Department of Applied Physics, Chalmers, Göteborg

FKA121/FIM540 Computational Physics

Time: 16 December 2011, 14:00 - 18:00
Place: M-building
Teacher: Göran Wahnström, 031 - 772 3634, 076 - 10 10 523, 031 - 827264
Göran will be available to answer questions at about 15:00
No allowed materials or tools (besides pencil etc)

For more information on the grading and on the inspection of the outcome of the exam, please see the homepage.

1. Consider Newton's equation of motion for a harmonic oscillator

$$m\frac{d^2x(t)}{dt^2} = -kx(t)$$

   Rewrite this as a set of first-order ODEs. (4p)

2. The Hamiltonian for the Fermi-Pasta-Ulam problem can be written as

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[\frac{\kappa}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3}(u_{i+1} - u_i)^3\right]$$

   It can be solved using the velocity Verlet algorithm

$$u_i(n+1) = u_i(n) + \Delta t v_i(n) + \frac{\Delta t^2}{2} a_i(n)$$
$$v_i(n+1) = v_i(n) + \frac{\Delta t}{2}\left[a_i(n+1) + a_i(n)\right]$$

   with

$$a_i(n) = ?$$

   Can you add what is missing at the question mark. (4p)

3. Consider a one-dimensional integral

$$I = \int_0^1 dx f(x)$$

   Explain how you evaluate this by simple Monte Carlo integration. This should include an explanation of how you estimate the error. (4p)

4. Explain the idea behind error estimate for correlated values using block averaging. (4p)

5. Consider the wave equation

$$\frac{\partial^2 y}{\partial t^2} = c^2 \left(\frac{\partial^2 y}{\partial x^2} - \epsilon L^2 \frac{\partial^4 y}{\partial x^4} \right)$$

with the boundary conditions, for $x = 0$ and $x = L$,

$$y = \frac{\partial^2 y}{\partial x^2} = 0$$

and discretize $y(x, t)$ according to

$$y_j^n = y(x_j, t_n)$$

Describe how the boundary conditions can be implemented. (4p)

6. Consider Poisson's equation

$$\frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} = \rho(x, y)$$

with the discretization

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta^2} = \rho_{i,j}$$

Introduce the transform

$$u_{i',j} = \frac{1}{J^2} \sum_{m=0}^{J-1} \sum_{n=0}^{J-1} \hat{u}_{m,n} \, e^{-2\pi i m i'/J} \, e^{-2\pi i n j/J}$$

and compute $\hat{\rho}_{m,n}$ according to

$$\hat{\rho}_{m,n} = \sum_{i'=0}^{J-1} \sum_{j=0}^{J-1} \rho_{i',j} \, e^{2\pi i m i'/J} \, e^{2\pi i n j/J}$$

One can then express $\hat{u}_{m,n}$ as

$$\hat{u}_{m,n} = A_{m,n} \hat{\rho}_{m,n}$$

Give the expression for $A_{m,n}$. (4p)

7. Describe the difference between the Jacobi and the Gauss-Seidel relaxation method for the solution of an elliptic PDE. (4p)