Runge-Kutta method

Let a system of functions $x_\beta(t)$ be the solutions of the system of coupled differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}x_\beta = \dot{x}_\beta = f_\beta\left(x_1, \ldots, x_N, t\right) \equiv f_\beta\left(\{x_\gamma\}, t\right).$$

We wish to numerically integrate those equations, thus we take $t \to t_k = k\Delta t$ as a discrete parameter and, therefore, $x_\beta(t) = x_{\beta,k}$.

I. SECOND ORDER

We use the Taylor series so that

$$\begin{aligned} x_{\beta,k+1} &= x_{\beta,k} + \frac{\mathrm{d}x_{\beta,k}}{\mathrm{d}t}\Delta t + \frac{1}{2!}\frac{\mathrm{d}^2 x_{\beta,k}}{\mathrm{d}t^2}\left(\Delta t\right)^2 + \ldots \\ &= x_{\beta,k} + f_{\beta,k}\Delta t + \frac{1}{2!}\frac{\mathrm{d}f_{\beta,k}}{\mathrm{d}t}\left(\Delta t\right)^2 + \mathcal{O}\left(f_{\beta,k}^{(2)}\left(\Delta t\right)^3\right). \end{aligned}$$

Since $\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \sum_\beta \frac{\partial x_\beta}{\partial t}\frac{\partial}{\partial x_\beta} = \frac{\partial}{\partial t} + \sum_\beta f_\beta \frac{\partial}{\partial x_\beta}$, then

$$x_{\beta,k+1} = x_{\beta,k} + f_{\beta,k}\Delta t + \frac{1}{2}\left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k}\partial_\gamma f_{\beta,k}\right)\left(\Delta t\right)^2 + \mathcal{O}\left(f_{\beta,k}^{(2)}\left(\Delta t\right)^3\right). \tag{1}$$

Now we compare this expansion with the following expression

$$x_{\beta,k+1} = x_{\beta,k} + \Delta t\left(A_{\beta,1}F_{\beta,k,1} + A_{\beta,2}F_{\beta,k,2}\right) + \mathcal{O}\left(f_{\beta,k}^{(2)}\left(\Delta t\right)^3\right), \tag{2}$$

with

$$F_{\beta,k,1} = f_{\beta,k} = f_\beta\left(x_{1,k}, \ldots, x_{N,k}, t_k\right) \text{ and } F_{\beta,k,2} = f_\beta\left(\left\{x_{\gamma,k} + \frac{\Delta t}{B_2}f_{\gamma,k}\right\}, t_k + \frac{\Delta t}{B_2}\right).$$

In order to compare (1) with (2), we need to expand

$$\begin{aligned} F_{\beta,k,2} = f_\beta\left(\left\{x_{\gamma,k} + \frac{\Delta t}{B_2}f_{\gamma,k}\right\}, t_k + \frac{\Delta t}{B_2}\right) &= f_\beta\left(\left\{x_{\gamma,k}\right\}, t_k\right) + \sum_\gamma \partial_\gamma f_{\beta,k}\left(\frac{\Delta t}{B_2}f_{\gamma,k}\right) + \partial_t f_{\beta,k}\left(\frac{\Delta t}{B_2}\right) + \mathcal{O}\left(f_\beta^{(2)}\left(\Delta t\right)^2\right) \\ &= f_\beta\left(\left\{x_{\gamma,k}\right\}, t_k\right) + \frac{\Delta t}{B_2}\left(\sum_\gamma f_{\gamma,k}\partial_\gamma + \partial_t\right) f_{\beta,k} + \mathcal{O}\left(f_\beta^{(2)}\left(\Delta t\right)^2\right) \\ &= f_\beta\left(\left\{x_{\gamma,k}\right\}, t_k\right) + \frac{\Delta t}{B_2}\frac{\mathrm{d}}{\mathrm{d}t}f_{\beta,k} + \mathcal{O}\left(f_\beta^{(2)}\left(\Delta t\right)^2\right). \end{aligned}$$

