CS 624: Numerical Solution of Differential Equations
Spring 2004
Problem Set 3

Handed out: Mon., Mar. 1.

Due: Wed., Mar. 10 in lecture.

1. Consider the Kepler problem, which describes the motion of a light body orbiting a heavy body:

$$\frac{d^2\mathbf{x}}{dt^2} = -\frac{\mathbf{x}}{\|\mathbf{x}\|^3}.$$

Here, $\mathbf{x}$ is a vector in $\mathbf{R}^2$. Let

$$H(\mathbf{x}, \mathbf{v}) = \frac{\|\mathbf{v}\|^2}{2} - \frac{1}{\|\mathbf{x}\|}.$$

It is easy to check that the above 2nd order ODE, when converted to a first order system using the standard trick of defining $\mathbf{v} = d\mathbf{x}/dt$, is a Hamiltonian system of ODE's for the above energy function.

(a) Show that if the leapfrog method is used to integrate the Kepler system, then

$$H(\mathbf{x}^{n+1}, \mathbf{v}^{n+1}) - H(\mathbf{x}^n, \mathbf{v}^n) = k^2 \left(-\frac{1}{2\|\mathbf{x}\|^4} - \frac{3(\mathbf{v}^T\mathbf{x})^2}{2\|\mathbf{x}\|^5} + \frac{\mathbf{v}^T\mathbf{v}}{2\|\mathbf{x}\|^3} \right) + O(k^3).$$

(b) Construct a perturbed energy function $\bar{H}(\mathbf{x}, \mathbf{v})$ (that may also depend on k) with the property that if the sequence $(\mathbf{x}^n, \mathbf{v}^n)$ is defined as above (i.e., as the solution computed by leapfrog to the original Kepler problem), then $\bar{H}(\mathbf{x}^{n+1}, \mathbf{v}^{n+1}) - \bar{H}(\mathbf{x}^n, \mathbf{v}^n) = O(k^3)$. Your function $\bar{H}(\mathbf{x}, \mathbf{v})$ should have the form

$$\bar{H}(\mathbf{x}, \mathbf{v}) = H(\mathbf{x}, \mathbf{v}) + kf(\mathbf{x}, \mathbf{v}),$$

where $f(\mathbf{x}, \mathbf{v})$ is a function that you determine explicitly. [This problem can be solved without any outside reading, but if you get stuck on (b), you will find a related solved example in the Sanz-Serna & Calvo book on reserve, pp. 129–131. A hint for part (b) is to first regard x and v as scalars and guess that in the scalar analog of this problem, f has the form $f(x, v) = Ax^d v^e$. Once the solution to the scalar analog is found, see if you can generalize to the case that $\mathbf{x}$ and $\mathbf{v}$ are vectors.]

2. (a) Write down the Newton system of linear equations that must be solved to get $\mathbf{v}^{n+3}$ in the BDF3 method. In particular, what is the Jacobian of the nonlinear system describing BDF3?

(b) Suppose the Newton system is solved via LU factorization. Suppose it desired to reuse the LU factors from one iteration on the next, which is possible if f^{n+1} is not too different from f^n (and hence the Jacobians of f are close). This reuse is possible if plain BDF is used. But it is not possible to reuse the factors if the interpolation definition of BDF is used to frequently change time-step size. Explain why not. [Hint: consider the role of β_3 in the Jacobian of BDF3, and what happens if the time-step is changed.]

(c) The version of BDF used by DASSL described in lecture and in Brenan et al. interpolates an interpolant instead of the original function when it changes step size. In light of (b), explain why this is an attractive option. You can focus on the stiff ODE case instead of the more general DAE case. (Ref: K. Jackson and S. Sacks-Davis, "An alternative implementation of variable step-size multistep formulas for stiff ODEs," ACM Transactions on Mathematical Software 6 (1980) 295-318.)

3. Consider applying the leapfrog method to the partitioned Hamiltonian problem whose Hamiltonian is given by $H(\mathbf{p}, \mathbf{q}) = (\mathbf{p}^T A\mathbf{p} + \mathbf{q}^T B\mathbf{q})/2$ where A, B are positive-definite diagonal matrices. Determine the condition that assures that the numerical method is stable (i.e., does not exhibit unbounded growth as $n \to \infty$). Your condition should be in as simple form as possible, involving k and the diagonal entries of A, B.

4. Symplectic integrators for Hamiltonian problems do not conserve energy, as mentioned in lecture. One way to get exact energy conservation for Hamiltonian problems is to drop one of the equations in the ODE system, and replace it with a constraint that energy is conserved. Then the resulting problem can be solved as a DAE. This method often fails.

   Solve the Kepler problem (Q1) in this manner. Use `ode15s`. Note that `ode15s` solves index-one DAE's in semi-explicit form if you give it a diagonal matrix M as input that has a mixture of 1's (evolution equations) and 0's (constraints) on the main diagonal. Try replacing one of the x_i evolution equations with the constraint, and also one of the v_i evolution equations. Hand in m-file listings, plots, and a brief statement of your conclusions. Explain why this method doesn't work very well. (Hint: consider the index.)