Checking the Radioactive Decay Euler Algorithm

Review of the first example: radioactive decay

The radioactive decay equation

$$\frac{dN}{dt} = -\frac{N}{\tau}$$

has a well known solution in terms of the initial number of nuclei present at time $t = 0$

$$N(t) = N_0 \exp \frac{-t}{\tau}$$

Obviously, since there is an analytic solution readily available, we don't need computational physics methods to solve this problem. However, the radioactive decay serves as a good first example since it illustrates some of the techniques, and the pitfalls, in computational physics.

The Euler Method algorithm

From the Taylor series expansion we have the *Euler Method* or algorithm for solving the radioactive decay example

$$\frac{dN}{dt} \approx \frac{N(t + \Delta t) - N(t)}{\Delta t}$$

$$\implies N(t + \Delta t) \approx N(t) + \frac{dN}{dt}\Delta t = \text{ (substituting for dN/dt) } N(t)(1 - \frac{\Delta t}{\tau})$$

$$N(t + \Delta t) \approx N(t)(1 - \frac{\Delta t}{\tau})$$

In general, if you are given the equation for the derivative of any function $f(x)$ as df/dx, then you iterate in equidistant steps $x_1, x_2, \ldots, x_{n+1}$ to obtain

$$f(x_{n+1}) = f(x_n) + \frac{df}{dx}_{x=x_n} \Delta x$$

where $\Delta x = x_2 - x_1 = x_3 - x_2 = x_{n+1} - x_n$.

How do you know what value of Δx to choose? That depends on the nature of the problem and how does dN/dx behave mathematically. If you make Δx too large, then the results are more likely to be inaccurate. If you make Δx too small, you may be wasting computing time, or have stability problems as we shall see later.

Let's examine the book's solution using the Euler algorithm with $\Delta t = 0.05$ seconds.

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Book's solution, pages 11-13

The book's solution with the Euler algorithm using $\Delta t = 0.05$ s as shown in Fig. 1.1 and checked in Fig. 1.2 is depicted here in the top half of Fig. 1 The initial glance at the top half, or the

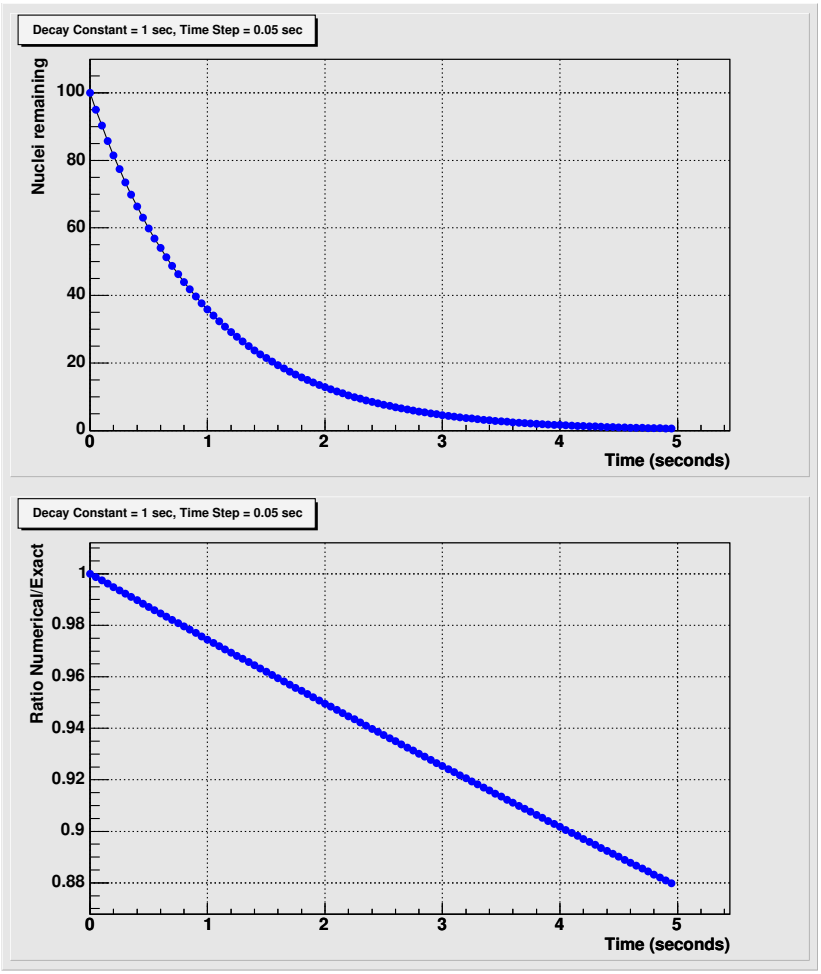

Figure 1: Check of Euler method for radioactive decay with $\Delta t = 0.05$ s.

