I, ____________________________, pledge that this exam is completely my own work, and that I did not take, borrow or steal any portions from any other person. I understand that if I violate this honesty pledge, I am subject to disciplinary action pursuant to the appropriate sections of the San Diego State University Policies.

____
Signature

Be sure to show all your work or include a copy of your programs.

1. Consider the matrix A and vector b given by

$$A = \begin{pmatrix} 1 & -1 & \alpha \\ -1 & 2 & -\alpha \\ \alpha & 1 & 1 \end{pmatrix} \qquad \text{and} \qquad b = \begin{pmatrix} -2 \\ 3 \\ 2 \end{pmatrix}.$$

a. The **Direct Method** for solving this system is **Gaussian elimination**. For this part of the problem, ignore any partial pivoting (as there are many cases). The process of Gaussian elimination is written compactly in the LU factorization of A, given by $A = LU$, where L is a lower triangular matrix representing the row operations of the Gaussian elimination and U is an upper triangular matrix. Find L and U for the matrix A above.

b. Use your LU factorization in Part a to solve the system of linear equations:

$$Ax = b,$$

for A and b given above. Note particular values of α resulting in cases other than a unique solution and give details on what occurs.

c. Find the condition number, $\kappa_1(A)$. You may want to use the information on p. 19 of the text to help find the 1-norm of the matrices used to compute $\kappa_1(A)$.

d. Let $\alpha = 1.01$. Perform the LU factorization, including partial pivoting, so $PA = LU$. List the matrices P, L, and U. Find the condition number, $\kappa_1(A)$, and find the exact solution to this problem. If your computer has only 3-digit arithmetic, then find the solution through LU factorization with partial pivoting with this restricted computer and determine the absolute error in the 1-norm between the actual solution and the solution obtained with your 3-digit computer.

2. In Chemical Engineering, the steady state diffusion in a quiescent fluid body with a first order chemical reaction may be modeled by the following boundary value problem.

$$D\frac{d^2w}{dx^2} - Kw = 0, \quad \text{with} \quad w(0) = C, \quad w(1) = 0, \quad \text{and} \quad x \in (0,1),$$

where w is the concentration of the substance, D is the diffusivity, K is the reaction rate, and C is the fixed boundary concentration at $x = 0$. For this problem, we assume that $D = 0.01$ cm^2/s, $K = 0.1$ s^{-1}, and $C = 5.0$ g/cm^3. It can be shown that the continuous solution to this boundary value problem is

$$w(x) = \frac{5\ \sinh(\sqrt{10}(1-x))}{\sinh(\sqrt{10})}.$$

Often the diffusion operator is discretized with a second order difference. This allows the **boundary value problem** to be written as a matrix system, which can be solved.

a. Let the interval $(0, 1)$ be divided into n even steps with $h = \frac{1}{n}$, so $x_0 = 0$, $x_1 = h$, ... $x_n = 1$. The discrete system can be written $AW = b$, where

$$A = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & -q & 1 & 0 & \cdots & 0 \\ 0 & 1 & -q & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -q & 1 \\ 0 & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad b = \begin{pmatrix} C \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

with $q = 2 + Kh^2/D$. Let $n = 4$ and perform an LU factorization of A. Give your matrices A, L, and U. Solve the system $AW = b$, where $W = [w(x_0), w(x_1), ..., w(x_n)]^T$. Write your solution W. What is the absolute error of this discrete solution at $x = 0.25$, 0.5, and 0.75, as compared to the actual continuous solution?

b. Repeat the process in Part a with $n = 8$ and 16. However, don't write your matrices A, L, and U. Write your solutions W and determine what is the absolute error of these discrete solutions at $x = 0.25$, 0.5, and 0.75, as compared to the actual continuous solution. Create a single graph showing the discrete solutions, W, from both Parts a and b ($n = 4$, 8, and 16) along with the exact solution. Use the **3** calculations at $x = 0.5$ to estimate the order of convergence with respect to the stepsize h.

c. In HW 5, we introduced **Jacobi's iterative method**, where A, a diagonally dominant matrix, was decomposed into a diagonal matrix D, a strictly lower triangular matrix L, and a strictly upper triangular matrix U, so that $A = D - L - U$. By defining $T_j = D^{-1}(L + U)$ and $c_j = D^{-1}b$, then a convergent iterative scheme was produced by

$$x^{(k+1)} = T_j x^{(k)} + c_j, \qquad k = 0, 1, ...,$$

where x^0 is an initial vector. Let $x^0 = [0, ..., 0]^T$ (initially clear solution). Use Jacobi's iterative method to approximate the equilibrium solution $w(x)$ with $n = 8$, so A is a 9×9 matrix. List your iterates, $w^{(k)}$, at $k = 4, 10, 20$, and 50. Create a single graph showing the first 10 iterates of $w^{(k)}$ along with the exact solution.

