AME 60614: Numerical Methods
Fall 2007, Solution Set 2

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1. The population growth of many kinds of insects is sometimes modeled by the following ordinary differential equation:

$$\frac{dN}{dt} = \alpha N - \beta N^2, \qquad N(0) = N_o,$$

where N is the population, α is the birth rate coefficient, and β is the death rate coefficient. If $N_o = 10^5$ *insect*, $\alpha = 0.1$ day^{-1}, and $\beta = 8 \times 10^{-7}$ $insect^{-1} day^{-1}$, what is the population of this kind after 20 years?

Solution:
This problem has analytical solution. So, there is no excuse to solve it numerically.

$$\begin{aligned} \int \frac{dN}{\alpha N - \beta N^2} &= \int dt, \\ \frac{N}{\alpha - \beta N} &= \mathcal{C} e^{\alpha t}, \\ N(t) &= \frac{\mathcal{C} \alpha e^{\alpha t}}{1 + \mathcal{C} \beta e^{\alpha t}}. \end{aligned}$$

where, $N(0) = N_o \Longrightarrow \mathcal{C} = 5 \times 10^6$ day. So, after 20 $years$, 7300 $days$, the population will be 1.25×10^5 $insects$.

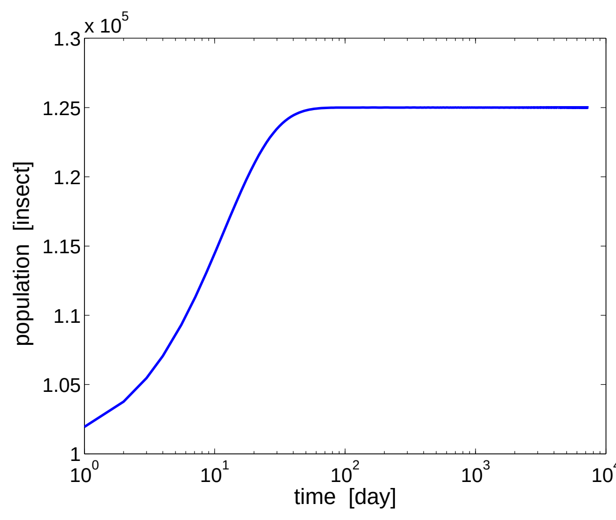

Figure 1: The evolution of the insect population.

2. The following ordinary differential equation model a simple one-step chemical reaction:

$$\frac{d\lambda}{dt} = 2500(1-\lambda)\exp\left[\frac{-E}{T}\right],$$

where T is the temperature, E is the activation energy, and λ is the reaction progress variable, $0 \le \lambda \le 1$. For a specific case $E = 50$ and $T = 12 + 1.9\sqrt{1-\lambda} - 9(1-\lambda)$,

(a) using any explicit scheme, plot the temperature distribution, for $\lambda(0) = 0$, $t \in [0, 1.5]$.

(b) perform a convergence study by plotting the norm of the relative error L_2 vs. the grid size h.

Solution:
(a) First order Euler scheme with $\Delta t = 10^{-6}$ will be used to solve this problem

$$\frac{\lambda_{n+1} - \lambda_n}{\Delta t} = 2500(1-\lambda_n)\exp\left[\frac{-50}{12 + 1.9\sqrt{1-\lambda_n} - 9(1-\lambda_n)}\right], \qquad \lambda_o = 0.$$

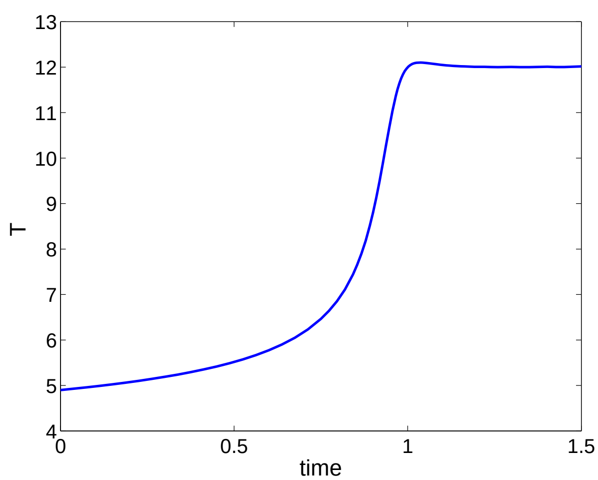

Figure 2: The temperature distribution, the solution of problem 2.

