Final Written Exam
University of Jordan
Physics Department

Date: 6-6-2005
Time: one hour

Software Packages in Physics
Final Exam

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Q1. In the course of this semester you took 7 lab sheets presenting problems from all sorts of fields, but the problems they posed can be classified into the five categories you know very well by now:

1. Numerical analysis.
2. Symbolic algebra.
3. Simulation.
4. Visualization.
5. Collection and analysis of data.

Mention what categories were involved in each of the 7 sessions.

Q2. Suppose a researcher wants to study a phenomenon that requires performing the following two tasks:

1. Conducting experiments in the lab, and collecting data using a computer.
2. Analyzing the resulting data on a computer, based on certain theoretical models.

In the various stages of this research, what general guidelines you think our researcher should follow in order to minimize the effect of errors?

Q3. Solve the following equation numerically for x.

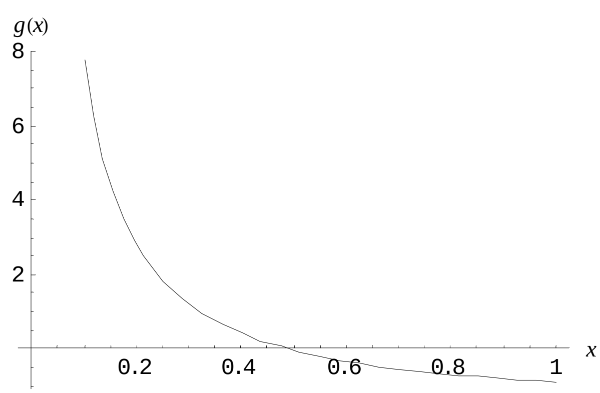
$$\int_1^2 J_1(y^2 - 1)y\,dy \equiv \xi = \frac{1}{2}\frac{e^{-x}}{x}$$

Where $J_1(x)$ is Bessel's function of the first kind.

Proposed algorithm:

1. This problem can be divided into two parts; evaluating the constant ξ, then solving the remaining equation for *x*.
2. We propose that you use the 1/3-Simpson rule to evaluate the integral. <u>Three</u> subdivisions are sufficient to get a good estimate of the integral.
3. As for the equation to be solved, we propose applying Newton's method on the function $g(x) = 2\xi - \dfrac{e^{-x}}{x}$. For this step, use as many iterations as needed to reach a tolerance for $|x_{n+1} - x_n|$ no greater than 0.0005.
4. You might find the following information useful:

x	$J_1(x)$
0.5	0.242268
1.0	0.440051
1.5	0.557937
2.0	0.576725
2.5	0.497094
3.0	0.339059



Q4. Seminars: True or False?

1. A property of complex systems is *emergence*. Friction, real gases, electrons, and society are usually considered examples of emergent structures or emergent phenomena. ( )

2. The Monte-Carlo method works because it uses randomness to scan through the space of the problem. ( )

3. Typically, a Linux installation requires four partitions to work. ( )

4. A classical bit of memory can hold a one or a zero or a superposition of both. ( )

5. In architecture, CAD has existed for a relatively long time, but only recently have there been major software and hardware breakthroughs that made sophisticated CAM in that field possible. ( )

6. MATLAB is best known for its use of real-mathematics notation. ( )

7. FORTRAN is so messy, that in writing a large programme it is not a bad idea to seek clarity over efficiency. ( )

8. CUPS is a scientific programming language. ( )

9. The following is a valid Maple statement: `>1+1;` ( )

10. Optica is a Mathematica package that has both educational and industrial uses. ( )

11. A Linux cluster can be thought of as a parallel computing system. ( )

12. A FLOP is a measure of the speed of a quantum computer. ( )

Solution and Marking

What follows is the model solution for the problems above along with the marks put on each item:

Q1: The following table classifies the type of problem addressed in each session.

Session	Numerical Techniques	Symbolic Algebra	Simulation	Visualization	Collection and Analysis of Data
1	✓	✓	×	✓	×
2	✓	✓	×	×	×
3	✓	✓	✓	✓	×
4 and 5	Even though some of the programmes in these sessions could be classified according to the provided categories, the emphasis, and main idea in these two sessions were on programming techniques, and as such cannot be described by the given categories.				
6	✓	×	×	✓	✓
7	✓	×	×	✓	×

Q2: The situation depicted has several sources of errors, none of which can be completely eliminated, but many of them can certainly be reduced significantly by carrying out things carefully. One can perhaps divide the sources of errors in this experiment into three categories:

1. **Errors related to the actual measurement and design of the experiment**. Such errors are reduced by efficiently addressing aspects of the experiment-design that would be suspected as possible sources of error. Since, in the present situation a computer takes care of the data-collection process, the effect of human factor in the overall error in the measurement process is negligible.
2. **Errors related to the method of analysis used**, and whether it requires certain simplifying assumptions or approximations, and especially those due to the use of numerical techniques. The level of approximation depends greatly on the efficiency of the method of analysis used, it can also depend to some extent on the computer software used in analysis, where a computer-algebra-system (CAS) can reduce the adverse effects in some cases.
3. **Intrinsic computer-related errors**, which have to do with how a computer works, specifically; we mean round-off errors; also here, using a CAS is likely to reduce the effect of this problem.

