RK4 is an ODE solver similar to euler's method, with the iterator taking the form:

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

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

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

$$\begin{cases} k_1=f(y_t,t) \\ k_2=f(y_t+\frac{h}{2}k_{1,}t+\frac{h}{2}) \\ k_3=f(y_t+\frac{h}{2}k_{2,}t+\frac{h}{2}) \\ k_4=f(y_t+hk_{3,}t+h) \end{cases}$$

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 $k_{1,}k_{2,}k_{3,}k_{4.}$

$$y(t+h) = y(t) + a_1 k_1 + a_2 k_2 + a_3 k_3 + a_4 k_4 + O(h^5).$$

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

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

*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 ):

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

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

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

Giving up to:

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

and thus

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