# Belosov-Zhabotinsky Reaction Model Using Step Doubling

This project is due at 11 PM on Sunday, November 13.

You are to implement an ODE solver that uses the first order backward difference method (aka backward Euler) as its basic building block. The error control is done with step doubling which means that in going from $t_{now}$ to $t_{new} = t_{now} + dt$ you take two paths: one uses two steps of size $dt/2$ to produce $d_{new}$ and the other uses a single step of size $dt$ to produce $s_{new}$. The error indicator is a norm of $d_{new} - s_{new}$. Local extrapolation gives a second-order correct method with the approximate solution at $t_{new}$ being $2d_{new} - s_{new}$.

In solving the backward difference equations for the problem

$$\begin{aligned} y' &= f(t, y) \text{ on}(a, b) \\ y(a) &= d, \end{aligned}$$

one needs to solve a nonlinear system. This is done by using one step of Newton's method with a carefully chosen initial guess. The initial guess at $d_{mid}$ the half-step solution that leads to $d_{new}$ is based on linear extrapolation of the solution $Y_{now}$ at $t_{now}$ and the previously accepted step $Y_{old}$ at $t_{old}$ to the time $t_{now} + dt/2$. The initial guess at $d_{new}$ is $d_{mid} + (d_{mid} - Y_{now})$. The initial guess at $s_{new}$ is $d_{new}$. You will need to check that the residual is being appropriately reduced by the single step of Newton's method; this will be discussed some below.

You should define a problem dependent norm that divides each component of the solution (or residual) by a number that is representative of the maximum size of that component. This norm is used in checking the Newton's method and in measuring the distance between $s_{new}$ and $d_{new}$.

The initial value problem that you are to solve is a simple model of the Belosov-Zhabotinsky reaction given as a set of 3 ODE's with $f = (f_0, f_1, f_2)^T$ defined by

$$\begin{aligned} f_0(t, y) &= 77.27(y_1 - y_0 y_1 + y_0 - 8.375\text{e-}6 y_0^2), \\ f_1(t, y) &= (1/77.27)(-y_1 - y_0 y_1 + y_2), \\ f_2(t, y) &= 0.161(y_0 - y_2). \end{aligned}$$

The initial value that you are to use is $y(0) = (4, 1.1, 4)^T$, and the interval over which you solve the problem is (0,700).

You will need to not only program $f$, but also its derivative, a 3x3 matrix, $Df$. You should also calculate a version of $f$ called $f_a$ that has absolute values on each term. The rounding error in each component of $f$ is about 1e-15$f_a$. The knowledge of what size the rounding is important in determining whether you are doing a good job of solving the nonlinear equations. To get an estimate of the rounding in each component of the residual you will need to include the effect of the time difference too. It can happen that the initial guess at the solution is so good that the residual cannot be reduced much before it gets to the level of rounding error.

You should implement a step adjustment scheme that is similar to that used in the Adams Method project, but it needs to incorporate the ability to solve the nonlinear equations as well as keeping the error indicator small. Note that as the time step decreases it becomes easier to solve the nonlinear problem.

Normally, after determining approximately what the solution is you would adjust the constants in your problem dependent norm. For this example the norm is defined below. Also, if you see that you are running into the $dt_{min}$ often, it may be too large.

# Results to Show

Run a convergence study in which you use tolerances of 0.001, 0.0001 and 0.00001 and you require that the norm of the residual be reduced by a factor of 100. Repeat these three runs with the requirement that the residual be reduced by a factor of 200. If the residual is within a factor of 100 of the rounding error estimate, consider that you met the residual reduction test. In doing these runs use a problem dependent norm that is

$$|v| = |v(0)|/1.25e5 + |v(1)|/1800 + |v(2)|/3.0e4.$$

For each of the six cases make a table that shows three numbers for each component: $v_{max}$, $t_{max}$, $v(700)$, where $v_{max}$ is the maximum value of the component on the time interval $[500, 700]$, $t_{max}$ is a time at which that values is attained, and $v(700)$ is the value of the component at $t = 700$. Also record the number of steps attempted in each of the six cases.

Produce graphs of the solution components, and $\log dt$, for the case with the tolerance of 0.00001 and a reduction factor of 100. Describe in a a few sentences the changes you see in when you vary the tolerance and the reduction factor.

## Coding Remarks

In developing tools like this is a good idea to test them on problems where you know the answer. You may want to try a simple scalar equation like $y' = -y$. Another case we looked at when studying Adams methods was $y' = Ay$ where $A$ is a 2×2 diagonal matrix with entries $-1$ and $-1000$. This code can solve the problems you used to test the Adams method as well.

Posted with this project description is a collection of C++ codes that I used in producing my code.