Then, Eq. (2) becomes

$$x_{\beta,k+1} = x_{\beta,k} + \Delta t\left(A_{\beta,1} + A_{\beta,2}\right)f_{\beta,k} + \frac{A_{\beta,2}}{B_2}\left(\frac{\mathrm{d}}{\mathrm{d}t}f_{\beta,k}\right)\left(\Delta t\right)^2 + \mathcal{O}\left(f_{\beta,k}^{(2)}\left(\Delta t\right)^3\right),$$

from which we conclude that

$$A_{\beta,1} + A_{\beta,2} = 1 \text{ and } \frac{A_{\beta,2}}{B_2} = \frac{1}{2}. \tag{3}$$

Notice there are more than one solution.

As an example, consider the case in which $\dot{x} = f_x(x, v, t) = v$, and $\dot{v} = f_v(x, v, t)$. Thus, up to second order, we have that

$$
\begin{aligned}
x_{k+1} &= x_k + \Delta t \left(A_{x,1} v_k + A_{x,2} \left(v_k + \frac{\Delta t}{B_2} f_{v,k} \right) \right) \\
&= x_k + \Delta t \left(A_{x,1} + A_{x,2} \right) v_k + (\Delta t)^2 \frac{A_{x,2}}{B_2} f_{v,k} \\
&= x_k + \Delta t v_k + \frac{(\Delta t)^2}{2} f_{v,k},
\end{aligned}
$$

for all solutions of (3). This is just the equation of movement for a particle with a constant acceleration. The update for the velocity is

$$
v_{k+1} = v_k + \Delta t \left[A_{v,1} f_{v,k} + A_{v,2} f_v \left(x_k + \frac{\Delta t}{B_2} v_k, v_k + \frac{\Delta t}{B_2} f_{v,k}, t_k + \frac{\Delta t}{B_2} \right) \right].
$$

For instance, in the case which $f_v(x, v, t) = f_v(t)$, and using the solution $A_{v,1} = A_{v,2} = \frac{1}{2}$, and $B_2 = 1$, then

$$
v_{k+1} - v_k = \frac{\Delta t}{2} \left[f_{v,k} + f_v \left(t_k + \Delta t \right) \right] = \frac{\Delta t}{2} \left[f_{v,k} + f_{v,k+1} \right],
$$

which simply is the Trapezoidal rule for numerical integration.

II. THIRD ORDER

Let us consider the expansion in third order. Then,

$$
\begin{aligned}
x_{\beta,k+1} =& x_{\beta,k} + f_{\beta,k} \Delta t + \frac{(\Delta t)^2}{2} \left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k} \partial_\gamma f_{\beta,k} \right) + \\
& \frac{(\Delta t)^3}{3!} \left(\partial_{tt}^2 f_{\beta,k} + \sum_\gamma \partial_t f_{\gamma,k} \partial_\gamma f_{\beta,k} + 2 \sum_\gamma f_{\gamma,k} \partial_{t\gamma}^2 f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} \partial_\delta f_{\gamma,k} \partial_\gamma f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial_{\delta\gamma}^2 f_{\beta,k} \right) \\
& + \mathcal{O}\left(f_{\beta,k}^{(3)} (\Delta t)^4 \right).
\end{aligned}
$$

We now assume that

$$
x_{\beta,k+1} = x_{\beta,k} + \Delta t \left(A_{\beta,1} F_{\beta,k,1} + A_{\beta,2} F_{\beta,k,2} + A_{\beta,3} F_{\beta,k,3} \right) + \mathcal{O}\left(f_{\beta,k}^{(3)} (\Delta t)^4 \right),
$$

with

$$
F_{\beta,k,1} = f_{\beta,k}, \;\; F_{\beta,k,2} = f_\beta \left(\left\{ x_\gamma + \frac{\Delta t}{B_2} F_{\gamma,k,1}, t_k + \frac{\Delta t}{B_2} \right\} \right), \text{ and } F_{\beta,k,3} = f_\beta \left(\left\{ x_\gamma + \frac{\Delta t}{B_3} F_{\gamma,k,2}, t_k + \frac{\Delta t}{B_3} \right\} \right).
$$

