Assignment IV: Numerical Quadrature

Due 9/26/2016

1. Evaluate the following integral numerically:

$$\pi = \int_{-1}^{1} dx \frac{2}{1+x^2} \tag{1}$$

using Trapezoidal, Simpson and Gaussian quadrature.
Modify the program *integ1.f90* for this part of the homework.

Compare the relative error

$$\epsilon = \left| \frac{numeric - exact}{exact} \right| \tag{2}$$

for the trapezoidal rule, Simpson's rule, and Gaussian quadrature.

(a) Make a table of the following form

N	h	T-Rule	S-Rule	G-Quad	ϵ_T	ϵ_S	ϵ_G
10	0.1111	⋮	⋮	⋮	⋮	⋮	⋮

(b) Make a plot of $\log_{10} \epsilon$ versus $\log_{10} N$. Note that the ordinate is effectively the number of decimal places of precision.

(c) Use the plot to determine the power-law dependence of the error on the number of points N. (Notice that you may not be able to reach the roundoff error regime for the trapezoidal rule because the approximation error is so large.)

(d) See how your answers change for single precision. Check out at least Simpson and Gaussian quadrature.

(e) How would you analyze your integration results if you didn't know the exact answer? Use the methods from you first assignment to analyze one of the integration rules to find the approximation error in the evaluation of

$$\int_{0}^{1} dx \frac{x^4(1-x^2)^4 \ \cos(5x)}{1+x^2} \tag{3}$$

2. The integral

$$\int_0^\infty \frac{x^3}{e^x - 1} dx \tag{4}$$

appears in Planck's treatment of black body radiation.

(a) Perform the integral numerically with Gauss-Laguerre integration, using 2, 4, 6, 8, 10 points and assess the convergence in an error plot.

(b) Perform the integral numerically with Gauss-Legendre integration by mapping the interval $(0, 1) \to (0, \infty)$ by using your favorite map. How do the two schemes compare?

3. Evaluate the integral

(a)

$$I = \mathcal{P} \int_0^\infty \frac{e^{-2x}}{x^2 - \sigma^2}, \tag{5}$$

where $\sigma = 2.1$ with Gauss-Legendre integration. Make sure you regularize the singularity. Make error plots to find the optimum number of integration points so that your answer is stable with respect to 6 significant figures. Remember, if you map has a parameter, you also need to vary that to find your optimal grid.

(b)

$$I = \mathcal{P} \int_0^{x_{max}} \frac{e^{-2x}}{x^2 - \sigma^2}, \tag{6}$$

with the same value of σ. Take $x_{max} = 20$ for your first calculation. How does this calculation differ from the one in part **(a)**?

(c) Now vary x_{max} so that your answer in **(b)** approximate the 'exact' value of **(a)** to 0.1%, 0.01%, 0.001%, 0.0001%, 0.00001%. Give your answer in tabular form. How large do you have to choose x_{max} in order to obtain the same 6 significant figures you obtained in **(a)**?