

# PHYS 512 Problem Set 3

Teophile Lemay, 281081252

## 1

The 4th order Runge-Kutta (RK4) method is a well defined algorithm for solving ODEs. For some first order ODE  $\frac{dy}{dx} = f(x, y)$  and a step size  $h$ , RK4 is defined as

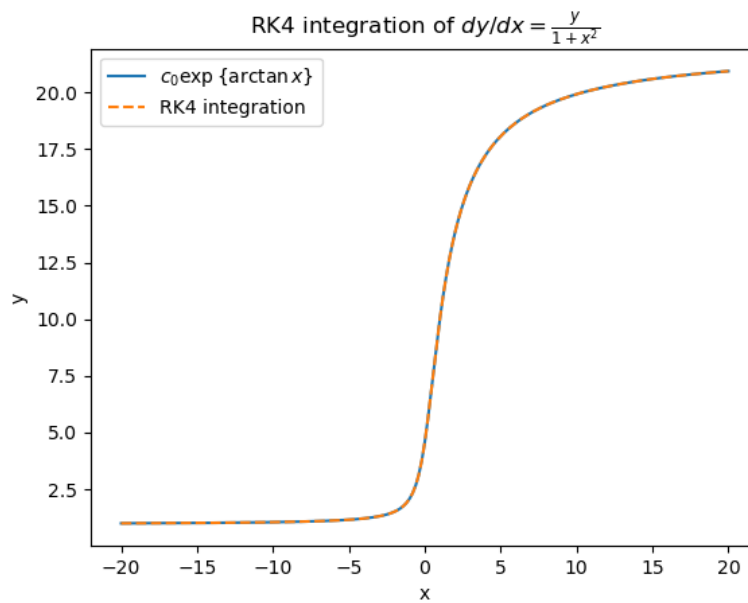
$$\begin{aligned}k_1 &= h \cdot f(y, x) \\k_2 &= h \cdot f(y + \frac{1}{2}k_1, x + \frac{1}{2}h) \\k_3 &= h \cdot f(y + \frac{1}{2}k_2, x + \frac{1}{2}h) \\k_4 &= h \cdot f(y + k_3, x + h) \\y(x + h) &= y(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\end{aligned}$$

This algorithm is implemented directly in my "rk4\_step" function which was used to evaluate

$$\frac{dy}{dx} = \frac{y}{1+x^2}$$

as shown in figure 1.

Figure 1: basic RK4 integration of  $\frac{dy}{dx} = \frac{y}{1+x^2}$  ( $N = 200$ )



Each of the RK4 terms after  $k_1$  can be described as a second order Taylor expansion using the previous term.

$$\begin{aligned}
k_1 &= h \cdot f(y, x) \\
k_2 &= h \cdot f\left(y + \frac{1}{2}k_1, x + \frac{1}{2}h\right) = h \cdot \left(f(y, x) + \frac{1}{2} \frac{d}{dx} k_1\right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2} \frac{d}{dx} f(y, x)\right) \\
k_3 &= h \cdot f\left(y + \frac{1}{2}k_2, x + \frac{1}{2}h\right) = h \cdot \left(f(y, x) + \frac{1}{2} \frac{d}{dx} k_2\right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2} \frac{d}{dx} \left(f(y, x) + \frac{h}{2} \frac{d}{dx} f(y, x)\right)\right) \\
&= h \cdot \left(f(y, x) + \frac{h}{2} \frac{d}{dx} f(y, x) + \frac{h^2}{4} \frac{d^2}{dx^2} f(y, x)\right) \\
k_4 &= h \cdot f(y + k_3, x + h) = h \cdot \left(f(y, x) + \frac{d}{dx} k_3\right) \\
&= h \cdot \left(f(y, x) + h \frac{d}{dx} \left(f(y, x) + \frac{h}{2} \frac{d}{dx} \left(f(y, x) + \frac{h}{2} \frac{d}{dx} f(y, x)\right)\right)\right) \\
&= h \cdot \left(f(y, x) + h \frac{d}{dx} f(y, x) + \frac{h^2}{2} \frac{d^2}{dx^2} f(y, x) + \frac{h^3}{4} \frac{d^3}{dx^3} f(y, x)\right) \\
y_{rk4}(x + h) &= y(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}$$

Given the proper coefficients, RK4 is equivalent to a 4th order polynomial so

$$y(x + h) = y_{rk4}(x + h) + \frac{h^5}{5!} \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6)$$