Q3: We start by looking at the given integral:

$$\int_1^2 J_1(y^2-1)y\,dy$$

To apply the Simpson rule on this integral, we need to know the values of the integrand at the points of subdivision, and by subdivision here, we mean the number *n*, which occurs in our Simpson's rule, and not the actual number of subdivisions, which happens to be double that number. We are given a table of values of the integrand, but for the form of the integral provided, it turns we are unable to use that table immediately, rather we need to transform the integral appropriately through a change of variables, as we shall see shortly.

Recall that the points at which the Simpson rule is evaluated are defined by the following formula:

$$x_i = a + \frac{b-a}{2n} i$$

where for the integral at hand, we have $a=1$, $b=2$, and *n* is proposed to be 3, so that $x_i = 1 + i/6$. Clearly, the values of x_i that would result, then, make the given table useless! So, we make a change of variables $y^2 - 1 \equiv z \Rightarrow 2y\,dy = dz$:

$$\int_1^2 J_1(y^2-1)y\,dy = \tfrac{1}{2}\int_0^3 J_1(z)\,dz\,,$$

in which case, the given table certainly gets useful, since the subdivisions would then lie exactly at each one of the points $x_i = i/2$ available in the table. Simpson's 1/3-rule reads:

$$\int_a^b f(z)\,dz = \frac{b-a}{6n}\sum_{i=1}^{3}(y_{2i-2} + 4y_{2i-1} + y_{2i}),$$

Thus, our integral can be approximated as:

$$\begin{aligned}\int_0^3 J_1(z)\,dz &\approx \frac{3}{6\times 3}\sum_{i=1}^{3}(y_{2i-2} + 4y_{2i-1} + y_{2i}) \\ &= \frac{1}{6}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + 4y_5 + y_6)\end{aligned},$$

Recalling that $y_n \equiv y(x_n)$, and using the tabulated values of the Bessel function, we get the following:

$$\begin{aligned}\int_0^3 J_1(z)\,dz &\approx \frac{1}{6}(J_1(0) + 4J_1(0.5) + 2J_1(1) + 4J_1(1.5) + 2J_1(2) + 4J_1(2.5) + J_1(3)) \\ &= \frac{1}{6}(0 + 4\times 0.242268 + 2\times 0.440051 + 4\times 0.557937 + 2\times 0.576725 \\ &\qquad +4\times 0.497094 + 0.339059) \\ &= 1.2603\end{aligned}$$

which means that:

$$\xi \approx 1.2603/2 = 0.63015$$

(The actual value of this integral can be obtained analytically, and in that case, our answer is fairly close: $\xi = 0.63015$).

Now we move to the next step of the solution; to solving the equation for *x*. By plugging the value of ξ we've just obtained in the original equation, we get the following:

$$1.2603 - \frac{e^{-x}}{x} = 0$$

To use Newton's method on this equation, we notice that in effect we're looking for the zeros of the function $g(x) = 1.2603 - e^{-x}/x$. For a close-enough initial guess of *x*, the Newton method iterations will be given by the following formula:

$$x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)} = x_n - \frac{2x_n^2 e^{x_n}\xi - x_n}{(1+x_n)}$$

Our initial guess is $x_0 = 0.5$, which we obtain from the supplied plot of $g(x)$. The following table shows the first couple of iterations:

Iteration	x_n	$\lvert x_{n+1} - x_n \rvert$
0	0.5	—
1	0.487019	0.013
2	0.487373	0.000354

If our programme is driven by tolerance, then it will have exited by now, since $0.000354 < 0.0005$. Incidentally, the actual answer is $x = 0.487438$.

Q4: The answers should be:

Problem	1	2	3	4	5	6	7	8	9	10	11	12
Answer	F	T	F	F	T	F	T	F	F	T	T	F

Marking: Students were asked to solve 3 out of 4 problems provided that Q3 and Q4 are two of them. Each problem was given 33.3% of the written exam's mark.