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 three (3) 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, Metropolis algorithm

In this exercise the aim is to set up an algorithm that employs the Metropolis algorithm with the Boltzmann distribution

$$w(\beta) = \frac{\exp\left(-\beta E\right)}{Z},$$

where $\beta = 1/kT$ is the inverse temperature, E is the energy of the system and Z is the partition function (a normalization constant).

We are going to study one single particle in equilibrium with its surroundings, the latter modelled via a large heat bath with temperature T. The model used to describe this particle is that of an ideal gas in **one** dimension and with velocity $-v$ or v. We are interested in finding $w(v)dv$, which expresses the probability for finding the system with a given velocity $v \in [v, v+dv]$. The energy for this one-dimensional system is

$$E = \frac{1}{2}kT = \frac{1}{2}v^2,$$

with mass $m = 1$.

a) Write down the Metropolis algorithm and explain the assumptions underlying its derivation (hint: think of Markov chains and detailed balance).

b) Write an algorithm which sets up the histogram $w(v)dv$, finds the mean velocity, energy and energy variance for a given temperature using the Metropolis algorithm. Use a step size δv for suggested changes of the velocity (note that your results may depend on the chosen step size). You can write the algorithm either as a pseucode or as a program.

   Explain the details of your algorithm.

c) In scientific computing (and science in general) validation and testing of a program are crucial ingredients. For this system, one can for example compute the energy and higher moments of the energy in closed form as

$$\langle E^i \rangle = \frac{\int E^i \exp{(-\beta E)} dE}{Z}.$$

   Discuss which tests you will need to implement in order to validate and test your code. How would you use the histogram $w(v)dv$ to test whether you have reproduced the Boltzmann distribution or not?

d) An important aspect of a Markov chain process is called equilibration. This means that a given number of so-called Markov chain steps are needed before the most likely state (steady state/stationary state) is reached. Explain how you could test whether a steady state has been reached or not. (hint: the covariance and the so-called auto-correlation time are important quantities in this discussion).

Exercise 2, Linear algebra

a) We have the linear set of equations

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

   where we assume that the matrix $\mathbf{A}$ is non-singular and that the matrix elements along the diagonal satisfy $a_{ii} \neq 0$. We let $\mathbf{A} \in R^{n\times n}$. The matrix is symmetric amd real. The vector $\mathbf{w} \in R^n$ is known while $\mathbf{x} \in R^n$ is unknown.

   Set up and explain the algorithms for Gaussian elimination and Lower-Upper (LU) decomposition. Find the number of floating point operations for LU decomposition and discuss the advantage og using LU decomposition for solving the above set of linear equations. We assume that the matrix is diagonally dominant and that pivoting is not necessary.

b) With an LU decomposed matrix, set up the algorithm for finding the determinant of the matrix and its inverse.

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

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

Show that, when discretizing y and x, that this equation can be rewritten as a linear algebra problem

$$\mathbf{Ay} = \mathbf{f},$$

where now $\mathbf{y}$ and $\mathbf{f}$ are discretized versions of the unknown $y(x)$ and the known function $f(x)$. Find the matrix $\mathbf{A}$. How does this matrix change if we modify the differential equation to

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} = f(x), \quad x \in (0,1), \quad y(0) = y(1) = 0,$$

where α is a constant.

d) Set up an algorithm for solving

$$\frac{d^2y}{dx^2} = f(x), \quad x \in (0,1), \quad y(0) = y(1) = 0,$$

using Gaussian decomposition. Explain why you would not use LU decomposition and count the number of floating point operations for your most optimal algorithm. Discuss also how you would validate and test your algorithm.

e) The algorithm from the previous exercise for solving a linear set of equations with a tridiagonal matrix $\mathbf{A}$ can be used to interpolate a function using what is called cubic spline. We assume that we have a function $f(x)$ with function values at specific values of x, that is $f(x_1), f(x_2), \dots f(x_n)$ with the arguments $x_1, x_2, \dots, x_n$ arranged in ascending order, that is $x_1 < x_2 < \dots x_{n-1} < x$. Derive the cubic spline equations for interpolating the function f at a given value x in the interval $x \in [x_1, x_n]$. Show that it ends up in solving a system of linear equations with a tridiagonal matrix and set up an algorithm for interpolating the function f at a value $x \in [x_1, x_n]$.