NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER II EXAMINATION 2013-2014

PAP455/PH4505 – Computational Physics

April 2014 Time Allowed: 2½ Hours

SEAT NUMBER:

MATRICULATION NUMBER:

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FIVE (5)** questions and comprises **SEVENTEEN (17)** pages.

2. Answer **ALL FIVE (5)** questions.

3. This is **NOT** an **OPEN BOOK** examination.

4. Candidates may use calculators. However, they should write down systematically the steps in the workings.

5. All your solutions should be written in this examination paper within the space provided after each question.

For examiners:

Questions	**1** (15)	**2** (15)	**3** (20)	**4** (25)	**5** (25)	**Total** (100)
Marks						

1. **Matrix multiplication** (15 marks total)

This question is about the runtimes of different matrix multiplication operations. You should specify runtimes in Big-O notation, e.g. $O(N^2)$.

(a) Let A be a full $M \times N$ matrix, and B be a full $N \times P$ matrix. What is the runtime of $C = AB$, computed using the standard row-times-column algorithm? Give a brief explanation.

(3 marks)

(b) Let A be an $N \times N$ tridiagonal matrix (i.e., non-zero only along the main diagonal, and one element above/below); let B be a full $N \times P$ matrix. What is the runtime of $C = AB$? Give a brief explanation.

(3 marks)

Note: Question no. 1 continues on Page 3.

(c) Suppose there is no `dot` function, or any other function for matrix multiplication. Write Scipy code to do the operation discussed in part (b) (i.e., $C = AB$ where A is $N \times N$ tridiagonal and B is $N \times P$ full), starting from the line below. Assume that `A`, `B`, `N`, and `P` are defined, and that `A` is indeed tridiagonal.

(3 marks)

```
C = zeros((N, P))
```

(d) Let L be an $N \times N$ lower triangular matrix (i.e., elements above the diagonal are zero), and U an $N \times N$ upper triangular matrix (i.e., elements below the diagonal are zero). What is the runtime of $C = LU$? Give a brief explanation.

(3 marks)

Note: Question no. 1 continues on Page 4.

(e) For the operation $C = LU$ discussed in part (d), suppose the runtime is 1ms for matrix size $N = 1000$. In Fig. 1 below, sketch the log-log plot of the runtime t versus N.

(3 marks)

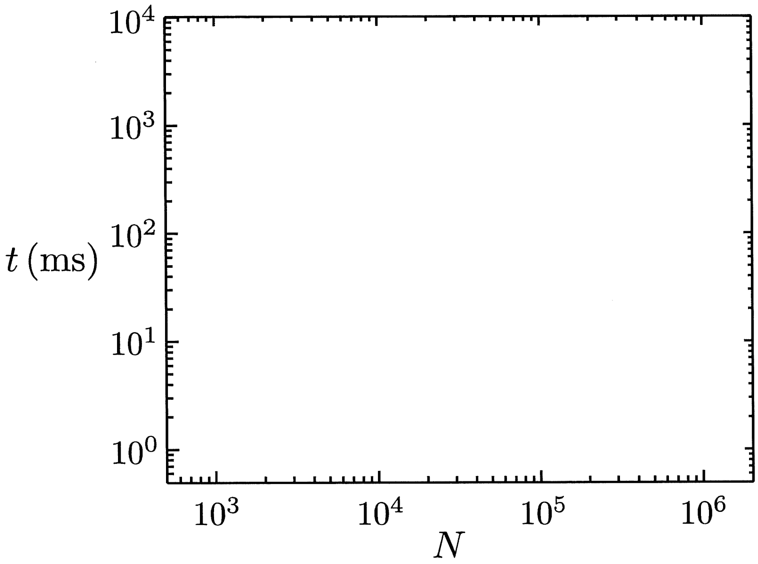


FIG. 1: Log-log plot of runtime t vs matrix size N.

2. **Debugging** (15 marks total)

In each of the code examples shown below, there is *one* incorrectly-written line. Circle the line containing the mistake, and state how it should be re-written. Assume all necessary `import` statements, variable definitions, etc. have been done.

(a) Plotting the mean energy $\langle E \rangle$ as a function of temperature T, with each value of $\langle E \rangle$ averaged over 200 Monte Carlo runs. The function `mc_sim(T)` performs one run at temperature `T`, and returns the energy.

(3 marks)

```
T = linspace(10, 100, 1000)
E = zeros(len(T))
nsamples = 200
energies = zeros(nsamples)

for k in range(len(T)):
    for m in range(nsamples):
        energies[m] = mc_sim(T[k])
        E[k] = energies[m]

plt.plot(T, E)
plt.show()
```

(b) Plotting the potential $V(x) = kx^2$ for $k = 10$.