3. Consider

$$\int_0^3 0.4\, x^3 \cos(x^4)\, dx$$

a. Find the exact value of the integral above. Show the steps for obtaining this answer using techniques from your Calculus course, (*i.e.*, an answer from Wolfram Alpha or Maple is not adequate). Also, provide a graph of this function for the interval of interest.

b. Use the Composite Midpoint and Composite Simpson's Rules with $n = 12$ or $h = 0.25$ to approximate the integral above, and find the absolute errors for these approximations.

c. Use the Composite Midpoint and Composite Simpson's Rules starting with $n = 12$ or $h = 0.25$ to approximate the integral above and halving the stepsize until the accuracy is less than a tolerance of 10^{-6}. Give the value of the stepsizes and state how large the values of n are to achieve this tolerance for each of these methods. The **order of convergence**, p, satisfies:

$$err \approx Ch^p, \qquad \text{which implies} \qquad \ln(err) \approx \ln(C) + p\ln(h),$$

where err is the absolute error, which is absolute value of the method minus the exact solution. It follows that the slope of the log-log plot for err and h approximates the order of convergence. Create a log-log plot of err and h from this halving of the stepsize for each procedure and determine the best fitting p-values.

d. Use the Adaptive Composite Simpson's Rule program provided in class and determine how much this reduces the number of intervals required to be used for the tolerance of 10^{-6} as compared to the even intervals used in Part c.

4. Consider

$$\int_0^4 2\,x^2 e^{-0.6x}\,dx$$

a. Find the exact value of the integral above. Show the steps for obtaining this answer using integration by parts from your Calculus course, (*i.e.*, an answer from Wolfram Alpha or Maple is not adequate). Also, provide a graph of this function for the interval of interest.

b. Use Gaussian Quadrature with 2, 3, 4, and 5 points to approximate the integral above. Find the absolute error is for each of these approximations.

c. Use the Composite Simpson's Rule with $n = 4$ or $h = 1$ to approximate the integral above, and find the absolute error.

d. Use the Composite Simpson's Rule starting with the solution in Part c and halve the stepsize until the accuracy just exceeds that of the Gaussian Quadrature with 5 points. Give the value of that stepsize and state how large the value of n is to achieve this degree of accuracy. Repeat the order of convergence process from Problem 3. Create a log-log plot of err and h from this halving of the stepsize for this procedure and determine the best fitting p-value.

5. a. Suppose, using the Trapezoid rule on the interval $[a, b]$ with step size

$$\Delta x = \frac{b-a}{N},$$

that

$$\int_a^b f(x)dx = T_{\Delta x} f + K_2(\Delta x)^2 + K_4(\Delta x)^4 + \cdots,$$

where

$$T_{\Delta x} f = \frac{\Delta x}{2}\left(f(a) + f(b) + 2\sum_{j=1}^{N-1} f(x_j)\right), \quad x_j = a + j\Delta x.$$

Note, you are making assumptions about how the error behaves very much like the ones we used to derive the Composite Simpson's Rule (see pg. 4, Chapter 6 for discussion). Based on this assumption, if we double the number of points $2N$ in our mesh, or if we cut the mesh width Δx in half, we have that

$$\int_a^b f(x)dx = T_{\Delta x/2}f + \frac{K_2}{4}(\Delta x)^2 + \frac{K_4}{16}(\Delta x)^4 + \cdots$$

So, you now have two approximations, one better than the other. Using these two approximations, show how you get the approximation

$$\int_a^b f(x)dx = \frac{1}{3}\left(4T_{\Delta x/2}f - T_{\Delta x}f\right) - \frac{K_4}{4}(\Delta x)^4 + \cdots$$

This shows that by finding two approximations, we can generate a third which should be of higher order than either. Use the code for the Composite Trapezoid method as a starting point.

b. Write code which implements your new method.

c. Consider the function $f(x) = 0.5 + \sin(x^2)e^{-0.4x}$ on $[0, 10]$. Graph this function and evaluate the integral (with Maple or some similar program). Evaluate your new method with $h = 0.5$ and compare this to the Composite Simpson's rule. For your given test function, compare the performance of your method to the Composite Simpson's method. Which is faster in terms of clock time? Are they as accurate as the other? Is one better in any clear way? Give the absolute error for both of them with this stepsize.

d. Modify your codes in Part c to approximate the integral of $f(x)$ on $[0, 10]$ to a tolerance of 10^{-8} by starting with $h = 0.5$ and halving the stepsize until successive approximations are within the tolerance. What stepsize is required for this integral to be accurate to the tolerance of 10^{-8}? These codes should create log-log plots, which determine the order of convergence for your new method and the Composite Simpson's rule for comparison.

