Examination, Computational Physics (FYTN03), October 27 2008

Allowed calculational aids: "TEFYMA" and pocket calculator.
The examination consists of eight problems of each five points.

1. Determine the weights A_1, A_2 and abscissas x_1, x_2 in the Gauss formula
$$\int_{-1}^{1} x^2 f(x)dx \approx A_1 f(x_1) + A_2 f(x_2)$$

2. Let r, θ and ϕ be spherical coordinates, $r = \sqrt{x^2+y^2+z^2}$, $\cos\theta = z/\sqrt{x^2+y^2+z^2}$ and $\tan\phi = y/x$. Using uniformly distributed random numbers between 0 and 1, describe how random points (r, θ, ϕ) can be generated to be uniformly distrubuted in the unit sphere, i.e. with the probability distribution $p(x, y, x) = 3/4\pi$ inside the unit sphere and zero outside. Describe both how to do it with the transformation method, and with the accept/reject method.

3. Derive a second-order Runge–Kutta method for the initial value problem $dy/dx = f(x, y)$, $y(0) = y_0$.

4. Consider the initial value problem
$$\mathbf{y}'(x) = \mathbf{A}\mathbf{y}(x) \qquad \mathbf{y}(0) = \mathbf{y}_0 \qquad \mathbf{A} = \begin{pmatrix} -2 & -1 \\ -1 & -2 \end{pmatrix}$$
where $\mathbf{y}(x)$ is a two-component vector. Write down the trapezoidal update for this problem and determine for which positive step sizes $(h > 0)$ it is stable.

5. One wants to sample a discrete probability distribution $P(t)$ by using the Metropolis method. Explain how stationarity of $P(t)$ is achieved in this method.

6. Describe the *Simulated Annealing* method and argue for when it is useful.

7. Suppose $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}\cdot\mathbf{A}\mathbf{x} - \mathbf{b}\cdot\mathbf{x}$, where $\mathbf{x}$ and $\mathbf{b}$ are n-component vectors and $\mathbf{A}$ is a symmetric, positive definite $n \times n$-matrix. Let $\mathbf{x}_0$ be an arbitrary initial point and put:
   (i) $\mathbf{h}_0 = \mathbf{g}_0 = -\nabla f(\mathbf{x}_0)$
   (ii) $\mathbf{x}_1 = \mathbf{x}_0 + \lambda_0\mathbf{h}_0$, where λ_0 is the minimum of the function $\lambda \to f(\mathbf{x}_0 + \lambda\mathbf{h}_0)$
   (iii) $\mathbf{g}_1 = -\nabla f(\mathbf{x}_1)$

   Show that if $\mathbf{h}_1 = \mathbf{g}_1 + \gamma_0\mathbf{h}_0$ for some number γ_0, then
$$\mathbf{h}_1 \cdot \mathbf{A}\mathbf{h}_0 = \frac{1}{\lambda_0}(\gamma_0\mathbf{g}_0^2 - \mathbf{g}_1^2)\,.$$
   How is γ_0 chosen in the steepest-descent and conjugate-gradient methods, respectively? *Hint:* Show that $\mathbf{g}_1 = \mathbf{g}_0 - \lambda_0\mathbf{A}\mathbf{h}_0$.

8. Consider the finite-difference approximation
$$\frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{h^2} = v^2\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{a^2}$$
of the wave equation $\partial^2 u/\partial t^2 = v^2\partial^2 u/\partial x^2$, where $u_j^n = u(x_j, t_n)$, $x_j = ja$, $t_n = nh$. Use von Neumann analysis to find a stability condition on v, a and h.