Fig. 1.1 in the book, might lead you to conclude that the numerical solution is OK. However, the bottom half of this figure plots the ratio of the numerical result to the exact result. This ratio plot shows that the numerical solution is *systematically and progressively bad* as the time increases. At the $t = 5$ seconds the numerical result is more than 10% too low. Can you deduce why this systematic problem occurs?

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Step size check

The previous figure indicates the importance of checking the numerical solution for accuracy. In most cases, however, you will not have the true analytic result against which to compare. Nonetheless, one thing that you can typically do is to change the parameters of the calculation. In particular since a steps size such as Δt is usually involved, then one should always check that the results are stable for a change in step size. So the first thing which can be checked here is a change in step size from say 0.05 to 0.005 seconds. This result is shown in Fig. 2 By

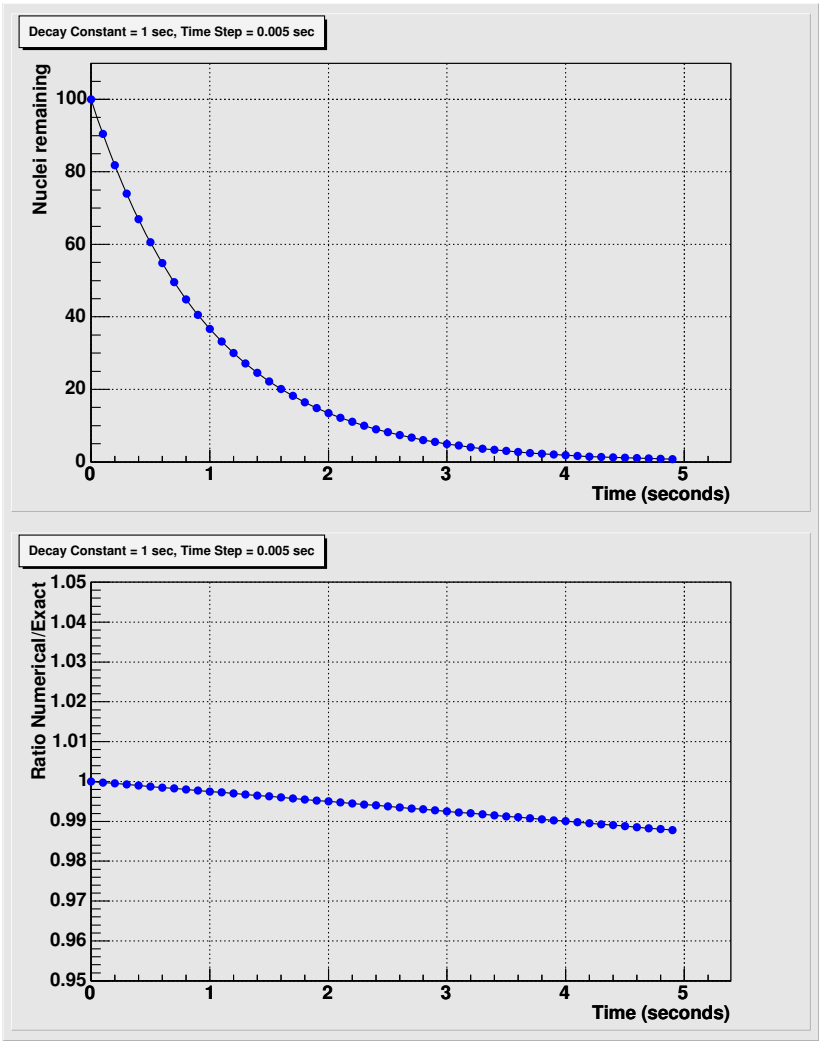

Figure 2: Check of Euler method for radioactive decay with $\Delta t = 0.005$ s.

decreasing the step size an order of magnitude, the numerical error has dropped to about 1% at $t = 5$ seconds, compared to about 11% in the previous figure.