We now need to expand these function:

$$
F_{\beta,k,2} = f_{\beta,k} + \frac{\Delta t}{B_2} \left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k} \partial_\gamma f_{\beta,k} \right) + \frac{(\Delta t)^2}{2! B_2^2} \left(\partial_{tt}^2 f_{\beta,k} + 2 \sum_\gamma f_{\gamma,k} \partial_{t\gamma}^2 f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial_{\delta,k}^2 f_{\beta,k} \right) + \dots
$$

$$
\begin{aligned}
F_{\beta,k,3} =& f_\beta \left(\left\{ x_\gamma + \frac{\Delta t}{B_3} \left(f_{\beta,k} + \frac{\Delta t}{B_2} (\star) + \dots \right), t_k + \frac{\Delta t}{B_3} \right\} \right) \\
=& f_{\beta,k} + \frac{\Delta t}{B_3} \left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k} \partial_\gamma f_{\beta,k} \right) + \frac{(\Delta t)^2}{2! B_3^2} \left(\partial_{tt}^2 f_{\beta,k} + 2 \sum_\gamma f_{\gamma,k} \partial_{t\gamma}^2 f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial_{\delta,k}^2 f_{\beta,k} \right) \\
& + \frac{(\Delta t)^2}{B_2 B_3} \left(\sum_\gamma \left(\partial_t f_{\gamma,k} + \sum_\delta f_{\delta,k} \partial_\delta f_{\gamma,k} \right) \partial_\gamma f_{\beta,k} \right) + \mathcal{O}\left(\Delta t \right)^4.
\end{aligned}
$$

Then,

$$\begin{aligned}
x_{\beta,k+1} =& x_{\beta,k} + \Delta t \left(A_{\beta,1} + A_{\beta,2} + A_{\beta,3}\right) f_{\beta,k} \\
&+ (\Delta t)^2 \left(\frac{A_{\beta,2}}{B_2} + \frac{A_{\beta,3}}{B_3}\right) \left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k} \partial_\gamma f_{\beta,k}\right) \\
&+ (\Delta t)^3 \left(\frac{A_{\beta,2}}{2B_2^2} + \frac{A_{\beta,3}}{2B_3^2}\right) \left(\partial^2_{tt} f_{\beta,k} + 2\sum_\gamma f_{\gamma,k} \partial^2_{t\gamma} f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial^2_{\delta,k} f_{\beta,k}\right) \\
&+ (\Delta t)^3 \frac{A_{\beta,3}}{B_2 B_3} \left(\sum_\gamma \partial_t f_{\gamma,k} \partial_\gamma f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} \partial_\delta f_{\gamma,k} \partial_\gamma f_{\beta,k}\right) + \mathcal{O}\left(f^{(3)}_{\beta,k} (\Delta t)^4\right).
\end{aligned}$$

Comparing the expansions, then

$$\left(A_{\beta,1} + A_{\beta,2} + A_{\beta,3}\right) = 1, \ \left(\frac{A_{\beta,2}}{B_2} + \frac{A_{\beta,3}}{B_3}\right) = \frac{1}{2!}, \text{ and } \frac{A_{\beta,3}}{B_2 B_3} = \frac{1}{3!} = \left(\frac{A_{\beta,2}}{2B_2^2} + \frac{A_{\beta,3}}{2B_3^2}\right).$$

As in the 2nd order case, there is more than one real solution. Maybe a simpler one is that in which $A_{\beta,2} = 0$. In this case

$$A_{\beta,1} = \frac{1}{4}, \ A_{\beta,2} = 0, \ A_{\beta,3} = \frac{3}{4}, \ B_2 = 3, \text{ and } B_3 = \frac{3}{2}.$$

III. FOURTH ORDER

Until now, we have seen there is no difference weather the number of components are $N = 1$ or $N > 1$. We can therefore use $N = 1$ and lighten the notation. We however choose to keep the more cumbersome and complete notation.

