**Homework 1**

PHZ 3151

Due Friday, January 23, 2009

1. Solve the following differential equations:

a) $\frac{dN}{dt} = -\frac{N}{\tau}$

b) $\frac{d^2y}{dt^2} = -\omega_0^2 y$

In a), write your answer in terms of N at $t = 0$, $N(t = 0)$. For b), write your answer in terms of the $t = 0$ position and velocity, $y(t = 0) = y_0$ and $\frac{dy}{dt}|_{t=0} = v_0$ respectively. Notice for the second-order differential equation, two initial conditions are needed to determine a particular solution.

2. Implement the Fortran radioactive decay program using the Euler method. You may directly copy the code given in Giordano. Choose for the time constant $\tau = 1.0s$. Run the code and generate a picture like Fig. 1.1. What happens if you choose a time step of $\Delta t = 0.05s$? Does the code compare well with the exact solution when $\Delta t = 0.1s$, or $\Delta t = 0.5s$?

3. Consider the following rate equations that describe a second-order chemical reaction $A + B \longleftrightarrow C$

$$\frac{dn_A}{dt} = -k_{AB} n_A n_B + k_C n_C$$

$$\frac{dn_B}{dt} = -k_{AB} n_A n_B + k_C n_C$$

$$\frac{dn_C}{dt} = k_{AB} n_A n_B - k_C n_C$$

where $k_{AB}$ and $k_C$ are rate constants that typically depend on temperature (and perhaps other conditions as well). The concentrations of the chemical species are $n_A$, $n_B$, and $n_C$. A second-order reaction occurs at a rate dependent on either a second-order concentration (e.g. $n_A^2$) or the product of two first-order concentrations (e.g. $n_A n_B$).

Write a code using the Euler method to integrate the three equations above. Run the code for a few different starting conditions and plot the results. Examine in particular the cases $n_A = 1$, $n_B = 1$, and $n_C = 0$ at $t = 0$, and also the case $n_A = 1$, $n_B = \frac{1}{2}$, and $n_C = \frac{1}{2}$.

Determine the appropriate conservation laws for the above equations, and verify that you code is obeying it. In particular, mass cannot be created or destroyed, so as $A$ and $B$ are consumed, $C$ must be created in predictable amounts. The same considerations apply as $C$ decomposes into $A$ and $B$.

For simplicity, choose $k_{AB} = k_C = 1$, and determine an appropriate time step $\Delta t$ for which the code runs accurately and efficiently.