(3 marks)

```
def potential(k):
    def f(x):
        return k*x**2
    return f

k, x = 10, linspace(-5, 5, 100)
plt.plot(x, potential(x))
plt.show()
```

Note: Question no. 2 continues on Page 6.

(c) Computing $\sum_n |\langle x|n\rangle|^2$, where $|x\rangle$ is a complex vector and $\{|n\rangle\}$ are the eigenvectors of a matrix H. The variables `H` $\equiv H$ and `x` $\equiv |x\rangle$ are already defined.
(3 marks)

```
u, v  = scipy.linalg.eig(H)

value = 0.
for n in range(len(u)):
    dotprod = x * v[:,n]
    value   += abs(dotprod)**2

print(value)
```

(d) Plotting the energy eigenvalues of an $N \times N$ Hamiltonian $H = H_0 + \lambda V$, as λ is varied over the range $[0, 1]$. Assume `H0`, `V`, and `N` are already defined.
(3 marks)

```
lambd = linspace(0,1,100)
E = zeros((N,len(lambd)))

for n in range(len(lambd)):
    H = H0 + lambd[n] * V
    E[:,n] = sort(scipy.linalg.eigvalsh(H))

for n in range(N):
    plt.plot(lambd, E[:,n], 'b')
plt.show()
```

Note: Question no. 2 continues on Page 7.

(e) Computing the circulation of a vector field $\vec{A}(x, y)$,

$$C = \oint \vec{A} \cdot d\vec{\ell},$$

over a loop of radius R centered at position (x_0, y_0).

(3 marks)

```
# An example vector field A(x,y)
def A(x, y):
    return -y, 0*x


# Function to compute the circulation
def circulation(vecfield, R, x0, y0):
    phi = linspace(0, 2*pi, 1000)
    x   = x0 + R * cos(phi)
    y   = y0 + R * sin(phi)

    vx, vy = vecfield(x, y)
    vphi   = -vx * sin(phi) + vy * cos(phi)
    return trapz(vphi, phi)


print(circulation(A, 1, 0, 0))
```

3. **The Finite-Difference Method** (20 marks total)

(a) In class, we discussed the three-point formula for the second derivative $f''(x_0)$:

$$f''(x_0) \approx \frac{1}{a^2}\Big[f(x_0 - a) - 2f(x_0) + f(x_0 + a)\Big].$$

Suppose we want f'' at a position x_0 *between* sampling points. We can use a finite-difference formula with four points $[x_0 - 3a/2,\ x_0 - a/2,\ x_0 + a/2,\ x_0 + 3a/2]$:

$$f''(x_0) = Af(x_0 - 3a/2) + Bf(x_0 - a/2) + Cf(x_0 + a/2) + Df(x_0 + 3a/2) + O(a^p).$$

Find the constants $[A, B, C, D]$, and find the order of the truncation error.

(7 marks)

Note: Question no. 3 continues on Page 9.

(b) In electrostatics, the potential $\phi(x)$ obeys Poisson's equation

$$-\frac{d^2\phi}{dx^2} = \rho(x)$$

where $\rho(x)$ is the charge density. Let $\rho_n \equiv \rho(x_n)$, where $\{x_0, x_1, \dots, x_{N-1}\}$ are equally-spaced points with $a = x_{n+1} - x_n$. Let $\phi_n = \phi(x_n - a/2)$ denote the potential at the *mid-point* positions. Poisson's equation can be written as

$$M \begin{bmatrix} \phi_0 \\ \vdots \\ \phi_{N-1} \end{bmatrix} = \vec{y}.$$

Find an appropriate matrix M and vector $\vec{y}$, ignoring boundary conditions. You may give your answer in terms of $\{A, B, C, D\}$ from part (a).

(5 marks)

Note: Question no. 3 continues on Page 10.

(c) Now consider the boundary conditions

$$\phi'(x_0 - a) = -E$$
$$\phi(x_{N-1} + a) = 0,$$

where E is a constant and a is the previously-defined point spacing. $\phi'(x)$ is the first derivative of $\phi(x)$. For these boundary conditions, derive the modified finite-difference matrix equation.

(8 marks)

4. **Fourier Analysis** (25 marks total)

(a) A damped harmonic oscillator obeys the equation

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0.$$

Suppose $\omega_0 > \gamma$, with initial conditions $x(0) = x_0$, $\dot{x}(0) = 0$. Let the Fourier transform of $x(t)$ be $X(\omega)$. Sketch $|X(\omega)|^2$ versus ω. Derive the frequency, height and width of the Fourier peak, in terms of γ, ω_0, and/or x_0.

