

FKA121/FIM540 Computational Physics

Time: 20 December 2013, 8:30 - 10:30

Place: M-building

Teacher: Göran Wahnström, 031 - 772 3634, 076 - 10 10 523, 031 - 827264

Göran will be available to answer questions at about 9:00

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

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

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

$$\begin{aligned} u_i(n+1) &= u_i(n) + \Delta t v_i(n) + \frac{\Delta t^2}{2} a_i(n) \\ v_i(n+1) &= v_i(n) + \frac{\Delta t}{2} [a_i(n+1) + a_i(n)] \end{aligned}$$

with

$$a_i(n) = ?$$

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

3. In a molecular-dynamics program one can sometimes find the following (pseudo-)code.

$$\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$$

$$\mathbf{r}_{ij} = \mathbf{r}_{ij} - L * [\mathbf{r}_{ij}/L]$$

It implements a certain useful technique. Explain the technique and state when it can be used. (5p)

4. In molecular-dynamics simulations the temperature and pressure can be adjusted. Explain how that can be done. Only the very basic principle, no explicit formulas are required. (5p)

5. Explain the idea behind error estimate for correlated values using block averaging. No explicit formulas are required. (5p)

6. 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. (5p)