Midterm
Computational Physics
October 18, 2005

You may not use books, notes, or calculators. For full credit show all of your work and give complete explanations.

1. The set of functions $u_n(x) = \sqrt{2}\sin n\pi x$, with $n = 1, 2, 3, \ldots$, forms an orthonormal basis on $0 \le x \le 1$ using the usual inner product

$$\langle f|g\rangle = \int_0^1 f^*(x)\, g(x)\, dx.$$

Expand the function $f(x) = x$ in this basis. Possibly useful information:

$$\int x \sin kx\, dx = -\frac{1}{k} x \cos kx + \frac{1}{k^2} \sin kx$$
$$\int x \cos kx\, dx = \frac{1}{k} x \sin kx + \frac{1}{k^2} \cos kx$$
$$\int x^2 \sin kx\, dx = \frac{1}{k}\left(\frac{2}{k^2} - x^2\right) \cos kx + \frac{2x}{k^2} \sin kx$$
$$\int x^2 \cos kx\, dx = \frac{1}{k}\left(x^2 - \frac{2}{k^2}\right) \sin kx + \frac{2x}{k^2} \cos kx$$
$$\int x \sin^2 x\, dx = \frac{x^2}{4} - \frac{x}{4} \sin 2x - \frac{1}{8} \cos 2x$$
$$\int x \cos^2 x\, dx = \frac{x^2}{4} + \frac{x}{4} \sin 2x + \frac{1}{8} \cos 2x$$

2. Why is the above expression for $\langle f|g\rangle$ acceptable as an inner product?

3. Write the operator d^4/dx^4 in the above basis, truncated to keep only $n = 1, 2, 3$.

4. Suppose you have calculated approximate values of a function $f(x)$ at a grid of points. That is, you have

$$f_0, f_1, f_2, \ldots, f_{n-1}$$

where f_j is (approximately) $f(x)$ at $x = x_j \equiv jh$. Write pseudocode to calculate the derivative $f'(x)$ evaluated at $x = x_j$ for $j = 1, 2, \ldots, n-2$. Discuss the algorithmic error in your approach.

5. Consider the coupled ordinary differential equations

$$\frac{dy}{dt} = -Ay, \text{ where } y(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix}, \quad A = \begin{pmatrix} -98.00 & -198.02 \\ 99.01 & 199.00 \end{pmatrix},$$

with initial conditions $y_1(0) = 3, y_2(0) = 4$. Discuss the stability of the Euler algorithm applied to this problem. If you needed to solve this numerically for $0 \leq t \leq 1000$, what approach would you use? (You do not need to write pseudocode.)

6. Sketch the Metropolis algorithm applied to the Ising model. What is its chief source of error? No pseudocode is necessary.

7. **(Counts as two problems.)** Consider the ordinary differential equation

$$\frac{d^2x}{dt^2} = -7\cos x - 3\left|\frac{dx}{dt}\right|\sin(3x^5)$$

with initial conditions

$$x(0) = 1, \quad \left.\frac{dx}{dt}\right|_{t=0} = 2.$$

Write pseudocode that implements the 4th order Runge Kutta method to solve this for $x(t)$ for $0 \leq t \leq 8$.