In forth order, the Taylor expansion is

$$\begin{aligned}
x_{\beta,k+1} =& x_{\beta,k} + f_{\beta,k}\Delta t + \frac{(\Delta t)^2}{2} \left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k} \partial_\gamma f_{\beta,k}\right) + \\
& \frac{(\Delta t)^3}{3!} \left(\partial^2_{tt} f_{\beta,k} + \sum_\gamma \partial_t f_{\gamma,k} \partial_\gamma f_{\beta,k} + 2\sum_\gamma f_{\gamma,k} \partial^2_{t\gamma} f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} \partial_\delta f_{\gamma,k} \partial_\gamma f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial^2_{\delta\gamma} f_{\beta,k}\right) + \\
& \frac{(\Delta t)^4}{4!} \Bigg(\partial^3_{ttt} f_{\beta,k} + \sum_\gamma \partial^2_{tt} f_{\gamma,k} \partial_\gamma f_{\beta,k} + 3\sum_\gamma \partial_t f_{\gamma,k} \partial^2_{t\gamma} f_{\beta,k} + 3\sum_\gamma f_{\gamma,k} \partial^3_{tt\gamma} f_{\beta,k} + \sum_{\delta,\gamma} \partial_t f_{\delta,k} \partial_\delta f_{\gamma,k} \partial_\gamma f_{\beta,k} \\
& + 2\sum_{\delta,\gamma} f_{\delta,k} \partial^2_{t\delta} f_{\gamma,k} \partial_\gamma f_{\beta,k} + 3\sum_{\delta,\gamma} f_{\delta,k} \partial_\delta f_{\gamma,k} \partial^2_{t\gamma} f_{\beta,k} + 3\sum_{\delta,\gamma} f_{\gamma,k} \partial_t f_{\delta,k} \partial^2_{\delta\gamma} f_{\beta,k} \\
& + 3\sum_{\delta,\gamma} f_{\delta,k} f_{\gamma,k} \partial^3_{t\delta\gamma} f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k} \partial_\eta f_{\delta,k} \partial_\delta f_{\gamma,k} \partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k} f_{\delta,k} \partial^2_{\eta\delta} f_{\gamma,k} \partial_\gamma f_{\beta,k} \\
& +3\sum_{\eta,\delta,\gamma} f_{\eta,k} f_{\delta,k} \partial_\delta f_{\gamma,k} \partial^2_{\eta\gamma} f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k} f_{\delta,k} f_{\gamma,k} \partial^3_{\eta,\delta\gamma} f_{\beta,k}\Bigg) \\
& + \mathcal{O}\left(f^{(4)}_{\beta,k} (\Delta t)^5\right).
\end{aligned}$$

Now, we assume that

$$x_{\beta,k+1} = x_{\beta,k} + \Delta t \left(A_{\beta,1} F_{\beta,k,1} + \cdots + A_{\beta,4} F_{\beta,k,4}\right) + \mathcal{O}\left(f^{(4)}_{\beta,k} (\Delta t)^5\right),$$

with

$$F_{\beta,k,1} = f_{\beta,k}, \ F_{\beta,k,2} = f_\beta\left(\left\{x_{\gamma,k} + \frac{\Delta t}{B_2} F_{\gamma,k,1}\right\}, t_k + \frac{\Delta t}{B_2}\right), \ \ldots, \ F_{\beta,k,4} = f_\beta\left(\left\{x_{\gamma,k} + \frac{\Delta t}{B_4} F_{\gamma,k,3}\right\}, t_k + \frac{\Delta t}{B_4}\right).$$