6. Cadmium is a toxic heavy metal used in nickel-cadmium batteries and cadmium telluride solar panels. However, because of its toxicity its use has significantly decreased in other applications. Human exposure to cadmium (Cd) comes from two primary sources. It can be ingested, often with leafy vegetables, raw potatoes, and certain meats, where about 0.5-1.0 μg/day are retained. It is much more readily absorbed through the lungs from cigarette smoke, often doubling the intake in the body. The metal concentrates in the kidney tissue. High exposure can cause itai-itai disease and renal failure (cadmium poisoning). Lower exposure has been linked to the increased risk of cancer (cadmium and smoking).

a. Cadmium is poorly removed from the body and accumulates in the kidney. A differential equation describing the amount of Cd, $C(t)$, in the kidney of a nonsmoker (in mg) is given by:

$$\frac{dC}{dt} = A - kC, \qquad C(0) = 0,$$

where A represents the amount of Cd entering by ingestion of food, k represents the removal rate, and t is in years. The solution of this differential equation in terms of A and k is

$$C(t) = \frac{A}{k}\left(1 - e^{-kt}\right),$$

where the best fitting model to data for the total Cd in the kidney (in mg) for an average nonsmoker at different ages[1] gives

$$A = 0.074 \qquad \text{and} \qquad k = 0.039.$$

The risk of cancer from cadmium is computed by the exposure to this element. The exposure, $E(t)$, is found by the amount of Cd in the tissue times the amount of time that it remains in the tissue. This is readily computed by the integral, which is given by:

$$E(t) = \int_0^t C(s)ds.$$

Use this formula and the computed model, $C(t)$, to determine the exposure of the average nonsmoker at ages 30, 50, and 70. Find the exact value of the integral, then use both the Composite Trapezoid and Composite Simpson's Rules with a stepsize of $h = 5$ to approximate each of the integrals, giving the absolute errors.

b. Find the age to a tolerance of 10^{-2} at which the average nonsmoker achieves an exposure level of 100 mg-yr. Detail how you find this exposure level using the Composite Simpson's Rule along with one of our techniques from the root finding methods. (Note that you could simply use a root finding method if you used the exact solution, but I want you to combine numerical techniques and think about what is contributing most to the error.)

c. As noted above, lungs absorb cadmium much more readily than the gut, so the Cd in cigarettes can easily double the intake of Cd. Because of the carcinogenic properties of Cd, this further increases the cancer risk from smoking. Assume that a smoker begins at age 16. As a simplifying assumption, we will assume that the smoker smokes the same amount of cigarettes annually, and that this increases the Cd intake by a factor of 1.9. For the first 16 years, the amount of Cd entering the body of the smoker is the same as the nonsmoker, following the differential equation in Part a above. For the remainder of the time in this problem, the differential equation describing the amount of Cd, $C_1(t)$, in the kidney of the smoker (in mg) satisfies:

$$\frac{dC_1}{dt} = 1.9A - kC_1, \qquad C_1(16) = C(16),$$

where A and k are the values presented above. This gives the solution of this initial value problem for $t \geq 16$.

$$C_1(t) = \frac{A}{k}\left(1.9 + \left((1 - e^{-16k}) - 1.9\right)e^{-k(t-16)}\right),$$

Again, the exposure, $E_1(t)$, is found by the amount of Cd in the tissue times the amount of time that it remains in the tissue. The first 16 years are found with the same formula as given in Part c, so $E_1(t) = E(t)$. However, the increased Cd in tobacco results in a new formula for $E_1(t)$ for $t \geq 16$. This is computed by the integral, which is given by:

$$E_1(t) = \int_0^{16} C(s)ds + \int_{16}^t C_1(s)ds.$$

Use this formula and the models, $C(t)$ and $C_1(t)$, to determine the exposure of this smoker at ages 30, 50, and 70. Find the exact value of the integral, then use both the Composite

[1] Lars Friberg, Cadmium and the kidney, *Environ. Health Persp.* (1984), **54**, 1-11.

Trapezoid and Composite Simpson's Rules with a stepsize of $h = 1$ to approximate all of the integrals.

d. Find the age to a tolerance of 10^{-2} at which this smoker achieves an exposure level of 100 mg-yr. Detail how you find this exposure level using the Composite Simpson's Rule along with one of our techniques from the root finding methods.

e. Create a graph of the two models, $E(t)$ and $E_1(t)$, for exposure to Cd for $t \in [0, 80]$. Label your axes and curves appropriately. Briefly describe what this graph is saying about the relative risk of cancer from Cd for a smoker compared to a nonsmoker as they age. Include in this discussion a comparison of the ages of a smoker versus a nonsmoker when they achieve the exposure level of 100 mg-yr. Also, compare the risk for someone age 30 to someone age 60 (both smoker and nonsmoker), assuming risk is directly related to exposure.