Checking the Radioactive Decay Euler Algorithm

Defect in the Euler Method

Although the authors of this textbook defend the use of the Euler method, and continues to use it in the next chapter, almost all other computational references do not use the Euler method except as an introductory exercise. The systematic error of the Euler method for the radioactive decay is actually a good illustration of the basic defect of the Euler method.

> *The Euler method only evaluates the derivative at the beginning of the step. If the derivative at the beginning of the step is systematically incorrect, either too high or too low, then the numerical solution will be similarly systematically incorrect. Moreover the relative error in the numerical calculation will continue to grow with each iteration.*

To improve upon the Euler method we need to use the derivative function at more than one point in the step size.

The Runge-Kutta method, a better algorithm

The four point Runge-Kutta(RK4) method is much more widely used than the Euler method for integrating ordinary differential equations. As its name implies, the RK4 method uses the derivative at four positions in the step. The RK4 equations are given in the Appendix A on page 459, for a function $x(t)$ which has a first derivative function $f(t, x)$, that is $dx/dt = f(t, x)$. The basic iteration equation is

$$x(t + \Delta t) = x(t) + \frac{1}{6}\left[f(x_1, t_1) + 2f(x_2, t_2) + 2f(x_3, t_3) + f(x_4, t_4)\right]\Delta t$$

The four (t, x) pairs of points are

$$\begin{aligned} x_1 &= x(t) & t_1 &= t \\ x_2 &= x(t) + \frac{1}{2}f(x_1, t_1)\Delta t & t_2 &= t + \frac{1}{2}\Delta t \\ x_3 &= x(t) + \frac{1}{2}f(x_2, t_2)\Delta t & t_3 &= t + \frac{1}{2}\Delta t \\ x_4 &= x(t) + f(x_3, t_3)\Delta t & t_4 &= t + \Delta t \end{aligned}$$

Essentially the RK4 method evaluates the derivative at the two endpoints, and twice in the middle with different values of the dependent variable, in order to get a more accurate algorithm. The error in the RK4 method scales as $(\Delta t)^5$ while the error in the Euler method scales as $(\Delta t)^2$.

Using the RK4 Algorithm

Improved result

We can see the dramatic improvement with the use of the RK4 algorithm instead of the Euler method algorithm in the following figure The RK4 method produce a result which is accurate

