APPLIED MATHEMATICS and STATISTICS

DOCTORAL QUALIFYING EXAMINATION

in COMPUTATIONAL APPLIED MATHEMATICS

Summer 2005 (January)

(CLOSED BOOK EXAM)

This is a two part exam.
In part A, solve 4 out of 5 problems for full credit.
In part B, you must also solve 4 out of 5 problems for full credit.

Indicate below which problems you have attempted by circling the appropriate numbers:

Part A:	1	2	3	4	5
Part B:	6	7	8	9	10

NAME ______________________________

Start each answer on its corresponding question page. Print your name, and the appropriate question number at the top of any extra pages used to answer any question. Hand in all answer pages.

Date of Exam: Tues., May 31, 2005

Time: 9:00 – 1:00 PM

Place: Physics Rm. P-118

A1. Let f and g be linearly independent solutions of the differential equation

$$u'' + p(x)u' + q(x)u = 0,$$

where p and q are continuous functions. Define the Wronskian of f and g by

$$W(x) = f'(x)g(x) - f(x)g'(x).$$

Prove that $W(x) \neq 0$ for all x.

A2. Find all solutions to the differential equation

$$y' = 3y^{2/3}, \qquad \text{with } y(0) = 0.$$

A3. Solve

$$u_x^2 + yu_y - u = 0,$$

subject to the initial condition

$$u(x,1) = 1 + x^2/4.$$

A4. Solve

$$u_{tt} - c^2 u_{xx} = 2t,$$

subject to the initial conditions

$$u(x,0) = x^2, \qquad u_t(x,0) = 1.$$

A5. a) Find the linear (fractional) transformation

$$w = \frac{az+b}{cz+d},$$

which maps the upper half-plane $Im(z) \geq 0$ on to the unit disk $\mid w \mid \leq 1$ in such a way that the "point at infinity" in the $z-$plane corresponds to the point $\frac{1}{2} + \frac{i}{2}$ in the $w-$plane.

b) Using contour integration in a complex plane, show that for $0 < a < 1$,

$$\int_0^\infty \frac{x^{a-1}}{1+x} dx = \frac{\pi}{\sin(a\pi)}.$$

B6. Consider finding the roots of the equation $f(x) = x^2 - 2 = 0$.

a) Show graphically how Newton's method behaves when the starting guess x_1 is near zero.

b) Show graphically how the secant method behaves when $x_1 \approx -0.3$ and $x_2 \approx 0.3$

c) If the secant iteration is converging to a zero of f then, due to rounding errors, it is possible to have $f(x_k) = f(x_{k-1}) \approx 0$. In this case, what is x_{k+1}. When programming the secant method, what would you do when $f(x_k) = f(x_{k-1}) \approx 0$?

B7.

a) Consider the GMRES algorithm to solve the linear system $Ax = b$ for an $m \times m$ matrix A.

Algorithm GMRES (Note: $\|\cdot\|$ denotes $\|\cdot\|_2$.)
$q_1 = b/\|b\|$
for $n = 1, 2, 3 \ldots$
  compute $\tilde{H}_n$ from Arnoldi iteration
  Find y to minimize $\|\tilde{H}_n y - \beta e_1\|$, where $\beta \equiv \|b\|$
  $x_n = Q_n y$

At each step n, we are finding $x_n \in \mathcal{K}_n$ to minimize the residual norm $\|b - Ax_n\|$. One way of doing this is to find y which minimizes $\|AQ_n y - b\|$, where Q_n is an $m \times n$ matrix whose columns $q_1, q_2, \ldots$ span the successive Krylov subspaces $\mathcal{K}_n$. Explain that how the GMRES algiritihm finds the same solution at a reduced cost.

b) Consider the following algorithm to solve $Ax = b$ for a real, symmetric, positive definite matrix A. Prove that the algorithm generates the sequence $r_n = b - Ax_n$.

Conjugate Gradient (CG) Iteration
$x_0 = 0$, $r_0 = b$, $p_0 = r_0$
for $n = 1, 2, 3 \ldots$
  $\alpha_n = (r_{n-1}^T r_{n-1})/(p_{n-1}^T A p_{n-1})$
  $x_n = x_{n-1} + \alpha_n p_{n-1}$
  $r_n = r_{n-1} - \alpha_n A p_{n-1}$
  $\beta_n = (r_n^T r_n)/(r_{n-1}^T r_{n-1})$
  $p_n = r_n + \beta_n p_{n-1}$

B8. Consider the integral

$$I(f) \equiv \int_a^b f(x)dx$$

approximated by the numerical quadrature scheme $I_h(f)$ on a partition of intervals of size $h = (b - a)/N$. Assume that we know

$$I(f) = I_h(f) + Ch^r + o(h^r), \tag{1}$$

where C is a constant.

a) How do you use the information in (1) to make a more accurate scheme, $I_h^*(f)$?

b) Suppose $I_h(f)$ is the trapezoid rule. What is the value of r? What is the expression for your new rule $I_h^*(f)$ written out in terms of values of f at partition points?

B9. Derive

(a) the local (one step) error and

(b) the stability

of the implicit Simpson scheme

$$y_{n+1} - y_{n-1} = \frac{h}{3}(f(y_{n+1}) + 4f(y_n) + f(y_{n-1}))$$

when applied to first order ODE's.

B10. NOTE: This question has 5 parts; it is continued on the next page.

a) Write the most common form of the classical potential energy expression used in computer simulations that employ a Molecular Mechanics force field. Explicitly label all variables and constants that appear in this standard expression.

b) Draw a thermodynamic cycle commonly used to determine the relative free energy of binding ($\Delta\Delta G_b$) between two ligands A and B with a protein receptor P. Clearly label all parts of your figure. Write a simple expression which shows how two legs of the cycle (computed using techniques such as free energy perturbation) are equivalent to the difference in the experimental binding energies $\Delta G_b(\mathrm{A})$ and $\Delta G_b(\mathrm{B})$ between the two ligands.

c) Answer the following questions about molecular modeling.

1. Name a commonly used molecular dynamics (MD) program.

2. Name a commonly used explicit water model.

3. Name a commonly used implicit water model.

4. Give two examples of data plots (property vs. time) often used in MD simulation analysis.

5. What is a typical time step (with units) used in MD simulations?

d) Answer the following question about proteins. use 3 letter codes if appropriate.

1. How many standard amino-acids are there?

2. Name 2 common secondary structure elements.

3. Name 2 types of noncovalent interactions that help stabilize folded proteins.

4. Name 5 amino-acids side chains.

5. Name 2 hydrophobic side chains.

6. Name 2 hydrophillic side chains.

7. Name 1 negatively charged side chain.

8. Name 1 positively charged side chain.

9. Name the side chain that can form disulfide bonds.

10. Name 2 aromatic side chains.

e) Draw each of the following molecules: 1) methane, 2) ethane, 3) methanol, 4) benzene, 5) water. Show and label all the atoms. Show stereochemistry when appropriate.