Computational Mathematics

Exercises Set: 3 (deadline Jan 8/2012)

1. Integrate the four 1st-order equations of motion derived from the Hamiltonian:
$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{x^2}{2} + 2y^2 - 0.05\ x\ y^2$ for $x(0)=0.2$, $y(0)=0$, $p_x(0)=0$ and $p_y(0)=0.4$, using **(a)** the 4th-order Runge-Kutta (RK4) method and **(b)** the Milne multistep method. For each method, use a proper value of the time-step, h, so that the relative error in the value of H is initially smaller than 10^{-6}, perform 10^5 steps and compare the time evolution of the energy function $H(t)$. Which method is faster? Which method has better accuracy, in terms of preserving the value of H ?

2. Integrate the 2nd-order differential equation $q'' - a q' + b q^3 = 0$ (Duffin's equation), for $q(0)=0$ $q'(0)=0.001$ and a and b taking values **(a)** $a=-1$, $b=0.05$ and **(b)** $a=4$, $b=0.05$. Use the Runge-Kutta-Felberg (RKF) method and compute 10^4 steps, with h chosen such that the relative error in each step is $\varepsilon<10^{-9}$. For the same value of h, integrate the equation using the Adams-Moulton predictor-corrector scheme, demanding that the predicted and corrected values agree within 10^{-9}. What is the maximum number of iterations needed by the corrector? Which method is faster? Plot the phase-space diagram (q_n, q'_n) of the trajectory.

<u>**Note:**</u> use appropriate formulae to compute the extra initial steps needed by the multistep methods.