PW #1: 1st-order ordinary differential equations

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We are interested in comparing different numerical schemes to solve 1st-order ODEs from an engineer point of view. Hence we shall focus on accuracy and efficiency.

1 Linear ODEs

We first consider a linear case over the time interval $[0,1]$:

$$\begin{cases} y'(t) = 3y(t) - 1, \\ y(0) = y_0. \end{cases} \tag{1}$$

Constant y_0 is assumed to be known.

1. Recall the exact solution to the Cauchy problem (1) – to do so, you can multiply the equation by e^{-3t} and integrate. In particular, what is the solution for $y_0 = \frac{1}{3}$?

2. **Euler schemes**

   (a) Apply the explicit Euler scheme to Eq. (1). Solve the resulting difference equation.

   (b) Given a homogeneous discretization of $[0,1]$ $t_n = n\Delta t$ for some $\Delta t > 0$, implement the resolution of (1) according to the aforementioned scheme.

   (c) Redo the same process for the implicit Euler scheme. Is any time step Δt admissible?

   (d) Show on the same plot the exact solution and the solutions obtained by means of the 2 Euler schemes for $\Delta t = 0.2, 0.1, 0.01$.

3. **Higher order schemes**

   (a) Apply the enhanced Euler scheme and the Crank-Nicolson scheme to Eq. (1) and solve the difference equations.

   (b) Implement these two schemes as well as the RK3 schemes and compare the numerical solutions (for $\Delta t = 0.2, 0.1, 0.01$) to the exact solution.

4. **Comparisons**

   (a) Plot the error $\max_n |y_n - y(t_n)|$ for the 5 schemes and for $\Delta t = 0.2, 0.1, 0.05, 0.02, 0.01$.

   (b) Which scheme seems to be the most suitable one?

2 Lotka-Volterra equations

These equations model the evolution of an isolated predator-prey system (for instance rabbits and lynx):

$$\begin{cases} x'(t) = x(t)\big(3 - y(t)\big), & x(0) = 1, \\ y'(t) = y(t)\big(x(t) - 2\big), & y(0) = 2. \end{cases} \tag{2}$$

We assume global-in-time existence for solutions to (2).

1. Determine which variable corresponds to the number of preys.
2. Rewrite Eqs. (2) as $\mathbf{Y}'(t) = \mathbf{F}\big(\mathbf{Y}(t)\big)$, where $\mathbf{Y} = (x, y)$.
3. We set $H(x, y) = x - 2\ln x + y - 3\ln y$. H is called the *Hamiltonian* of the system. Show that for all $t \geq 0$, $H\big(x(t), y(t)\big) = H\big(x(0), y(0)\big)$.
4. Implement the Heun method and the RK4 scheme to solve (2).
5. Plot the graph $\big(x(t), y(t)\big)$ for $\Delta t = 0.01$ and $T_{final} = 10$.
6. Show the evolution of $H\big(x(t), y(t)\big)$ with respect to t. Is this result in accordance with Question 3?
7. Determine the only constant solution to (2). Do you obtain numerically the expected result?

3 Chemical reactions

We consider the following system which models three coupled chemical reactions involving species E_1, E_2 and E_3:

$$\begin{cases} y_1' = -k_1 y_1 + k_3 y_2 y_3, & y_1(0) = 1, \\ y_2' = k_1 y_1 - k_3 y_2 y_3 - k_2 y_2^2, & y_2(0) = 0, \\ y_3' = k_2 y_2^2, & y_3(0) = 0. \end{cases} \tag{3}$$

We set: $k_1 = 0.04$, $k_2 = 3{\cdot}10^7$ and $k_3 = 10^4$ the velocities of reactions. y_k denotes the chemical concentration of species E_k. We assume that all components remain positive.

1. Rewrite Eqs. (3) as $\mathbf{Y}'(t) = \mathbf{F}\big(\mathbf{Y}(t)\big)$, where $\mathbf{Y} = (y_1, y_2, y_3)$.
2. What are the stationary states (constant solutions).
3. Show that $y_1(t) + y_2(t) + y_3(t) = 1$ for any time t. Interpret this result from a physical point of view.
4. Write the implicit Euler scheme applied to Syst. (3). Show that no inversion algorithm is required to apply the scheme to this case.
5. Compare results with the RK4 scheme. What do results tend to show about species 1? species 3?