Now we need to expand

$$
\begin{aligned}
F_{\beta,k,2} =& f_{\beta,k} + \frac{\Delta t}{B_2}\left(\partial_t f_{\beta,k} + \sum_{\gamma} F_{\gamma,k,1}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_2^2}\left(\partial^2_{tt} f_{\beta,k} + 2\sum_{\gamma} F_{\gamma,k,1}\partial^2_{t\gamma} f_{\beta,k} + \sum_{\gamma,\delta} F_{\gamma,k,1}F_{\delta,k,1}\partial^2_{\gamma\delta} f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{3!B_2^3}\left(\partial^3_{ttt} f_{\beta,k} + 3\sum_{\gamma} F_{\gamma,k,1}\partial^3_{tt\gamma} f_{\beta,k} + 3\sum_{\gamma,\delta} F_{\gamma,k,1}F_{\delta,k,1}\partial^3_{t\gamma\delta} f_{\beta,k} + \sum_{\eta,\gamma,\delta} F_{\gamma,k,1}F_{\eta,k,1}F_{\delta,k,1}\partial^3_{\eta\gamma\delta} f_{\beta,k}\right)\\
=& f_{\beta,k} + \frac{\Delta t}{B_2}\left(\partial_t f_{\beta,k} + \sum_{\gamma} f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_2^2}\left(\partial^2_{tt} f_{\beta,k} + 2\sum_{\gamma} f_{\gamma,k}\partial^2_{t\gamma} f_{\beta,k} + \sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial^2_{\gamma\delta} f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{3!B_2^3}\left(\partial^3_{ttt} f_{\beta,k} + 3\sum_{\gamma} f_{\gamma,k}\partial^3_{tt\gamma} f_{\beta,k} + 3\sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial^3_{t\gamma\delta} f_{\beta,k} + \sum_{\eta,\gamma,\delta} f_{\gamma,k}f_{\eta,k}f_{\delta,k}\partial^3_{\eta\gamma\delta} f_{\beta,k}\right) + \mathcal{O}\left(\Delta t\right)^4.
\end{aligned}
$$

$$
\begin{aligned}
F_{\beta,k,3} =& f_{\beta,k} + \frac{\Delta t}{B_3}\left(\partial_t f_{\beta,k} + \sum_{\gamma} F_{\gamma,k,2}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_3^2}\left(\partial^2_{tt} f_{\beta,k} + 2\sum_{\gamma} F_{\gamma,k,2}\partial^2_{t\gamma} f_{\beta,k} + \sum_{\gamma,\delta} F_{\gamma,k,2}F_{\delta,k,2}\partial^2_{\gamma\delta} f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{3!B_3^3}\left(\partial^3_{ttt} f_{\beta,k} + 3\sum_{\gamma} F_{\gamma,k,2}\partial^3_{tt\gamma} f_{\beta,k} + 3\sum_{\gamma,\delta} F_{\gamma,k,2}F_{\delta,k,2}\partial^3_{t\gamma\delta} f_{\beta,k} + \sum_{\eta,\gamma,\delta} F_{\gamma,k,2}F_{\eta,k,2}F_{\delta,k,2}\partial^3_{\eta\gamma\delta} f_{\beta,k}\right)\\
=& f_{\beta,k} + \frac{\Delta t}{B_3}\left(\partial_t f_{\beta,k} + \sum_{\gamma} f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_3^2}\left(\partial^2_{tt} f_{\beta,k} + 2\sum_{\gamma} f_{\gamma,k}\partial^2_{t\gamma} f_{\beta,k} + \sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial^2_{\gamma\delta} f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{3!B_3^3}\left(\partial^3_{ttt} f_{\beta,k} + 3\sum_{\gamma} f_{\gamma,k}\partial^3_{tt\gamma} f_{\beta,k} + 3\sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial^3_{t\gamma\delta} f_{\beta,k} + \sum_{\eta,\gamma,\delta} f_{\gamma,k}f_{\eta,k}f_{\delta,k}\partial^3_{\eta\gamma\delta} f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^2}{B_2B_3}\left(\sum_{\gamma}\partial_t f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\gamma,\delta} f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_\gamma f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{2!B_2^2B_3}\left(\sum_{\gamma}\partial^2_{tt} f_{\gamma,k}\partial_\gamma f_{\beta,k} + 2\sum_{\delta,\gamma} f_{\delta,k}\partial^2_{t\delta} f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k}f_{\delta,k}\partial^2_{\eta\delta} f_{\gamma,k}\partial_\gamma f_{\beta,k}\right)\\
&+ \frac{(\Delta t)^3}{B_2B_3^2}\left(\sum_{\gamma}\left(\partial_t f_{\gamma,k} + \sum_{\delta} f_{\delta,k}\partial_\delta f_{\gamma,k}\right)\partial^2_{t\gamma} f_{\beta,k} + \sum_{\gamma,\delta}\left(\partial_t f_{\gamma,k} + \sum_{\eta} f_{\eta,k}\partial_\eta f_{\gamma,k}\right) f_{\delta,k}\partial^2_{\gamma\delta} f_{\beta,k}\right) + \mathcal{O}\left(\Delta t\right)^4.
\end{aligned}
$$

