Numerical Solution of Ordinary Differential Equations
(MTH 452/552)
Homework due Wednesday, March1, 2017

Problem 1. (30 points). Consider the IVP

$$u'' = -19u - 20u', \quad y(0) = \eta_1, \quad y'(0) = \eta_2.$$

a) Rewrite the differential equation as a first order system and compute the exact solution of the IVP. Show that the exact solution converges to zero for $x \to \infty$. Show your work.

b) Assume that the IVP is solved numerically, using Euler's method $U^{n+1} = U^n + \Delta t f(t_n, U^n)$, where of course $f(t_n, U^n) = AU^n$ corresponds to the equivalent linear first order system. Derive a condition that the step size Δt must satisfy for the computed solution U^n to converge to zero for $n \to \infty$. Show your work.

Hint. Write U^n in the form $U^n = c_n v_1 + d_n v_2$, where $c_n, d_n \in \mathbf{R}$, and v_1, v_2 are two linearly independent eigenvectors of A. Then find a condition for Δt such that c_n and d_n converge to zero as $n \to \infty$.

Problem 2. (40 points) The so-called Oregonator is the following system of differential equations describing an oscillating chemical reaction involving five substances.

$$\begin{aligned}
c_1' &= -k_1 c_1 c_2 - k_3 c_1 c_3 \\
c_2' &= -k_1 c_1 c_2 - k_2 c_2 c_3 + k_5 c_5 \\
c_3' &= k_1 c_1 c_2 - k_2 c_2 c_3 + k_3 c_1 c_3 - 2k_4 c_3^2 \\
c_4' &= k_2 c_2 c_3 + k_4 c_3^2 \\
c_5' &= k_3 c_1 c_3 - k_5 c_5.
\end{aligned}$$

The reaction rate coefficients k_i are given by

$$k_1 = 1.34, \quad k_2 = 1.6 \cdot 10^9, \quad k_3 = 8 \cdot 10^3, \quad k_4 = 4.0 \cdot 10^7, \quad k_5 = 1.0,$$

and the initial conditions are

$$\begin{aligned}
&c_1(0) = 0.06, \quad c_2(0) = 3.3 \cdot 10^{-7}, \quad c_3(0) = 5.01 \cdot 10^{-11} \\
&c_4(0) = 0.03, \quad c_5(0) = 2.4 \cdot 10^{-8}.
\end{aligned}$$

a) Familiarize yourself with MATLAB's current family of ODE solvers (e.g., by typing help ode45). Solve this IVP for $t \in [0, 1]$ using ode15s, ode23s, ode45, as well as the older ode45v4.m. Compare the number of evaluations of f and the number of time steps that are needed to get reasonably accurate results for all concentrations. For each program present the results as follows. State the needed number of evaluations of f and the number of time steps. Then use the subplot command (subplot(231), subplot(232), etc.) to produce one figure with the following six plots: The five concentrations (using semilogy), as well as the vector of times t_n where the numerical solution was computed. Observe where the different programs take small timesteps and how the solution behaves in those intervals.

b) Find out why this ODE system has the name Oregonator.