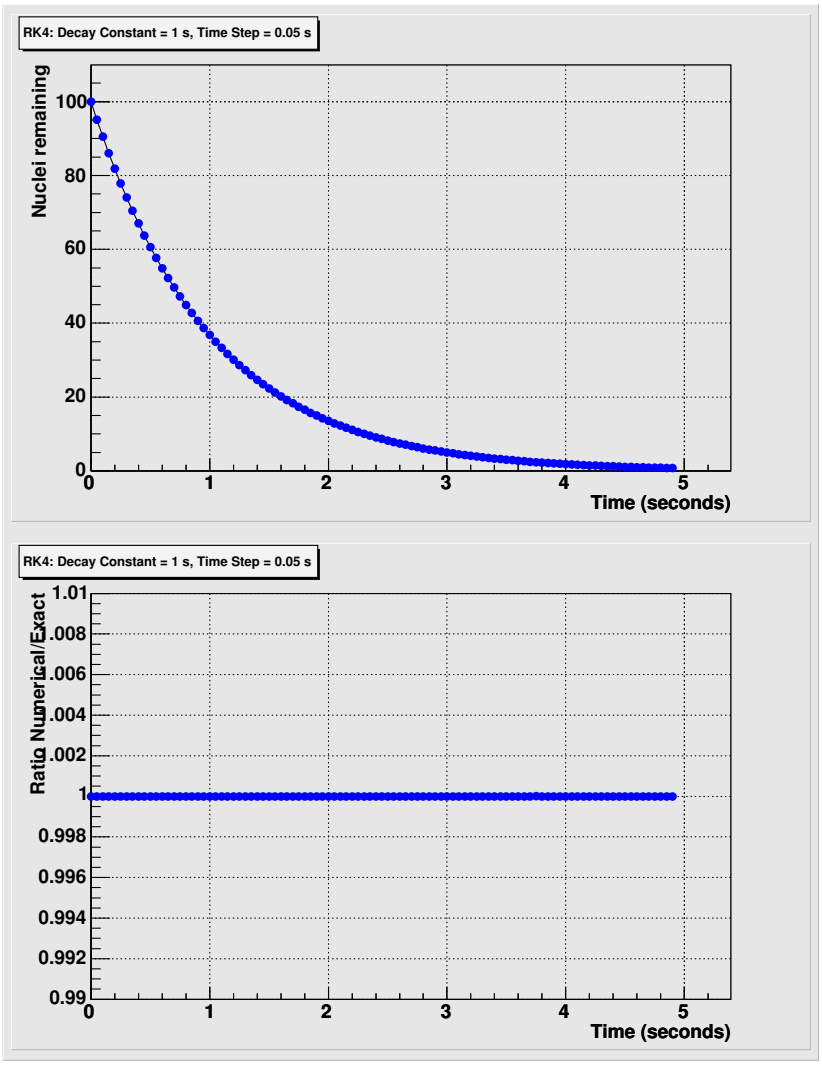

Figure 3: Check of RK4 method for radioactive decay with $\Delta t = 0.05$ s.

to better than one part in one million compared to the one part in ten accuracy of the Euler method with the same step size.

Numerical Stability Issues

Double vs Single Precision

Numerical computations are always done with double precision variables instead of single precision variables. A single precision variable uses 32 bits of memory storage, while a double precision variable uses 64 bits. Roughly speaking, a single precision variable is accurate to one part in 10^7 whereas a double precision variable is accurate to one part in 10^{15}. A single precision variable has a range -3.4×10^{-38} to $+3.4\times10^{+38}$ while the double precision range is -1.7×10^{-308} to $+1.7\times10^{+308}$

An example of how a single precision calculation will fail is in the radioactive decay program when the time step is set to 5×10^{-5} seconds. The result is

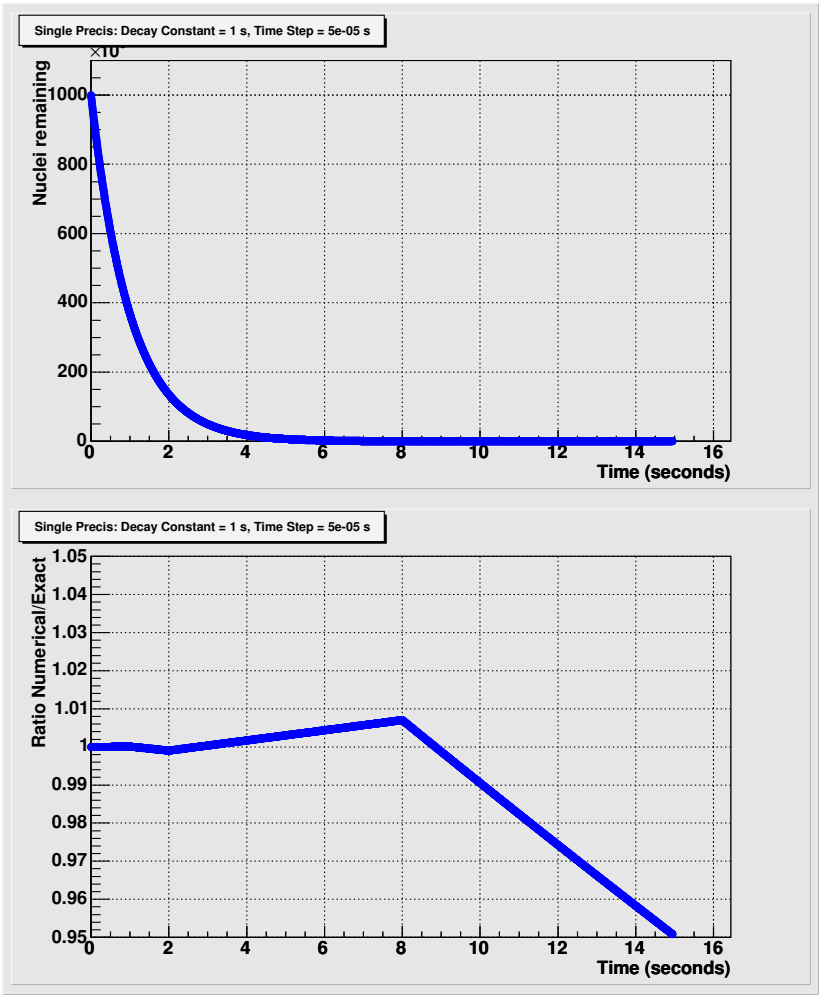

Figure 4: Check of Single Precision Euler method for radioactive decay with $\Delta t = 0.00005$ s showing a numerical instability as a function of time. The same program written in double precision does not have this numerical instability.