Department of Applied Physics, Chalmers, Göteborg

FKA121/FIM540 Computational Physics

Time: 12 January 2015, 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. The equation

$$\frac{d^2y(t)}{dt^2} = f(y,t)$$

can be solved using the Verlet algorithm

$$y_{n+1} = 2y_n - y_{n-1} + h^2 f_n + O(h^4)$$

where

$$f_n = f(y_n, t_n)$$

The Verlet algorithm can also be written on the "velocity Verlet" form

$$\begin{aligned} y_{n+1} &= y_n + hv_n + (h^2/2)f_n \\ v_{n+1} &= v_n + (h/2) \quad ? \end{aligned}$$

This algorithm was used when you solved the Fermi-Pasta-Ulam problem. Can you add what is missing at the question mark. (3p)

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

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

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

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

3. Consider the molecular dynamics simulation technique and temperature scaling. You would like the temperature to decay exponentially to T_{eq},

$$T(t) = T_{eq} + (T(0) - T_{eq})e^{-t/\tau_T}$$

with some decay time constant τ_T. The instantaneous temperature can be changed by scaling the velocities at each time-step according to

$$\boldsymbol{v}_i^{new} = \alpha_T^{1/2} \boldsymbol{v}_i^{old}$$

Give the expression for α_T. (5p)

4. 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. (5p)

5. Consider a one-dimensional integral

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

that you would like to solve using the Monte Carlo method. Explain how the error can be reduced using a weight function

$$p(x) \quad \text{with} \int_0^1 p(x)dx = 1$$

(5p)

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