CS 624: Numerical Solution of Differential Equations

Spring 2006

**Problem Set 2**

Handed out: Fri., Feb. 10.

Due: Mon., Feb. 20 in lecture.

1. (a) Consider applying AB2 to compute $v^{n+2}$ in the case that $k_2 \neq k_1$, where $k_2 = t_{n+2} - t_{n+1}$ and $k_1 = t_{n+1} - t_n$. Note that in order to derive a formula for AB2 in this case of unequal time steps, you must go back to the definition of AB2 given in lecture based on interpolation.

   (b) *Catastrophic cancellation* means subtraction of two nearly equal numbers in floating point arithmetic, with the result being a loss of significant digits in the answer. Show that the formula for AB2 that you derived in (a) could be prone to catastrophic cancellation if $k_2 \gg k_1$. In particular, pinpoint the operation in which two large numbers are subtracted, leaving an answer that is much smaller (and hence may have many fewer significant digits).

2. Exercise 1.8.1 of the text. Restrict attention to consistent, D-stable explicit LMS formulas. [Hints: (1) First, argue that any D-stable consistent LMS has at least one nonzero $\beta_j$. This is established by arguing that $C_0 = 0 \Rightarrow \rho(1) = 0$, then D-stability $\Rightarrow \rho'(1) \neq 0$, then $\rho'(1) \neq 0, C_1 = 0 \Rightarrow$not all $\beta_j$'s are zero. (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

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

3. An IVP can change from being stiff to nonstiff (or vice versa) as the solution evolves. Consider, e.g., the system $u' = -u; v' = -v/u$ with initial conditions $u(0) = v(0) = 1$. Write a paragraph or two in which you analyze whether this system is stiff and why. Then try the Matlab IVP solver `ode23` on it. Integrate it out to $t = 10$ and plot both components using a log-scale for the y-axis (i.e., use the `semilogy` function). This solver ode23 is not intended for stiff problems and exhibits some pathology on this problem.

4. Consider the reactions taking place in a homogeneous solution described by the chemical formulas $A \leftrightarrow B + C$ and $C \leftrightarrow D$, where $A, B, C, D$ are chemical species. There are four reactions here (namely $A \rightarrow B + C$, $B + C \rightarrow A$, $C \rightarrow D$ and $D \rightarrow C$); let the four rate constants be $m_1, m_2, m_3, m_4$ respectively. Let $\alpha, \beta, \gamma, \delta$ be the concentrations of $A, B, C, D$ as functions of $t$. Then the equations governing this system are

$$\alpha' = -m_1\alpha + m_2\beta\gamma,$$

$$
\begin{aligned}
\beta' &= m_1\alpha - m_2\beta\gamma, \\
\gamma' &= m_1\alpha - m_2\beta\gamma - m_3\gamma + m_4\delta, \\
\delta' &= m_3\gamma - m_4\delta.
\end{aligned}
$$

Suppose the initial conditions are $a^0 = 1$, $\beta^0 = \gamma^0 = \delta^0 = 0$. Suppose the rate constants are $m_1 = 1$, $m_2 = .5$, $m_3 = 100000$, $m_4 = .1$. This means that $A$ is slowly converted to $B$ and $C$ which are even more slowly converted back, $C$ 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 $B$ and $D$.

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 $B$ 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.