UNIVERSITY OF OSLO

FACULTY OF MATHEMATICS AND NATURAL SCIENCES

Exam in FYS3150 Computational Physics, Fall 2011
Day of exam: Tuesday December 13, 9am
Exam hours: Four (4) hours
This examination paper consists of five (5) pages.

Allowed material:	Rottmann: Matematische Formelsamlung (In Norwegian, English or German) Two A4 sheets with own notes (totaling 4 pages). Approved numerical calculator.

Make sure that your copy of this examination paper is complete before answering. Check the number of pages. You can answer in English or Norwegian. The final written exam counts 50% of the final mark. The remaining 50% is accounted for by project 5.

Exercise 1, Ordinary differential equations

We have the second-order differential equation for a so-called RLC electric circuit

$$L\frac{d^2Q}{dt^2} + \frac{Q}{C} + R\frac{dQ}{dt} = A\cos(t),$$

where t stands for time. The other quantities are the charge Q, the resistance R, the current I, the inductance L, the capacitance C and the applied voltage $V(t) = A\cos(t)$, with A the amplitude of the applied voltage.

a) Rewrite the above second-order differential equation as two coupled first-order differential equations (hint: you will need one equation for the derivative of the charge $dQ/dt = I$ and one for the current I, namely $dI/dt = d^2Q/dt^2$).

b) Derive the equations for Euler's algorithm with an estimate for the error in Δt for the two coupled differential equations. Set up the essential steps in the algorithm for solving the equation. The algorithm for solving the equations can be written out as pseudocode or as a program.

c) Repeat the steps from the previous exercise but derive now the equations for the second-order and the fourth-order Runge-Kutta methods. Find also the error Δt. Write down the final algorithm either as pseudocode or as a program.

Exercise 2, Numerical integration

We have the three-dimensional integral

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdydz\frac{\exp(-r)}{r},$$

with $r = \sqrt{x^2+y^2+z^2}$. The integral is easy to solve and the result is, using spherical coordinates,

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdydz\frac{\exp(-r)}{r} = 4\pi\int_0^{\infty}\exp(-r)rdr = 4\pi.$$

There is no depedence on the angles θ, ϕ in the integrand.

a) Derive the equations for the Trapezoidal rule (with an error estimate) and set up an algorithm for integrating the above integral, either in cartesian or spherical coordinates. Explain the basic philosophy behind methods based on Newton-Cotes quadrature.

b) We switch now to integration by Gaussian quadrature. Explain the basic philosophy behind the determination of integration points x_i and derive the equation for finding the integration weights w_i.

c) We choose now to perform the integration using Gaussian quadrature and Legendre polynomials. These are orthonormal polynomials defined in the interval $x \in [-1,1]$. However, for a general interval $t \in [a,b]$ we can always use the mapping

$$t = \frac{b-a}{2}x + \frac{b+a}{2}.$$

If we have an integral on the form

$$\int_0^{\infty} f(t)dt,$$

we can choose new integration points using the mapping

$$t_i = \tan\left\{\frac{\pi}{4}(1+x_i)\right\},$$

and integration weights

$$\xi_i = \frac{\pi}{4}\frac{\omega_i}{\cos^2\left(\frac{\pi}{4}(1+x_i)\right)},$$

Table 1: integration points and weights for the interval $x \in [-1, 1]$ with $N = 2$ using Legendre polynomials.

i	x_i	ω_i
1	$-1/\sqrt{3}$	1
2	$1/\sqrt{3}$	1

where x_i and ω_i are the original integration points and weights in the interval $[-1, 1]$, while t_i and ξ_i are the new integration points and weights for the interval $[0, \infty)$, respectively. The polynomials obey the orthogonality relation

$$\int_{-1}^{1} L_i(x) L_j(x) dx = \frac{2}{2i+1} \delta_{ij}.$$

The first three Legendre polynomials are

$$L_0(x) = 1,$$

$$L_1(x) = x,$$

and

$$L_2(x) = (3x^2 - 1)/2.$$

Set up the algorithm for computing the above integral, using either cartesian or spherical coordinates. Explain your choices of integration domains. Assume that the function which sets up the integration points and weights is known (you don't need to write the algorithm for that). Calculate thereafter the integral using two integration points only, using the integration points and weights set up for $x \in [-1, 1]$ in Table 1.

d) The integrand in

$$I = 4\pi \int_0^\infty \exp(-r) r dr,$$

is well suited for using Laguerre polynomials. In that case, we identify a weight function $W = \exp(-r) r$. Set up the algorithm for computing the integral using Laguerre polynomials (again either in pseudocode form or as a program) and find the value of the integral using $N = 2$ integration points and the values for the integration points and weights listed in Table 2. Again, assume that the function which sets up the integration points and weights is known (you don't need to write the algorithm for that).

Table 2: integration points and weights for the interval $x \in [0, \infty)$ with $N = 2$ only using Laguerre polynomials with a weight function $\exp(-r)r$.

i	x_i	ω_i
1	1.26795	0.788675
2	4.73205	0.211325

e) Explain then the philosophy behind Monte Carlo integration and set up an algorithm for brute force calculation of

$$I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdydz \frac{\exp(-r)}{r}.$$

using the uniform distribution. Discuss thereafter how you could rewrite the above integral using spherical coordinates and importance sampling (hint: you need to map your random variables generated with the uniform distribution to the exponential distribution). Set up the final algorithm for performing importance sampling.

f) Discuss finally also which method you would prefer for calculating this particular integral, that is, discuss the pros and cons of the methods discussed in exercises a), c), d) and e).

Exercise 3, Eigenvalue Problems

a) We have the eigenvalue problem

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x},$$

where we assume that the matrix $\mathbf{A}$ is non-singular and $\mathbf{A} \in R^{n\times n}$. The matrix is symmetric and real. The vector $\mathbf{x} \in R^n$ and the eigenvalues λ are unknown.

To obtain the eigenvalues of $\mathbf{A} \in R^{n\times n}$, the strategy is to perform a series of so-called similarity transformations on the original matrix $\mathbf{A}$, in order to reduce the matrix to a diagonal form. Show that such similarity transformations do not change the eigenvalues λ.

b) We have the following two-point boundary value differential equation

$$\frac{d^2y}{dx^2} + v(x)y(x) - \epsilon y(x) = 0, \quad x \in (0,1), \quad y(0) = y(1) = 0.$$

The function $v(x)$ and the constant ϵ are real. The function $v(x)$ is known while ϵ is unknown. Show that (when discretizing y and x) this equation can be rewritten as an eigenvalue problem

$$\mathbf{A}\mathbf{y} = \lambda \mathbf{y},$$

where now $\mathbf{y}$ is a discretized version of the unknown $y(x)$. Find the matrix $\mathbf{A}$. How does this matrix change if we modify the differential equation to

$$\frac{d^2y}{dx^2} + \alpha \frac{dy}{dx} + v(x)y(x) - \epsilon y(x) = 0, \qquad x \in (0,1), \qquad y(0) = y(1) = 0,$$

where α is a constant.

c) Set up an algorithm for solving

$$\frac{d^2y}{dx^2} + v(x)y(x) - \epsilon y(x) = 0, \qquad x \in (0,1), \qquad y(0) = y(1) = 0,$$

using Jacobi's method. Explain the basic steps in the algorithm and how you would choose the similarity transformations. Write up a final algorithm (only for finding the eigenvalues and without the computation of the eigenvenctors) either as a pseudocode or as a program.

Discuss at least one point in favour and one against using the Jacobi algorithm.