Runge-Kutta methods

In this activity we will solve an initial value differentail equation by various explicit methods and compare them with each other.

Let us first establish a common language. A first order ordinary differental equation is an equation of the form

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

These problems have as solution a mathematical function $y(x)$ and can be solved numerically (and sometimes analytically) when the initial condition $y(x_0)$ is known. In this activity we will use an explicit method (i.e., a numerical method that constructs the solution at a further position $\bar{x} + \Delta x$ by knowing the properties at the position $\bar{x}$).

A first approach, known as the Euler method, is that of using the first derivative at a position $\bar{x}$ to predict the value of the mathematical function y at a further position $\bar{x} + \Delta x$.

One can write:

$$y(\bar{x} + \Delta x) = y(\bar{x}) + \left.\frac{dy}{dx}\right|_{x=\bar{x}} \Delta x \tag{2}$$

Armed with this equation, once we have tabulated an array of positions $\{x_i\}_{i=0 \ldots n}$, we can write a simple *for* loop and compute

$$y_{i+1} = y_i + f(x_i, y_i)(x_{i+1} - x_i) \tag{3}$$

Notice that all the quantities on the right hand side are known and therefore the value of y at the advanced position can be calculated.

You may also have noticed that Equation (2) looks a lot like a Taylor series truncated at the first order. For that reason the Euler method is called a "first order" method.

We have learned in our previous activity that the more terms we add to the series, the more precise is the approximation. Fortunately, that can be extended to the solution of differential equations. Let us, for example, devise a second order method. From the Taylor series we have:

$$y(\bar{x} + \Delta x) = y(\bar{x}) + y'(\bar{x})\Delta x + \frac{y''}{2}(\bar{x})\Delta x^2 \tag{4}$$

we do not know directly $y''(x)$, but we know that

$$y''(x) = \frac{df'(x)}{dx} = \frac{d}{dx} f(x, y) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f \tag{5}$$

This may not seem great progress, since we do not know the partial derivatives of f. However, it can be shown that this is equivalent to calculating $y(\bar{x} + \Delta x)$ as:

$$y(\bar{x} + \Delta x) = y(\bar{x}) + (k_1 + k_2)\frac{\Delta x}{2} \tag{6}$$

where

$$k_1 = f(x_i, y_i) \tag{7}$$

$$k_2 = f(x_i + \Delta x, y_i + k_1 \Delta x) \tag{8}$$

A very commonly used ethod is the 4^{th} order method (RK4) that uses:

$$y(\bar{x} + \Delta x) = y(\bar{x}) + (k_1 + 2k_2 + 2k_3 + k_4)\frac{\Delta x}{6} \tag{9}$$

where

$$\begin{aligned} k_1 &= f(x_i, y_i) && (10)\\ k_2 &= f(x_i + \Delta x/2, y_i + k_1 \Delta x/2) && (11)\\ k_3 &= f(x_i + \Delta x/2, y_i + k_2 \Delta x/2) && (12)\\ k_4 &= f(x_i + \Delta x, y_i + k_3 \Delta x) && (13) \end{aligned}$$

Activity We will consider the differential equation

$$y' = xy \tag{14}$$

and the initial condition:

$$y(0) = 1 \tag{15}$$

We know the analytical solution of this equation:

$$y(x) = e^{\frac{x^2}{2}} \tag{16}$$

1. Write a python script that tabulates and plot the analytical solution for $x \in [0, 5]$.
2. Add a block that uses the Euler method to compute the numerical solution. Use $\Delta x = 0.1$. Plot the Euler (1^{st} order solution) in the same graph. Add a legend.
3. Repeat the previous step but use a second order RK method.
4. Same as above but with RK4.

Questions to address during presentations:

1. How would you test accuracy of the solution if there is no known analytical result for the differential equation?
2. Is having a fixed step a necessity? Can a variable step be used?

Challenging:

1. Find three values of Δx that, used with Euler, RK2, and RK4, give solutions of the same accuracy.
2. Add time flags to your code and compare the run times of the three methods. Which is the faster to achieve the given accuracy?
3. Code an implicit method and compare the solution you get.

Physical equations:

- [**Velocity of falling object with drag**]: $\frac{dv}{dt} = -g + av + bv^2$, where $a < b$ are constants (pick your own)
- [**Number of atoms of a decaying isotope**]: $\frac{dN_2}{dt} = \frac{N_1}{\tau_1}e^{-\frac{t}{\tau_1}} - \frac{N_2}{\tau_2}e^{-\frac{t}{\tau_2}}$ where $N_1 \gg 1$ is the number of atoms of a parent species and τ_1 and τ_2 the decay times (pick your own).