pi$

   (c) $I = \int_0^2 x^{\frac{1}{3}} dx = 3 \cdot 2^{-2/3}$

   (d) $I = \int_0^1 (-\ln x)^{\frac{1}{2}}\,dx = \frac{1}{2}\pi^{1/2}$ (use only the open integration rules i.e. Midpoint and Gauss integration for this integral)

2. Consider the integral, which by Cauchy's integral formula, is given by

   $$\sin a = \frac{1}{2\pi i} \oint_\gamma \frac{\sin z}{z-a} dz$$

   where $\gamma = \partial B_r(b)$ is a circle with radius r and centre located at $z = b$. Use the

   change of variables $z = re^{i\phi} + b$ to arrive at a 1D integral, and evaluate it using Gauss-Legendge quadrature. Use $N = 10$ and 20 intervals, 3 points per interval, $a = i\pi/4$, $b = 1 + i$ and $r = 3$. Now repeat this process with the Composite Trapezium Rule. Compare the results to $\sin a$ by completing the following table.

$Method$	$N = 10$	$N = 20$
$\sin a$		
Gauss Quadrature		
Composite Trapezium Rule		

3. In class we showed that if we apply Richardson extrapolation to the Trapezium Rule then we obtain Simpson's rule. This idea can be extended to obtain higher order Newton-Cotes integration rules. As an example combine two estimates of the same integral using Simpson's Rule with h and $\frac{h}{2}$ and Richardson Extrapolation (recall that the error in the Composite Simpson's Rule is $O(h^4)$) to obtain the so-called Boole's Rule which is given under the list of closed Newton-Cotes formulae in the notes:

$$\int_{x_1}^{x_5} f(x)dx = \frac{h}{45}\left(7f_1 + 32f_2 + 12f_3 + 32f_4 + 7f_5\right) + O(h^7)$$

Repeated Richardson extrapolation applied to the Trapezium Rule is known as Romberg integration. Use the following asymptotic expansion for the error in the Trapezium rule:

$$I(0) - I(h_s) = \sum_{i=1}^{\infty} c_i h_s^{2i}$$

to derive the recursion for Richardson extrapolants for I in which $h_{s+1} = \frac{1}{2}h_s$. If we define $a_s^{(1)} = I(h_s)$ then by eliminating the $O(h^2)$ term in the expansion show that:

$$I(0) - \left\{ a_{s+1}^{(1)} + \frac{a_{s+1}^{(1)} - a_s^{(1)}}{2^2 - 1} \right\} = \sum_{i=2}^{\infty} c_i^{(2)} h_s^{2i}$$

where $c_i^{(2)} = \frac{c_i}{3}\left(\frac{1}{4^{(i-1)}} - 1\right)$. Now define

$$a_s^{(2)} = a_{s+1}^{(1)} + \frac{a_{s+1}^{(1)} - a_s^{(1)}}{2^2 - 1}$$

and use expressions for $a_s^{(2)}$ and $a_{s+1}^{(2)}$ to eliminate the $O(h^4)$ term. Now generalize this to obtain the following recursion for $a_s^{(m)}$ in terms of $a_s^{(m-1)}$:

$$a_s^{(m)} = a_{s+1}^{(m-1)} + \frac{a_{s+1}^{(m-1)} - a_s^{(m-1)}}{4^{m-1} - 1}$$

Modify the routine `trapez` posted on the course web site to perform repeated Richardson Extrapolation until a prescribed tolerance is reached. Call this new function

$$[\texttt{Integral}, \texttt{I}, \texttt{X}] = \texttt{Romberg}(\texttt{f}, \texttt{a}, \texttt{b}, \texttt{tol}, \texttt{kmax})$$

where the inputs are `f`=the integrand, `[a,b]`= the domain of integration, `tol` = the specified tolerance, and `kmax` = the maximum number of refinements. The outputs are: `Integral`= the approximate integral, `I`= the table of extrapolated values, and X= the sample points. Use this routine to evaluate the integral (a) in question 1.

4. Evaluate the Fresnel integral $I = \int_0^{\pi/2} x^{-\frac{1}{2}} \cos x dx$ =1.954902848583 directly using your Midpoint code and your 3-point Gauss-Legendre code. The singularity can sometimes be avoided all together by means of a judicious transformation of variables, which in this case involves the simple substitution $u = x^{\frac{1}{2}}$. Alternatively, the convergence of the numerical approximation can be improved by subtracting out the singularity as follows: $I = \int_0^{\pi/2} x^{-\frac{1}{2}} dx + \int_0^{\pi/2} x^{-\frac{1}{2}}(\cos x - 1)dx = (2\pi)^{\frac{1}{2}} + \int_0^{\pi/2} x^{-\frac{1}{2}}(\cos x - 1)dx$. Since the last integrand is no longer singular it can be evaluated without difficulty using all the routines developed above. Use the the midpoint rule, the repeated Trapezoidal rule, and the 3-point Gauss-Legendre rule to evaluate I by (a) using the transformation, (b) subtracting one and two terms in the Taylor series expansion for $\cos x$.Compare the results by completing the following table:

Integration Rule	$h = 2^{-4}$	$h = 2^{-6}$
Direct Midpoint		
Direct 3 pt Gauss		
Transform Midpoint		
Transform 3 pt Gauss		
Transform Trapezium		
Subtract 1 term Midpoint		
Subtract 1 term 3 pt Gauss		
Subtract 1 term Trapezium		
Subtract 2 terms Midpoint		
Subtract 2 terms 3 pt Gauss		
Subtract 2 terms Trapezium		

5. Consider the problem of evaluating the following integral numerically:

$$I = \int_0^{\infty} \cos^2(x) e^{-x} dx = 3/5$$

   (a) Evaluate the integral using your Romberg integration routine by dividing the integral into two parts $I = I_1 + I_2 = \int_0^c + \int_c^{\infty}$. Estimate how large c should be for $|I_2| < 10^{-5}$ so that $|I - I_1| < 10^{-5}$.

   (b) Now use the five point Gauss-Laguerre Quadrature rule (see http://mathworld.wolfram.com/Laguerre-GaussQuadrature.html to obtain the appropriate abscissae and weights)