(5 marks)

(b) Suppose ω_0 and γ are approximately known, and we wish to compute the Fourier spectrum. How should we choose the total sampling time interval T, and the number of sampling times N? Explain your reasoning.

(4 marks)

Note: Question no. 4 continues on Page 12.

(c) A driven harmonic oscillator obeys

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = F_0 \cos(\Omega t).$$

Supposing the system is in steady-state oscillation, let the Fourier transform of $x(t)$ be $X(\omega)$. Sketch $|X(\omega)|^2$ versus ω. Derive the frequency, height and width of the Fourier peak, in terms of γ, ω_0, Ω, and/or F_0.

(5 marks)

(d) Suppose we sample an unknown $x(t)$ at times $[t_0, t_1, \ldots, t_{N-1}]$, which are evenly-spaced with $t_{n+1} - t_n = \Delta t$. Using the mid-point or trapezium rule, derive an approximation for $X(\omega_k)$, where $X(\omega) = \int_{T_1}^{T_2} dt\, x(t)\, e^{-i\omega t}$ is a truncated Fourier integral. Specify the frequencies ω_k and the integral endpoints T_1 and T_2.

(4 marks)

Note: Question no. 4 continues on Page 13.

(e) Repeat part (d), but using Simpson's rule

$$\int_a^b f(z)\,dz \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Choose an appropriate set of discretized frequencies ω_k, and derive $X(\omega_k)$.

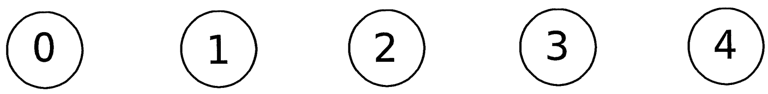
(7 marks)

5. <u>**Markov Chains**</u> (25 marks total)

Consider a Markov chain with N states, denoted $\{x_0, x_1, \ldots, x_{N-1}\}$, and transition probabilities given by

$$
\begin{aligned}
P(x_m|x_n) &= \left\{ \begin{array}{ll} a_n & \text{if } m = n+1 \\ b_n & \text{if } m = n-1 \\ 1 - a_n - b_n & \text{if } m = n \end{array} \right\} \qquad \text{for } 1 \le n \le N-2. \\
P(x_1|x_0) &= a_0, \qquad P(x_{N-2}|x_{N-1}) = b_{N-1} \\
P(x_0|x_0) &= 1 - a_0, \quad P(x_{N-1}|x_{N-1}) = 1 - b_{N-1}.
\end{aligned}
$$

(a) For $N = 5$, fill in the state diagram below, and label the transition probabilities. (3 marks)



(b) For $N = 5$, write down the transition matrix $P_{mn} \equiv P(x_m|x_n)$. (3 marks)

Note: Question no. 5 continues on Page 15.

(c) Using the principle of detailed balance, derive the steady-state distribution $[p(x_0), \ldots, p(x_{N-1})]$, in terms of the transition probabilities a_n and b_n.

(4 marks)

(d) Suppose the Markov chain represents a thermodynamic system, with state x_n having energy E_n. Let the temperature be T. How should a_n and b_n be chosen?

(4 marks)

Note: Question no. 5 continues on Page 16.

(e) Denote the state probabilities on turn j by $[p(x_0, t_j), \ldots, p_j(x_{N-1}, t_j)]$. We can regard $p(x_n, t_j)$ as a set of points sampled from a continuous function $p(x, t)$. Then the Markov chain is the finite-difference limit of a differential equation:

$$\frac{\partial p}{\partial t} = \left[D(x) \frac{\partial^2}{\partial x^2} + \mu(x) \frac{\partial}{\partial x} + V(x) \right] p(x, t).$$

Let the space and time steps be normalized to unity: $\Delta x = \Delta t = 1$. Let $a(x)$ and $b(x)$ be functions such that $a(x_n) = a_n$ and $b(x_n) = b_n$. Derive $D(x)$, $\mu(x)$ and $V(x)$ in terms of $a(x)$ and $b(x)$, ignoring boundary conditions.

(8 marks)

Note: Question no. 5 continues on Page 17.

(f) Suppose the transition amplitudes are all equal: $a_n = b_n = a$. Let $\langle T \rangle$ be the average number of steps required to reach state x_{N-1}, if the Markov chain is initially in state x_0. How does $\langle T \rangle$ scale with N?

(3 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.