(b) To perform a convergence study, the solution from the previous part will be considered as an "exact" solution for this problem. Also, several solutions are obtained by utilizing $\Delta t = [10^{-2}, 10^{-3}, 10^{-4},$ and $10^{-5}]$. The convergence criteria, the norm of the relative error L_2, is defined as:

$$L_2 = \sqrt{\sum_{i=1}^{N}\left(\frac{T_i^{numerical} - T_i^{exact}}{T_i^{exact}}\right)^2},$$

where, N represent the number of grid points.

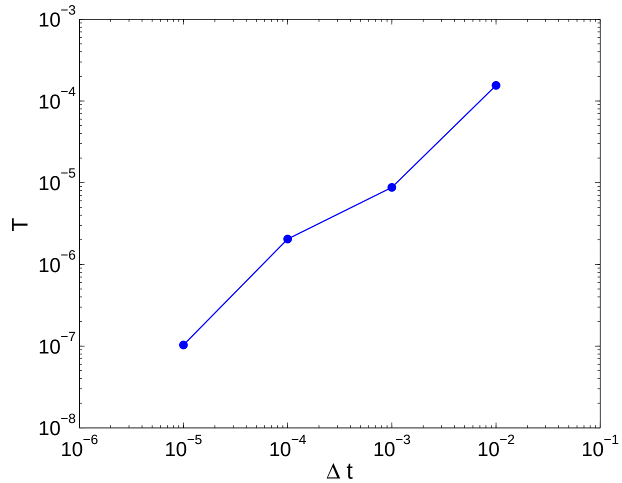

Figure 3: The convergence study for problem 2.

3. Solve the following ODE:

$$y' = t^2\ y\ \cos(y+t)^3, \quad y(0) = 1, \quad t \in [0,3],$$

(a) using the following schemes:

i. Leapfrog.

ii. Trapezoidal.

iii. Second order Runge-Kutta (RK2).

iv. Fourth order Runge-Kutta (RK4).

(b) Investigate experimentally the order of accuracy of each scheme by performing a convergence study. Plot the norm of the relative error L_∞ vs. the grid size h on a log-log scale and estimate the order of accuracy. (At least show five solutions.)

(c) Discuss your results.

Solution:
(a) This problem can be solved using the four listed schemes with a grid size $\Delta t = 10^{-7}$.

- The leapfrog scheme,

$$\frac{y_{n+1} - y_{n-1}}{2\Delta t} = t_n^2 y_n \cos\left(y_n + t_n\right)^3,$$

is a multi-step method. So, to initiate the solution for the first time step, the RK2 will be used since these two schemes have the same order of accuracy.

- The considered ODE is non-linear, which make it essential to use linearization technique first in order to employ the trapezoidal scheme

$$\frac{y_{n+1} - y_n}{\Delta t} = \frac{1}{2}\left[\frac{f(t_{n+1}, y_n) + f(t_n, y_n)}{1 - \frac{\Delta t}{2}\left.\frac{\partial f}{\partial y}\right|_n}\right],$$

$$\frac{y_{n+1} - y_n}{\Delta t} = \frac{1}{2}\left[\frac{t_{n+1} y_n \cos{(y_n + t_{n+1})}^3 + t_n y_n \cos{(y_n + t_n)}^3}{1 - \Delta t/2\left[t_n^2 \cos{(t_n + y_n)}^3 - 3y_n(y_n + t_n)^2 \sin{(t_n + y_n)}^3\right]}\right].$$

- For the RK2 and the RK4 schemes, no special treatment has to be considered.

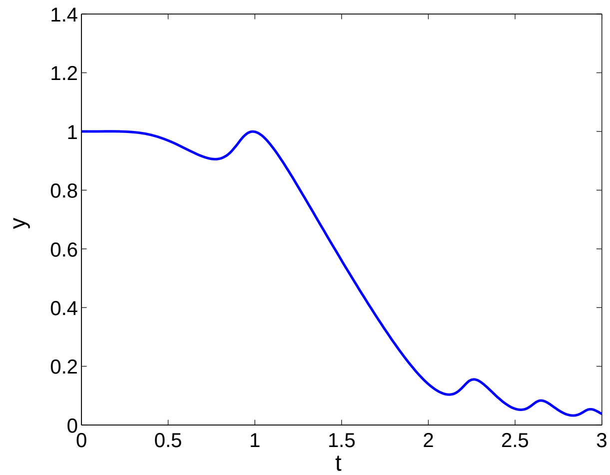

Figure 4: The solution of problem 3.