If the step size is reduced to  $h/2$ , repeating the second order expansion on  $k'_1, k'_2, k'_3$ , and  $k'_4$  (' designates the  $h/2$  step) produces

$$\begin{aligned}
y_{rk4}(x + h/2) &= y(x) + \frac{1}{6}(k'_1 + 2k'_2 + 2k'_3 + k'_4) \\
y(x + h/2) &= y_{rk4}(x + h/2) + \left(\frac{h}{2}\right)^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6) .
\end{aligned}$$

A second  $h/2$  step (') gives

$$\begin{aligned}
y_{rk4'}(x + h) &= y(x + h/2) + \frac{1}{6}(k'_1 + 2k'_2 + 2k'_3 + k'_4) \\
y(x + h) &= y(x + h/2) + \frac{1}{6}(k'_1 + 2k'_2 + 2k'_3 + k'_4) + \left(\frac{h}{2}\right)^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6) \\
y(x + h) &= y_{rk4}(x + h/2) + \left(\frac{h}{2}\right)^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6) + \frac{1}{6}(k'_1 + 2k'_2 + 2k'_3 + k'_4) + \left(\frac{h}{2}\right)^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6) . \\
y(x + h) &= y_{rk4}(x + h/2) + \frac{1}{6}(k'_1 + 2k'_2 + 2k'_3 + k'_4) + 2 \left(\frac{h}{2}\right)^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6) .
\end{aligned}$$

Thus, the leading error term for  $y(x + h)$  after 2 RK4 steps of  $h/2$  is  $\frac{h^5}{16} \frac{d^4}{dx^4} f(y, x)$  compared to  $h^5 \frac{d^4}{dx^4} f(y, x)$  for a single step of length  $h$ . Using this result, I can make use of both step lengths to eliminate the 5<sup>th</sup> order error term.

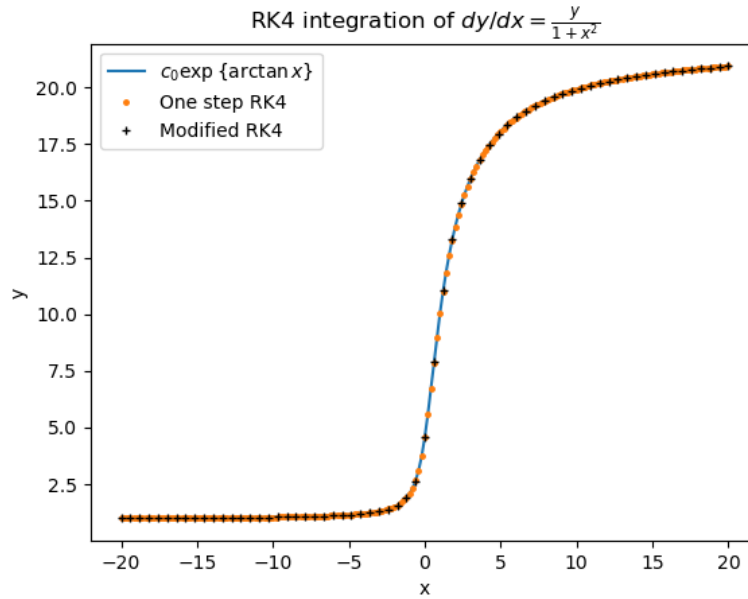
$$y_{h/2}(x + h) = y_{true}(x + h) - \frac{h^5}{16} \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6)$$

$$y_h(x+h) = y_{true}(x+h) - h^5 \frac{d^4}{dx^4} f(y, x) + \mathcal{O}(h^6)$$

$$\boxed{\frac{16y_{h/2}(x+h) - y_h(x+h)}{15} = y(x+h) + \mathcal{O}(h^6)}.$$

For each step  $H$ , this modified RK4 algorithm computes a one step RK4 3 times, requiring 12 function calls compared to the 4 required by a default RK4 implementation. Assuming that function evaluations are the most important complexity consideration, then the modified RK4 should be able to achieve greater accuracy than the one step RK4 while using  $N/3$  points. Figure 2 shows a comparison of the expected result, basic RK4 integration with  $N = 200$  steps, and my modified RK4 integration with  $N_{h/2} = 66$  steps. For the given ODE, the root mean squared deviation (RMSD) for the modified RK4 integration is more than 20 times smaller than for the default RK4, with values of  $RMSD_{h/2} \approx 1.04 \cdot 10^{-4}$  and  $RMSD_h \approx 2.32 \cdot 10^{-3}$  respectively. All code for this question can be found in the file "Q1\_runge\_kutta.py".s

