NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER II EXAMINATION 2014-2015

PH4505 – Computational Physics

Apr/May 2015 Time Allowed: 2.5 Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FIVE (5)** questions and comprises **SIX (6)** pages.
2. Answer **ALL FIVE (5)** questions.
3. Answer each question beginning on a **FRESH** page of the answer book.
4. This **IS NOT** an **OPEN BOOK** exam.

1. **Runtimes** (25 marks total)

For each of the following operations, state the runtime in big-O notation (e.g. $O(N)$, $O(N^2)$, etc.), and briefly explain why.

(a) The Scipy code `x = A[:,0]`, where `A` is a 2D array of size $M \times N$. (3 marks)

(b) The Scipy code `k = argmax(A, axis=0)`, where `A` is a 2D array of size $M \times N$. (3 marks)

(c) The Scipy code `C = dot(A,B)`, where `A` is a 3D array of size $M \times N \times P$ and `B` is a 2D array of size $P \times Q$. (3 marks)

(d) The Scipy code `X = solve(A, B)`, where `A` is a 2D array of size $N \times N$ and `B` is a 2D array of size $N \times M$. (3 marks)

(e) Solving $\sum_j A_{ij} x_j = b_i$ for $\vec{x}$, assuming we know the LU decomposition of the $N \times N$ matrix $\mathbf{A}$ into $\mathbf{A} = \mathbf{LU}$, where $\mathbf{L}$ is a lower-triangular $N \times N$ matrix and $\mathbf{U}$ is an upper-triangular $N \times N$ matrix. The vector $\vec{b}$ has length N. (4 marks)

(f) The Scipy code `C = A.dot(B)`, where both `A` and `B` are in the List-of-Lists (LIL) sparse matrix format, each with size $N \times N$, but *every element of these matrices is nonzero.* (5 marks)

(g) Calculating the value of the electric potential produced by N point charges, at M distinct positions, in a d dimensional space. (4 marks)

2. **Gaussian elimination** (10 marks total)

Solve the following system of linear equations using Gaussian elimination. (Show intermediate steps for full credit.)

$$\begin{bmatrix} 4 & 4 & 3 & 4 \\ 2 & 2 & 0 & 3 \\ -4 & -1 & 2 & 1 \\ 3 & 1 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 18 \\ 10 \\ 3 \\ 7 \end{bmatrix}$$

3. **Coding tasks** (15 marks total)

For each of the following programming tasks, complete the Python code to achieve the intended purpose. In your answer, you do not need to copy out the starter code.

You can use any standard Python/Scipy function previously used in the homework problems; assume they are already imported. If you have forgotten a function's name or calling convention, choose a name or calling convention and add a comment explaining the choice; you will not be penalized for that.

(a) After solving a discretized eigenvalue problem, normalize the discretized wavefunctions stored in `psi` so that $\int |\psi(x)|^2\, dx = 1$:

```
N = 100
x = linspace(0, 1, N)
H = discrete_hamiltonian(x)
E, psi = eigh(H)
## Insert code here to normalize psi
```

(5 marks)

(b) Given d-dimensional space, let `r` be an $N \times d$ array representing a set of N positions. Find the position in `r` that is closest to a reference position `r0`:

```
N, d = 100, 5
r0 = random.random(d)      # A reference position
r  = random.random((N,d)) # Positions to search
## Insert code here to find the position in r closest to r0
```

(5 marks)

(c) For a system of coupled 1D oscillators, find the trajectories $x_1(t)$ and $x_2(t)$, which are the solutions to

$$\ddot{x}_0 = -\lambda_0 \dot{x}_0 - k_0(x_0 - x_1)$$

$$\ddot{x}_1 = -\lambda_1 \dot{x}_1 - k_1(x_1 - x_0)$$

```
lambd0, lambd1, k0, k1 = 1., 2., 0.1, 0.2
x0i, v0i = 1.0, 0.0       # Initial position/velocity for x0
x1i, v1i = 0.5, 0.5       # Initial position/velocity for x1
t = linspace(0, 10, 1000) # Array of times.
## Insert code here to find x0(t) and x1(t)
```

(5 marks)

4. **Numerical integration** (20 marks total)

(a) Consider a function $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \cdots$ (i.e., a function which can be written as a MacLaurin series), and its integral from $-L$ to L:

$$I \equiv \int_{-L}^{L} f(x)\, dx.$$

Suppose we approximate I by sampling $f(x)$ at the points $x = \pm L$:

$$I_{\text{approx}} = pf(-L) + qf(L).$$

Find the values of p and q which give rise to the smallest numerical error, and derive the numerical error to lowest order in L (leaving your answer in terms of one or more of the unknown coefficients $a_0, a_1, a_2, \ldots$) (4 marks)

(b) Now suppose we approximate I by sampling $f(x)$ at two points $x = \pm h$, which need *not* coincide with the end-points of the integral:

$$I_{\text{approx}} = uf(-h) + vf(h).$$

Find the values of u, v, and h which give rise to the smallest numerical error, and derive the numerical error to lowest order in L (leaving your answer in terms of one or more of the unknown coefficients $a_0, a_1, a_2, \ldots$) (8 marks)

(c) Now consider a smooth function $f(x)$ and its integral between two arbitrary points A and B:

$$I \equiv \int_{A}^{B} f(x)\, dx.$$

We want to approximate I by sampling $f(x)$ at N points (where N is even). By extending your results in part (b), propose a method for performing this approximation, and derive how the numerical error scales versus N. Your answer should be given in terms of the constants A, B, and N.

(4 marks)

(d) In terms of numerical error, how does the method of part (c) compare with the trapezium rule and Simpson's rule? (4 marks)

5. **Markov chains** (30 marks total)

(a) Consider a modified Ehrenfest model. We have two boxes (A and B), a total of N particles to distribute between them, and the following Markov process:

i. Randomly choose one of the N particles (with equal probability).

ii. If the chosen particle was in box A, transfer it to B with probability p; whereas if the chosen particle was in B, transfer it to A with probability q. Otherwise, leave the particle in place.

For $N = 4$, draw the state diagram, and write down the transition matrix. Indicate clearly what your state labels correspond to. (4 marks)

(b) For the model described in part (a), find the stationary distribution for general N, in terms of p and q. For $N = 4$, show that it is an eigenvector of the transition matrix found in (a). (10 marks)

(c) The model described in part (a) maps onto a thermodynamic system of N particles at temperature T, where each particle has two possible states, with energies E_A and E_B respectively. Explain this mapping, and derive the relationship between the Markov parameters $\{p, q\}$ and the thermodynamic parameters $\{T, E_A, E_B\}$.

(4 marks)

(d) Consider a "grand canonical ensemble": similar to part (c), each particle has two possible states, with energies E_A and E_B respectively, but the number of particles N is now allowed to fluctuate. The probability to have N particles is proportional to $\exp(-\mu N)$, where μ is the chemical potential.

Describe a modified Ehrenfest model that maps onto this grand canonical ensemble. Explain how the Markov parameters in your model are related to the thermodynamic parameters μ, T, E_A, and E_B. (12 marks)

- End of Paper -

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Please read the following instructions carefully:

1. **Please do not turn over the question paper until you are told to do so. Disciplinary action may be taken against you if you do so.**

2. You are not allowed to leave the examination hall unless accompanied by an invigilator. You may raise your hand if you need to communicate with the invigilator.

3. Please write your Matriculation Number on the front of the answer book.

4. Please indicate clearly in the answer book (at the appropriate place) if you are continuing the answer to a question elsewhere in the book.