RK4 is an ODE solver important in numerical integration. Its working resembles that of Euler's method. The iterator takes the form:

$$y_{t+h}=y_t+\frac{h}{6}(k_1+2k_2+2k_3+k_4);$$

$$\Leftrightarrow\begin{cases} y_{t+h}=y_t+h<k> \\ <k>=\frac{1}{6}(k_1+2k_2+2k_3+k_4) \end{cases}$$

In this document we will focus on how to obtain $<k>=\frac{1}{6}(k_1+2k_2+2k_3+k_4)$.

RK-family method relies on finding k_n iteratively, in RK4 the iteration reads

$$\begin{cases} k_1=f(y_t,t) \\ k_2=f(y_t+\frac{h}{2}k_{1,}t+\frac{h}{2}) \\ k_3=f(y_t+\frac{h}{2}k_{1,}t+\frac{h}{2}) \\ k_4=f(y_t+h,k_{1,}t+h) \end{cases}$$

However, these relations are only useful to derive k2, not from k1 directly, but proxyed through a complicated y. We now seek to eliminate this proxy. We wonder what happened to the coefficients of k1 to k4. Thus, we should taylor-expand k1 to k4, exploiting the aforementioned preserved relation. Note this expansion has a 2D form if partial derivative is taken. However we can exploit the principle of total derivative to simplify the notation. (This is essentially dropping the dependency of "f" on "y" to achieve a simpler notation).

$$k_2=f(y_t+\frac{h}{2}k_{1,}t+\frac{h}{2})=f(y_t,t)+\frac{h}{2}k_1\frac{\partial}{\partial y}f(y_t,t)+\frac{h}{2}\frac{\partial}{\partial t}f(y_t,t)+O(h^2k^2,h^2);(I)$$

By the principle of total derivative:

$$\partial f=\frac{\partial f}{\partial y}\partial y+\frac{\partial f}{\partial t}\partial t$$

Take derivative wrt t:

$$\frac{df}{dt}=\frac{\partial f}{\partial y}\frac{dy}{dt}+\frac{\partial f}{\partial t}=\frac{\partial f}{\partial y}k_1+\frac{\partial f}{\partial t}$$

Exchange LHS with RHS, time both sides by $\frac{h}{2}$ gives:

$$\frac{h}{2}k_1\frac{\partial f}{\partial y}+\frac{h}{2}\frac{\partial f}{\partial t}=\frac{h}{2}\frac{df}{dt};(II)$$

substitue (II) into (I) gives:

$$k_2=f(y,t)+\frac{h}{2}\frac{df}{dt}$$

Note $f(y_t,t)=k_1$,in other words:

$$k_2=f(y,t)+\frac{h}{2}\frac{dk_1}{dt};$$

We have now obtained a direct iteravie relation from k_1 to k_2.We can iterate this approach to obtain k_3 and k_4. Note this iteration involves differentiating k_1 w.r.t. t. Now that k_1 is the first derivative of y against t, k_4 thus contains a fourth order derivative at highest by induction.

The fact that k_4 contains $\frac{d^{4y}}{dt^4}$ allows us to eliminate h^4 but leaves $O(h^5)$ untouched

We approximate $y(t+h)$ as a linear combination of $k_{1,}k_{2,}k_{3,}k_{4.}$

$$y(t+h)=y(t)+a_1k_1+a_2k_2+a_3k_3+a_4k_4+O(h^5).$$

Substituting $k_1 k_2 k_3 k_4$ *according* to *the iterated expression should give* :

$$y(t+h)=y(t)+b_1\frac{dy}{dt}h^1+b_2\frac{d^2y}{dt^2}h^2+b_3\frac{d^3y}{dt^3}h^3+b_4\frac{d^4y}{dt^4}h^4+O(h^5);(III),$$

where any b_n *is a function of* $a_1,a_2,a_3,a_{4.}$

Compare (III) against well-known Taylor expansion of y(t+h):

$$y(t+h)=y(t)+\frac{1}{1!}\frac{dy}{dt}h^1+\frac{1}{2!}\frac{d^2y}{dt^2}h^2+\frac{1}{3!}\frac{d^3y}{dt^3}h^3+\frac{1}{4!}\frac{d^4y}{dt^4}h^4+O(h^5);$$

We obtain

$$\begin{cases} b_1=\frac{1}{1!} \\ b_2=\frac{1}{2!} \\ b_3=\frac{1}{3!} \\ b_4=\frac{1}{4!} \end{cases}$$

Since any b_n is a function of $a_1,a_2,a_3,a_{4,}$ we now have 4 equations to solve for 4 unknowns.
Solving these should* give up to

$$\begin{cases} a_1=\frac{1}{6} \\ a_2=\frac{2}{6} \\ a_3=\frac{2}{6} \\ a_4=\frac{1}{6} \end{cases}$$

*According to Wikipedia, the full expansion of (III) looks like

$$\begin{aligned}
y_{t+h} &= y_t + h\left\{a \cdot f(y_t,\, t) + b \cdot \left[f\left(y_t,\, t\right) + \frac{h}{2}\frac{d}{dt}f\left(y_t,\, t\right)\right] + \right.\\
&\quad + c \cdot \left[f\left(y_t,\, t\right) + \frac{h}{2}\frac{d}{dt}\left[f\left(y_t,\, t\right) + \frac{h}{2}\frac{d}{dt}f\left(y_t,\, t\right)\right]\right] + \\
&\quad \left. + d \cdot \left[f\left(y_t,\, t\right) + h\frac{d}{dt}\left[f\left(y_t,\, t\right) + \frac{h}{2}\frac{d}{dt}\left[f\left(y_t,\, t\right) + \frac{h}{2}\frac{d}{dt}f\left(y_t,\, t\right)\right]\right]\right]\right\} + \mathcal{O}(h^5) \\
&= y_t + a \cdot hf_t + b \cdot hf_t + b \cdot \frac{h^2}{2}\frac{df_t}{dt} + c \cdot hf_t + c \cdot \frac{h^2}{2}\frac{df_t}{dt} + \\
&\quad + c \cdot \frac{h^3}{4}\frac{d^2 f_t}{dt^2} + d \cdot hf_t + d \cdot h^2\frac{df_t}{dt} + d \cdot \frac{h^3}{2}\frac{d^2 f_t}{dt^2} + d \cdot \frac{h^4}{4}\frac{d^3 f_t}{dt^3} + \mathcal{O}(h^5)
\end{aligned}$$

Giving up to:

$$\begin{cases}
a + b + c + d = 1 \\
\frac{1}{2}b + \frac{1}{2}c + d = \frac{1}{2} \\
\frac{1}{4}c + \frac{1}{2}d = \frac{1}{6} \\
\frac{1}{4}d = \frac{1}{24}
\end{cases}$$

and thus

$$\begin{cases}
a = \frac{1}{6} \\
b = \frac{2}{6} \\
c = \frac{2}{6} \\
d = \frac{1}{6}
\end{cases}$$