HOMEWORK 7

Reading:

- Suggested: Ascher & Petzold, Chapter 3 and Chapter 4.5, 4.8.

Code to turn in:

- Your code for Problem 5 (turning in the other code is optional for feedback).

Note: Questions marked [A&P] are adapted from Ascher & Petzold.

1. Problems

Problem 1 (continuation, A&P).
One three-stage RK method is **Heun's method**. For $y' = f(t, y)$, the method is

$$\begin{aligned} f_1 &= f(t_n, u_n) \\ f_2 &= f(t_n + \frac{h}{3}, u_n + \frac{h}{3} f_1) \\ f_3 &= f(t_n + \frac{2h}{3}, u_n + \frac{2h}{3} f_2) \\ u_{n+1} &= u_n + h(\frac{1}{4} f_1 + \frac{3}{4} f_3) \end{aligned}$$

a) Determine the region of absolute stability R (don't use the indirect e^z argument here).

b) The boundary of R can be computed in the following way: Given a value of θ, solve $q(z) = e^{i\theta}$ for z using Newton's method. Then increment θ by a small amount to get the next value of z on the boundary and so on. Use this method (starting at $\theta = 0$) to plot the boundary of R. *Note: If done correctly, this approach avoids having to find all the roots of $q(z) = e^{i\theta}$ for each θ.*

c) Estimate the interval of absolute stability $(-b, 0)$ from the numerical calculation.

(**Remark:** This technique is called 'continuation'. To solve $F(x; \alpha) = 0$ for $\alpha = \alpha_1$, instead solve the easy problem $F(x; \alpha_0) = 0$ and adjust α from $\alpha_0 \to \alpha_1$, solving each problem along the way and using the intermediate solutions from each step to help solve the next step. If it is easy to solve for α_0 and easy to go from α to α + small, then continuation lets you extend your solution reliably up to much harder problems.)

Problem 2 (stiff decay, A&P 4.8). Suppose a method produces an approximation $\{u_n\}$ for the test equation $y' = \lambda y$. If the solution is 'more stable', we would like u_n to decay faster. However, the region of absolute stability does not tell us 'how fast' u_n decays.

A method is said to have **stiff decay** (or **L-stability**) if approximations decay fast when the solution $y(t)$ to the test equation decays fast. To be precise, let $\rho(h\lambda)$ be the best 'rate' such that $u_n = O(\rho^n)$ as $n \to \infty$ (for instance, $\rho = 1 + h\lambda$ for Forward Euler).
Then the method has stiff decay if

$$\rho(h\lambda) \to 0 \text{ as } \mathrm{Re}(h\lambda) \to -\infty.$$

To illustrate the idea, consider the 'θ-method'

$$u_n = u_{n-1} + h(\theta f(u_n) + (1-\theta) f(u_{n-1})).$$

where $\theta \in [0, 1]$. The method is first order for $\theta \neq 1/2$ and second order for $\theta = 1/2$.

a) For which values of θ is the method A-stable?

b) For which values of θ does the method have stiff decay?

c) Implement this method for $\theta \neq 0$ Suppose you are tasked with obtaining a qualitatively correct solution to

$$y' = -1000(y - \sin t) + \cos t, \quad y(0) = 0$$

for $t \in [0, 2\pi]$ (the exact solution is $y(t) = \sin t$). How small must h to get a reasonable looking solution when using Backward Euler ($\theta = 1$) and when using the trapezoidal method ($\theta = 1/2$)?

Contrast the two methods - why does the stiff decay property matter?

Problem 3 (conserved quantities). Suppose an object in motion has position x and momentum p, with potential energy $U(x)$. The **Hamiltonian**

$$H(x, p) = \frac{1}{2}p^2 + U(x)$$

is a conserved quantity ($H(x(t), p(t)) = \text{const. for all } t$). The equations of motion are

$$x' = p, \quad p' = -f(x). \tag{1}$$

where $f(x) = dU/dx$. For this problem, let $H(t)$ denote, for short, $H(x(t), p(t))$.

a) Suppose $U(x) = 2x^2$ (so the solution is an elliptical orbit) and Backward Euler is used to compute the solution in $[0, T]$ when $x(0) = 1$ and $p(0) = 0$.

Prove that (i) $H(t)$ converges to $H(0)$ as $h \to 0$ but (ii) the computed solution is not periodic even when h is small (and is always bad for large enough t). *Hint: you can compare $H(t_n)$ and $H(t_{n-1})$ directly since U is not too complicated).*

b) Implement Backward Euler for systems and test your result from (a) by plotting $H(t) - H(0)$ for $t \in [0, 6\pi]$ for various values of h. What happens?

Problem 4 (a fix for P3) [AC]. A **symplectic integrator** preserves some of the structure of Hamiltonian system. The simplest is the **symplectic Euler method**, which uses Backward Euler on the x' equation and Forward Euler on the p' equation:

$$x_{n+1} = x_n + hp_{n+1}, \qquad p_{n+1} = p_n - hf(x_n).$$

a) Suppose $U = Ax^2/2$ (with $A > 0$). Define the 'perturbed' Hamiltonian

$$H^h(x,p) := \frac{1}{2}p^2 + \frac{A}{2}x^2 - \frac{A}{2}hxp.$$

Show that symplectic Euler with step size h conserves H^h **exactly**. Use this to conclude that if h is small enough then the computed solutions will be periodic. (This fact generalizes to more general Hamiltonians, but requires more effort to prove).

b) Implement SE to solve the system (1). Check that H^h is conserved. How well (qualitatively) does SE approximate the actual energy $H(t)$?

Remark: There is much more to symplectic methods and other techniques for preserving invariants of systems; see problems 4.9 and 4.11 and 4.15 in A&P, for instance.

Problem 5. A simplified model for the well-known Belousov-Zhabotinsky oscillating reaction is the 'Oregonator' model[1], in which there are three species with concentrations $u(t), v(t)$ and $w(t)$ governed by the ODEs

$$\begin{aligned} x' &= A(y - xy + x - Bx^2) \\ y' &= \frac{1}{A}(-y - xy + z) \\ z' &= C(x - z) \end{aligned}$$

with constants

$$A = 77.27, \quad B = 8.375 \times 10^{-6}, \quad C = 0.161.$$

Consider initial concentrations

$$x(0) = 4, \quad y(0) = 1.1, \quad z(0) = 4.$$

The solution exhibits oscillations. For the given initial conditions, there is a spike at an early time T_0 between 1 and 2, then another spike that reaches its maximum value at a time T_1 between 300 and 350.

Your task is to obtain a qualitatively correct solution showing both spikes in $x(t)$ (you don't need to plot v and w) and to estimate the value of T_1. *Note: plot $x(t)$ using a semi-log plot.*

Discuss your approach (what works, what doesn't, why your method is a good choice, etc.).

[AC] Obtaining a reliable solution takes effort. For additional credit, try to be precise - justify the accuracy for your value of T_1, or try to improve your method to be more efficient or accurate. Note that you should not invest too much time into this (there are diminishing returns both in solution quality and in things to learn by improving the method).

[1] Equations and parameters taken from Field & Noyes, "Oscillations in chemical systems. IV. Limit cycle behavior in a model of a real chemical reaction", J. Chem. Phys. (1974).