Math 228A, Fall 2006, Wilkening

Homework 7
due Thursday, Nov. 30

Consider a molecule consisting of two atoms of equal mass, one with a positive charge, the other neutral, flying into a time varying magnetic field. The distance between molecules is held nearly fixed by a rigid spring ($k = 10^8$) with a natural length $\ell = 0.1$. The magnetic field $\vec{B}$ points in the z direction with magnitude $B(t) = 5\exp(-t^4)$. The ODE for this system may be written

$$w' = f(t, w), \quad \text{or} \quad \begin{pmatrix} x_1 \\ y_1 \\ x_2 \\ y_2 \\ u_1 \\ v_1 \\ u_2 \\ v_2 \end{pmatrix}' = \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ k(r-l)\frac{x_2 - x_1}{r} + v_1 B(t) \\ k(r-l)\frac{y_2 - y_1}{r} - u_1 B(t) \\ k(r-l)\frac{x_1 - x_2}{r} \\ k(r-l)\frac{y_1 - y_2}{r} \end{pmatrix},$$

where $r = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$. The initial condition at $t = -3$ is

$$\begin{aligned} x_1 &= -2, & u_1 &= 1.75, \\ y_1 &= 1, & v_1 &= 0, \\ x_2 &= -2, & u_2 &= 1.75, \\ y_2 &= .9, & v_2 &= 0. \end{aligned}$$

We wish to track the trajectories of the atoms over the time interval $T = [-3, 3]$.

(1) Compute the Jacobian $Df(t, w) = \left(\frac{\partial f_i}{\partial w_j}\right)$.

(2) Implement the 4 step BDF method

$$\frac{25}{12} w_{n+1} - 4w_n + 3w_{n-1} - \frac{4}{3} w_{n-2} + \frac{1}{4} w_{n-3} = h f_{n+1}$$

using constant stepsizes $h = .008$, .004, .002 and .001. Implement Newton's method using linear extrapolation for the initial guess. (Do calculate the Jacobian on every iteration). Once $\|F\| \leq 1.0 \times 10^{-8}$, do one more Newton iteration and accept the step. (also accept the step if the number of iterations exceeds 10, but this never happened in my code for the above choices of h — don't put any stepsize control into your code). Since we don't know the exact solution, the best we can do is compare the solutions to each other.

Turn in 4 plots:
(a) plot the trajectories of the two particles for each of the simulations (plot them all on top of each other – they should agree pretty nicely).
(b) sample the $h = .004$ solution at every other point and plot the difference between one of the components of this solution and the $h = .008$ solution. For definiteness, choose the 5th component of w (which is u_1).
(c) do the same for $h = .002$ and $h = .004$.
(d) do the same for $h = .001$ and $h = .002$.
If the solution were converging at 4th order, we would expect these error estimates to decrease by a factor of 16 every time we cut the meshes in half. Instead they're decreasing by more than 30, indicating at least 5th order convergence. If you keep going with this, you run into a surprise: when $h = .000331$ or so, the method becomes unstable and the solution blows up badly. But when $h \leq .00001$, the method is stable again and gives very accurate answers (you need a pretty good computer to verify this!). The reason this happens, presumably, is that the stiff part of the system (the spring) leads to large imaginary eigenvalues of the Jacobian that pass through the unstable region of the 4 step BDF method (which is not A-stable) as $h \to 0$.