CS 624: Numerical Solution of Differential Equations  
Spring 2000  
Problem Set 2

Handed out: Fri., Feb. 18.

Due: Mon., Feb. 28 in lecture.

1. Exercise 1.8.1 of the text. Restrict attention to consistent, D-stable explicit LMS formulas. [Hints: (1) As mentioned in lecture, any D-stable consistent LMS formula has at least one nonzero $\beta_j$. (2) If $p(z) = z^s + a_{s-1}z^{s-1} + \cdots + a_0$ is a monic polynomial, then for each $i$, $a_{s-i}$ is the sum of all possible $i$-fold products of the roots, multiplied by a sign factor. In other words, if the roots of $p$ are $z_1, \ldots, z_s$, then

$$a_{s-i} = (-1)^i \sum_{\{j_1, \ldots, j_i\} \subseteq \{1, \ldots, s\}} z_{j_1} \cdots z_{j_i}.$$  

2. Find a $2 \times 2$ linear constant-coefficient IVP of the form

$$\begin{align*}
\frac{du}{dt} &= Au, \\
u(0) &= u_0
\end{align*}$$

such that, even though all the eigenvalues of $A$ have nonpositive real parts, the solution norm $\|u(t)\|$ tends to infinity as $t \to \infty$. [Hint: You will presumably need to use a non-diagonalizable matrix with repeated eigenvalues, else your example would contradict the theorem in lecture.]

3. Propose an integration rule for the harmonic oscillator that is

- explicit,
- exactly energy-conserving (except for rounding error), and
- at least first order or higher.

The harmonic oscillator is the simplest Hamiltonian ODE and is given by the equations $dp/dt = -q$, $dq/dt = p$. The energy (Hamiltonian) is $p^2 + q^2$. Your method does not have to be elegant, e.g., it can involve some kind of “brute force” correction. Be sure to argue that your method is at least first order. You are not restricted to LMS methods. Proposing a non-LMS formula means that you will have improvise a definition of “order”.

4. Consider the reactions taking place in a homogeneous solution described by the chemical formulas $A + B \rightarrow C$ and $C \leftrightarrow D$, where $A, B, C, D$ are compounds. There are three reactions here (namely $A + B \rightarrow C$, $C \rightarrow D$ and $C \leftrightarrow D$); let the three rate
constants be $m_1, m_2, m_3$. Let $\alpha, \beta, \gamma, \delta$ be the concentrations of $A, B, C, D$ as functions of $t$. Then the equations governing this system are

\begin{align*}
\alpha' &= -m_1 \alpha \beta, \\
\beta' &= -m_1 \alpha \beta, \\
\gamma' &= m_1 \alpha \beta - m_2 \gamma + m_3 \delta, \\
\delta' &= m_2 \gamma - m_3 \delta.
\end{align*}

Suppose the initial conditions are $\alpha^0 = \beta^0 = 1, \gamma^0 = \delta^0 = 0$. Suppose the rate constants are $m_1 = 1, m_2 = 10000, m_3 = 1$. This means that $A$ and $B$ are slowly converted to $C$, $C$ is very rapidly converted to $D$, and $D$ is slowly converted back to $C$. So at the end of the reaction, one would expect most of the product to be $D$.

Integrate the above equations out to $t = 6$ in Matlab using ode23 and ode15s. Note that ode15s is intended for stiff problems like this one. For ode15s, experiment with both numerical Jacobians (the default) and user-specified Jacobians. For user-specified Jacobians, you have to write code to provide the Jacobian. The help-files on these functions will explain how they work. Turn in plots of the concentrations of $C$ and $D$ for the various methods.

Hand in listings of all m-files, at least two interesting plots, and a couple of paragraphs describing your experience with these methods.