IVP with implicit timestepping

Computer Session C3

Background

The dG0 timestep method (backward Euler) for the initial value problem

$$\begin{aligned} \dot{u}(t) &= f(u(t)) \quad 0 < t < T \\ u(0) &= u^0 \end{aligned} \tag{1}$$

is, Find $U(t_n)$ successively for $n = 0, \ldots, N$ according to

$$U(t_n) = U(t_{n-1}) + k_n f(U(t_n)) \tag{2}$$

This is a nonlinear equation if f is nonlinear in u.

Before today's computer session, make sure that you understand and can answer the following question.

Question 1 Derive the equation for the backward Euler method (2) from the IVP (1).

Preparations

Create a new directory called `c3` and then create the subdirectory `problem`. Then download the following files to the subdirectory:

- `BackwardEulerNewton.m`,
- `akzonobelf.m`,
- `volterra.m`

The files are available on the web page of this session under *Programs and templates*.

Problem

Problem 1

Preparation

Go to the directory `problem`. For this problem you will need to edit your `BackwardEulerNewton.m`, and perhaps create new functions for testing your solver.

Problem

Create a program for solving general IVP with backward Euler (a frame of the program can be found in `BackwardEulerNewton.m`). You should use Newton iterations for solving the implicit difference equation that arises when computing u_{n+1} from u_n.

You should test your solver on three different IVP:s. First

$$\begin{aligned} \dot{u}(t) &= -u(t) \quad 0 < t < T \\ u(0) &= 1 \end{aligned} \tag{3}$$

Compare your result to the exact solution.

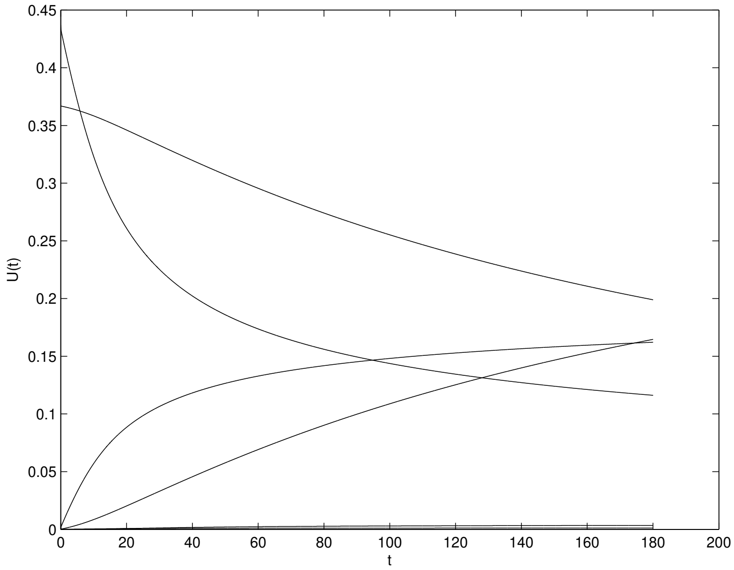

Figure 1: The computed solution to the Akzo-Nobel problem.

The second example is a stiff IVP, "Akzo-Nobel system of chemical reactions". Find the concentrations $u(t) = (u_1(t), u_2(t), \ldots, u_6(t))$ such that for $0 < t < T$,

$$\left\{\begin{array}{lcl} \dot{u}_1 & = & -2r_1 + r_2 - r_3 - r_4 \\ \dot{u}_2 & = & -0.5r_1 - r_4 - 0.5r_5 + F \\ \dot{u}_3 & = & r_1 - r_2 + r_3 \\ \dot{u}_4 & = & -r_2 + r_3 - 2r_4 \\ \dot{u}_5 & = & r_2 - r_3 + r_5 \\ \dot{u}_6 & = & -r_5 \end{array}\right. \tag{4}$$

where $F = 3.3 \cdot (0.9/737 - u_2)$ and the reaction rates are given by $r_1 = 18.7 \cdot u_1^4 \sqrt{u_2}$, $r_2 = 0.58 \cdot u_3 u_4$, $r_3 = 0.58/34.4 \cdot u_1 u_5$, $r_4 = 0.09 \cdot u_1 u_4^2$ and $r_5 = 0.42 \cdot u_6^2 \sqrt{u_2}$, with the initial condition $u_0 = (0.437, 0.00123, 0, 0, 0, 0.367)$. Compare your result to figure 1.

The third and last example is the "Volterra-Lotka" equations, also known as the prey-predator equations,

$$\begin{array}{lcl} \dot{u}_1 & = & u_1(a - bu_2) \\ \dot{u}_2 & = & -u_2(c - du_1) \end{array} \tag{5}$$

where u_1 is the number of some prey (for example rabbits) and u_2 is the number of its predator (for example foxes). a, b, c, d are parameters representing the interaction of the two species.

Compute solutions for different parameters. The solution should have a periodic behaviour.

Question 2 Can you notice any damping of the solution? What may be the cause of this?

Problem 2

Preparation

For this problem you will edit the solver you created in Problem 1.

Problem

Edit your solver so that it uses an adaptive procedure. This can be done by choosing an appropriate step length k_n,

$$k_n = \frac{\mathrm{TOL}}{S_c(t) \cdot R_n} \tag{6}$$

where TOL is your error tolerance, $S_c(t)$ the stability factor, and R_n the residual. A more useful approximation is to use R_{n-1} instead of R_n. In this session, you will assume that $S_c(t) = 1$.

Apply your adaptive solver to equation (3).
Question 3 Is there a change in the timestep? Explain this.

Hints

Problem 1

When updating u_n from u_{n-1} we use Newton iterations,

$$u_n^1 = u_n^0 - (\nabla g(u_n^0))^{-1} g(u_n^0) \tag{7}$$

where

$$g(u_n^0) = u_n^0 - u_{n-1} - k_n f(u_n^0) \tag{8}$$

Problem 2

The residual can be computed using

$$R_{n-1} = \|(U_{n-1} - U_{n-2})/k_n\| \tag{9}$$

Solutions

Make sure that you really try to solve each problem before looking at the solutions. Have you really tried to solve the problem or should you try again before looking at the solution?

The solutions are available on the web page of this session under *Solutions to problems*.

About

This Computer Session is part of the Body and Soul educational program. More information can be found at

`http://www.phi.chalmers.se/bodysoul/`

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