(b) Also, solutions from the previous part will be considered as "exact" solutions for this problem, and other solutions will be obtained by utilizing $\Delta t = [10^{-2}, 10^{-3}, 10^{-4}, 10^{-5},$ and $10^{-6}]$, except for RK4. Where it can be seen from Fig. (5) that the machine roundoff limit has been reached at $\Delta t = 10^{-4}$, and utilizing finer grid size will not improve the accuracy of the solution anymore. The relative error here is $\mathcal{O}\left(10^{-10}\right)$.

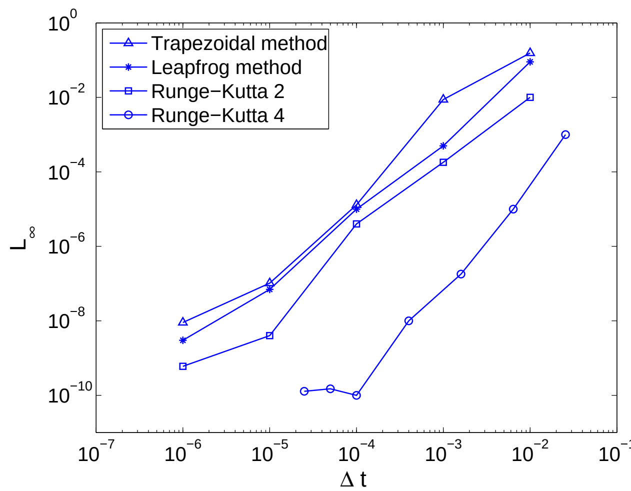

Figure 5: The convergence study for problem 3.

The convergence criteria, the norm of the relative error L_∞, is defined as:

$$L_\infty = max_{t_o \le t \le t_f} \left| \frac{y_i^{numerical} - y_i^{exact}}{y_i^{exact}} \right|, \qquad i = 1, \ldots, N,$$

where, N represent the number of grid points.

4. The following numerical scheme:

$$y_{n+1} = y_{n-1} + \frac{h}{3}\left[f_{n-1} + 4f_n + f_{n+1}\right],$$

is proposed. By utilizing the model problem, $y' = \lambda y$,

(a) classify this scheme in terms of consistency and order of accuracy.

(b) Derive the characteristic equation and find its roots. Find the order of accuracy of this scheme by expanding the roots of the characteristic equation in powers of h.

(c) Investigate the stability of this scheme for:

i. λ purely real.

ii. λ purely imaginary.

(d) Discuss your results.

Solution:
(a) To check for consistency, each term will be expand in terms of Taylor series,

$$\begin{aligned}
y_{n+1} &= y_n + hy_n' + \frac{h^2}{2!}y_n'' + \frac{h^3}{3!}y_n''' + \frac{h_n^4}{4!}y_n^{iv} + \frac{h_n^5}{5!}y_n^v + \ldots, \\
y_{n-1} &= y_n - hy_n' + \frac{h^2}{2!}y_n'' - \frac{h^3}{3!}y_n''' + \frac{h_n^4}{4!}y_n^{iv} - \frac{h_n^5}{5!}y_n^v + \ldots, \\
f_{n-1} &= f_n - hf_n' + \frac{h^2}{2!}f_n'' - \frac{h^3}{3!}f_n''' + \frac{h_n^4}{4!}f_n^{iv} - \frac{h_n^5}{5!}f_n^v + \ldots, \\
f_{n+1} &= f_n + hf_n' + \frac{h^2}{2!}f_n'' + \frac{h^3}{3!}f_n''' + \frac{h_n^4}{4!}f_n^{iv} + \frac{h_n^5}{5!}f_n^v + \ldots.
\end{aligned}$$

So, be substituting back onto the scheme, we get

$$2hy_n' + \frac{h^3}{3}y_n''' + \frac{2h^5}{125}y_n^v + \ldots = 2hf_n + \frac{h^3}{3}f_n'' + \frac{h^5}{72}f_n^{iv} + \ldots.$$

We can note that the error leading term is $\frac{21}{500}h^5 y_n^v$. It can be noted that as $h \to 0$ the error vanish. So, this scheme is consistent and it is 4^{th} order accurate.

