

**APPLIED MATHEMATICS and STATISTICS
DOCTORAL QUALIFYING EXAMINATION
in COMPUTATIONAL APPLIED MATHEMATICS**

Spring 2006 (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 6 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	11

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: Wed., Jan. 25, 2006

Time: 10:00 – 2:00 PM

Place: Stony Brook Union Auditorium Rm. 123

A1. Find a basis for the solution set to the equation $u'' + xu = 0$.

A2. Find all solutions to the equation $y' = y^2 - 1$. Provide solution sketches in the plane.

A3. In terms of the fundamental solution to the heat equation, write an explicit formula for the solution of

$$\begin{aligned}u_t - \nabla^2 u + cu &= f(x, t), & x \in R^n, t > 0, \\u(x, 0) &= g(x), & x \in R^n\end{aligned}$$

where $c \in R$ is a (non-zero) constant.

Hint: Consider functions $e^{\alpha t}v(x, t)$, for some α .

A4. Solve

$$\begin{aligned} & uu_x + u_y = 1, \\ \text{s.t. } & u(x, x) = x/2 \end{aligned}$$

A5. Calculate the integral

$$\frac{1}{2\pi i} \int_C \frac{dz}{z^3 - 1},$$

where the contour of integration C is the circle $|z - 1| = 1$ traversed in the clockwise direction.

B6. For the following matrix

$$A = \begin{pmatrix} -2.2 & 0.1 & 0.0 & 0.1 \\ 0.1 & 6.1 & 0.2 & 0.2 \\ 0.0 & 0.2 & -4.3 & 0.0 \\ 0.1 & 0.2 & 0.0 & 1.2 \end{pmatrix}$$

- a) Find the ranges in which the eigenvalues of A are located.
- b) Write a program using the shifted inverse power method to find all eigenvalues of A .

B7.

- a) Prove that the Frobenius norm of an $N \times N$ real matrix A equals the square root of the trace of A^2 .
- b) If Q is an $N \times N$ unitary matrix, prove $\|QA\|_F = \|AQ\|_F = \|A\|_F$.
- c) Suppose A is a 100×100 matrix with $\|A\|_2 = 50$ and $\|A\|_F = 51$. Find the lower bound of $\|A^{-1}\|_2$.
- d) Is the matrix in (c) well-conditioned? Why?

B8.

- a) Let P be an $N \times N$ projector. Show that $\|P\|_2 \geq 1$.
- b) If P is a projector and $\|P\|_2 = 1$, show that $I - 2P$ is unitary.
- c) If $a_1^T = (1, 1, 3)$, $a_2^T = (2, 1, 1)$, and $a_3^T = (2, 0, 1)$, find projectors P_2 and P_3 such that $P_2 a_2$ is orthogonal to a_1 and $P_3 a_3$ is orthogonal to a_1 and a_2 .
- d) Describe the Gram-Schmidt projection method and count the number of arithmetic operations needed to orthogonalize an $N \times N$ matrix.

B9. Determine α , β and γ such that the linear, multistep method

$$y_{j+4} - y_j + \alpha(y_{j+3} - y_{j+1}) = h[\beta(f_{j+3} - f_{j+1}) + \gamma f_{j+2}]$$

for the differential equation $y' = f(x)$ has global error of order 3. Is the resulting method stable? Justify your answer.

B10. Consider the quadratic interpolation polynomial $p_2(x)$ to the function $f(x)$ on the points x_n, x_{n-1}, x_{n-2} . We can obtain a point iterative scheme,

$$x_{n+1} = x_n - \frac{f(x_n)}{w(x_n, x_{n-1}, x_{n-2})},$$

by demanding that x_{n+1} be a root of $p_2(x)$. Determine the form of the function $w(\cdot)$. To simplify your work and presentation, do not expand any divided difference coefficients.

B11.

- a) List by name the five potential energy terms used in most classical Molecular Mechanics force fields.
- b) Draw a graph illustrating the shape of the standard Lennard-Jones potential commonly used in Molecular Mechanics simulations. Clearly label all portions of the graph including the axis. Indicate the attractive and repulsive regions and the most common values for the exponents.
- c) Solvent (water) dramatically reduces the interaction energy between two species. Using the data below compute the interaction energies (i.e. the binding energy) in kcal/mol between the ligand and receptor for both the gas-phase and the condensed-phase data. Which type of calculation most reflects what would occur in biological systems? Give a physics-based reason for the difference in the magnitude of the computed binding energies.

species	Molecular Mechanics Gas (MMgas) kcal/mol	Molecular Mechanics GBSA (MMwater) kcal/mol
ligand	-54.9	-142.21
receptor	-6594.6	-10037.69
complex	-6844.05	-10220.49

- d) Answer the following questions about molecular modeling.
- 1) Partial atomic charges are not needed for Generalized Born calculations. (True or False)
 - 2) A successful docking calculation should yield a high RMSD between the most favorably scored binding mode found in the calculation and the experimental pose. (True or False)
 - 3) Disulfide bonds help stabilize proteins. (True or False)
 - 4) RMSD vs. time analysis of MD trajectories help researchers determine if simulations are _____(fill in the blank).
 - 5) Does Generalized Born simulation require periodic boundary conditions? (Yes or No)

e) Draw the following 4 functional groups commonly used in SAR (structure activity relationships). Show and label all atoms and put an "R" at points of attachment. Show stereochemistry when appropriate.

- 1) hydroxyl group
- 2) Et group
- 3) Me group
- 4) benzyl group