Figure 2: Modified RK4 integration of  $\frac{dy}{dx} = \frac{y}{1+x^2}$  ( $N = 66$ )



## 2

### 2.1 a)

A single stage exponential decay relates can be described by the differential equation

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

with solution

$$N(t) = N_0 e^{-\frac{t}{\tau} \ln 2}$$

where  $\tau$  is the half-life. Using this description, the decay chain for uranium-238 (figure 3) can be translated into a series of differential equations:

$$\frac{dN_{U238}}{dt} = -\frac{\ln 2}{\tau_{U238}} N_{U238} \quad (1)$$

$$\frac{dN_{Th234}}{dt} = \frac{\ln 2}{\tau_{U238}} N_{U238} - \frac{\ln 2}{\tau_{Th234}} N_{Th234} \quad (2)$$

$$\frac{dN_{Pa234}}{dt} = \frac{\ln 2}{\tau_{Th234}} N_{Th234} - \frac{\ln 2}{\tau_{Pa234}} N_{Pa234} \quad (3)$$

$$\frac{dN_{U234}}{dt} = \frac{\ln 2}{\tau_{Pa234}} N_{Pa234} - \frac{\ln 2}{\tau_{U234}} N_{U234} \quad (4)$$

$$\frac{dN_{Th230}}{dt} = \frac{\ln 2}{\tau_{U234}} N_{U234} - \frac{\ln 2}{\tau_{Th230}} N_{Th230} \quad (5)$$

$$\frac{dN_{Ra226}}{dt} = \frac{\ln 2}{\tau_{Th230}} N_{Th230} - \frac{\ln 2}{\tau_{Ra226}} N_{Ra226} \quad (6)$$

$$\frac{dN_{Rn222}}{dt} = \frac{\ln 2}{\tau_{Ra226}} N_{Ra226} - \frac{\ln 2}{\tau_{Rn222}} N_{Rn222} \quad (7)$$

$$\frac{dN_{Po218}}{dt} = \frac{\ln 2}{\tau_{Rn222}} N_{Rn222} - \frac{\ln 2}{\tau_{Po218}} N_{Po218} \quad (8)$$

$$\frac{dN_{Pb214}}{dt} = \frac{\ln 2}{\tau_{Po218}} N_{Po218} - \frac{\ln 2}{\tau_{Pb214}} N_{Pb214} \quad (9)$$

$$\frac{dN_{Bi214}}{dt} = \frac{\ln 2}{\tau_{Pb214}} N_{Pb214} - \frac{\ln 2}{\tau_{Bi214}} N_{Bi214} \quad (10)$$

$$\frac{dN_{Po214}}{dt} = \frac{\ln 2}{\tau_{Bi214}} N_{Bi214} - \frac{\ln 2}{\tau_{Po214}} N_{Po214} \quad (11)$$

$$\frac{dN_{Pb210}}{dt} = \frac{\ln 2}{\tau_{Po214}} N_{Po214} - \frac{\ln 2}{\tau_{Pb210}} N_{Pb210} \quad (12)$$

$$\frac{dN_{Bi210}}{dt} = \frac{\ln 2}{\tau_{Pb210}} N_{Pb210} - \frac{\ln 2}{\tau_{Bi210}} N_{Bi210} \quad (13)$$

$$\frac{dN_{Po210}}{dt} = \frac{\ln 2}{\tau_{Bi210}} N_{Bi210} - \frac{\ln 2}{\tau_{Po210}} N_{Po210} \quad (14)$$

$$\frac{dN_{Pb206}}{dt} = \frac{\ln 2}{\tau_{Po210}} N_{Po210} \quad (15)$$

**2.2** b)

**3**

**3.1** a)

**3.2** b)

**3.3** c)

Figure 3: Uranium-238 decay chain (From slides)

	Half-Life	Time unit	Emitter
Uranium-238	4,468	billion of years	alpha
Thorium-234	24,10	days	beta -
Protactinium-234	6,70	hours	beta -
Uranium-234	245 500	years	alpha
Thorium-230	75380	years	alpha
Radium-226	1 600	years	alpha
Radon-222	3,8235	days	alpha
Polonium-218	3,10	minutes	alpha
Plomb-214	26,8	minutes	beta -
Bismuth-214	19,9	minutes	beta -
Polonium-214	164,3	microseconds	alpha
Plomb-210	22,3	years	beta
Bismuth-210	5,015	years	beta
Polonium-210	138,376	days	alpha
Plomb-206	Stable		