(b) To find the characteristic equation, we use $y_n = \sigma^n y_o$.

$$y_o \sigma^{n+1} = y_o \sigma^{n-1} + \frac{\lambda h y_o}{3}\left(\sigma^{n-1} + 4\sigma^n + \sigma^{n+1}\right),$$

by dividing over σ^{n-1},

$$\left(1 - \frac{\lambda h}{3}\right)\sigma^2 - \left(\frac{4\lambda h}{3}\right)\sigma - \left(1 + \frac{\lambda h}{3}\right) = 0. \tag{1}$$

This equation has two roots,

$$\sigma_{1,2} = \frac{-2\lambda h \pm \sqrt{3\left(\lambda^2 h^2 + 3\right)}}{\lambda h - 3}.$$

By expanding these two roots in terms of λh,

$$\begin{aligned} \sigma_1 &= -1 + \frac{\lambda h}{3} - \frac{\lambda^2 h^2}{18} - \frac{\lambda^3 h^3}{54} + \ldots, \\ \sigma_2 &= 1 + \lambda h + \frac{\lambda^2 h^2}{2} + \frac{\lambda^3 h^3}{6} + \frac{\lambda^4 h^4}{24} + \frac{\lambda^5 h^5}{72} + \ldots, \end{aligned}$$

we can note that first root is *spurious*, while the second roots assure, what we found in the previous part, that this scheme is 4^{th} order accurate.

(c) To investigate the stability of this scheme, lets take $\sigma = e^{i\theta}$ and substitute back into eq. (1). So, after arrangement it become

$$\lambda h = \frac{3e^{2i\theta} - 3}{e^{2i\theta} + 4e^{i\theta} + 1}.$$

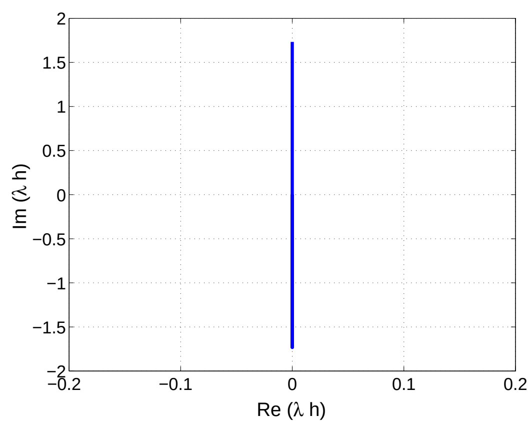

Figure 6: The stability region for the scheme in problem 4.

We can find the region where this scheme is stability by plot the stability boundary. It is clear from Fig. (6) that this scheme is not stable for any pure real λ. On the other hand, it is stabile for a pure imaginary λ; $Im(\lambda h) \in [-1.73205, 1.73205]$.

5. For the following set of ODEs:

$$\begin{aligned} y' &= -4z - 0.1y, \quad y(0) = 1, \\ z' &= -2 \times 10^4 z, \quad z(0) = 1, \end{aligned}$$

where $t \in [0, 1]$,

(a) Find the eigenvalues and the stiffness ratio for this system.

(b) Solve this system using any explicit Runge-Kutta scheme. In order to yield a solution, what is the largest grid size?

(c) Discuss your results.

Solution:
(a) This system of equation in matrix form is

$$\frac{d}{dt}\left[\begin{array}{c} y \\ z \end{array}\right] = \left(\begin{array}{cc} -0.1 & -4 \\ 0 & -20000 \end{array}\right)\left[\begin{array}{c} y \\ z \end{array}\right],$$

where it is clear that the system eigenvalues are $\{-0.1, -20000\}$, and the stiffness ratio is

$$\mathcal{S} = \left|\frac{\lambda_{max}}{\lambda_{min}}\right| = 2 \times 10^5.$$

(b) The largest grid size in order to get a solution is $h = 2/|\lambda_{max}| = 10^{-4}$. Using RK2 method with a grid size $h = 10^{-8}$, we where apply to solve this problem. The multi-scale nature of this problem is clearly noted the evolution of each variable, see Fig. (7).

6. For the following multi-step numerical scheme:

$$\begin{aligned} y^*_{n+1} &= y_n + hf_n, \\ y^{**}_{n+1} &= y_n + \frac{h}{2}\left[f^*_{n+1} - f_n\right], \\ y_{n+1} &= y_n + \frac{h}{2}\left[(1-\alpha)f^{**}_{n+1} + \alpha f^*_{n+1} + f_n\right]. \end{aligned}$$

(a) By using the model equation, $y' = \lambda y$, what is the maximum order of accuracy of this scheme?

(b) Plot the stability region for $\alpha = [0, 0.5, 0.75, \text{ and } 1]$.

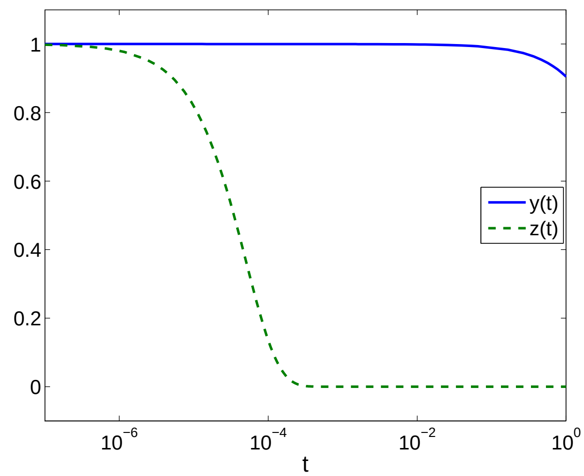

Figure 7: The solution of problem 5.

Solution:
(a) By substituting the model equation in y^*_{n+1}, y^{**}_{n+1} and y_{n+1}, and then substituting these equation into each other,

$$\begin{aligned} y^*_{n+1} &= y_n + \lambda h y_n, \\ y^{**}_{n+1} &= y_n + \frac{h}{2}\left[\lambda y_n + \lambda^2 h y_n - \lambda y_n\right], \\ y_{n+1} &= y_n + \frac{h}{2}\left[\lambda y_n + \alpha\lambda y_n + \alpha\lambda^2 h y_n + (1-\alpha)\left(\lambda y_n + \frac{\lambda^3 h^2 y_n}{2}\right)\right]. \end{aligned}$$

So,

$$y_{n+1} = y_n\left[1 + \lambda h + \frac{\alpha\lambda^2 h^2}{2} + (1-\alpha)\frac{\lambda^3 h^3}{4}\right],$$

for $\alpha = 1$ the scheme is second order accurate, which is the maximum order of accuracy.

(b) It is clear from the previous part that the amplification factor is

$$\sigma = 1 + \lambda h + \frac{\alpha\lambda^2 h^2}{2} + (1-\alpha)\frac{\lambda^3 h^3}{4}.$$

To plot the stability region, Fig. (8), we take $e^{i\theta} = \sigma,\ \theta = 0, \ldots, 2\pi$.

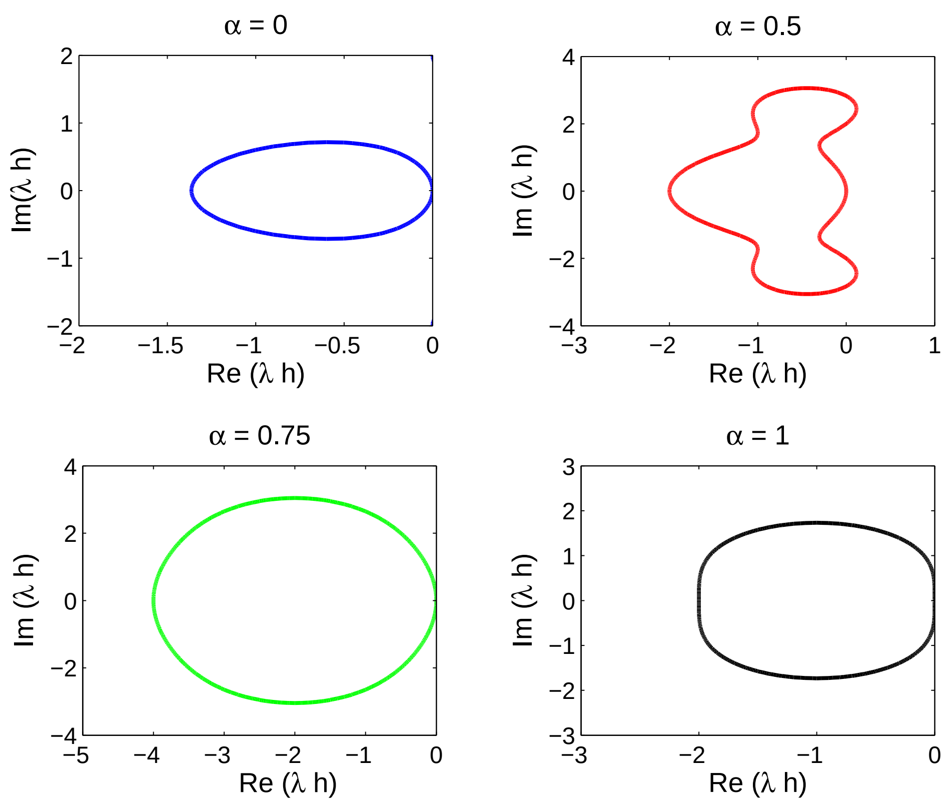

Figure 8: The stability boundary at different values of α.