$$
\begin{aligned}
F_{\beta,k,4} =& f_{\beta,k} + \frac{\Delta t}{B_4}\left(\partial_t f_{\beta,k} + \sum_\gamma F_{\gamma,k,3}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_4^2}\left(\partial_{tt}^2 f_{\beta,k} + 2\sum_\gamma F_{\gamma,k,3}\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\gamma,\delta} F_{\gamma,k,3}F_{\delta,k,3}\partial_{\gamma\delta}^2 f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{3!B_4^3}\left(\partial_{ttt}^3 f_{\beta,k} + 3\sum_\gamma F_{\gamma,k,3}\partial_{tt\gamma}^3 f_{\beta,k} + 3\sum_{\gamma,\delta} F_{\gamma,k,3}F_{\delta,k,3}\partial_{t\gamma\delta}^3 f_{\beta,k} + \sum_{\eta,\gamma,\delta} F_{\gamma,k,3}F_{\eta,k,3}F_{\delta,k,3}\partial_{\eta\gamma\delta}^3 f_{\beta,k}\right) \\
=& f_{\beta,k} + \frac{\Delta t}{B_4}\left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) + \frac{(\Delta t)^2}{2!B_4^2}\left(\partial_{tt}^2 f_{\beta,k} + 2\sum_\gamma f_{\gamma,k}\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial_{\gamma\delta}^2 f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{3!B_4^3}\left(\partial_{ttt}^3 f_{\beta,k} + 3\sum_\gamma f_{\gamma,k}\partial_{tt\gamma}^3 f_{\beta,k} + 3\sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial_{t\gamma\delta}^3 f_{\beta,k} + \sum_{\eta,\gamma,\delta} f_{\gamma,k}f_{\eta,k}f_{\delta,k}\partial_{\eta\gamma\delta}^3 f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^2}{B_3B_4}\left(\sum_\gamma \partial_t f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\gamma,\delta} f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{2!B_3^2B_4}\left(\sum_\gamma \partial_{tt}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k} + 2\sum_{\delta,\gamma} f_{\delta,k}\partial_{t\delta}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k}f_{\delta,k}\partial_{\eta\delta}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{B_2B_3B_4}\left(\sum_{\delta,\gamma} \partial_t f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\delta,k}\partial_\delta f_{\eta,k}\partial_\eta f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{B_3B_4^2}\left(\sum_\gamma\left(\partial_t f_{\gamma,k} + \sum_\delta f_{\delta,k}\partial_\delta f_{\gamma,k}\right)\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\gamma,\delta}\left(\partial_t f_{\gamma,k} + \sum_\eta f_{\eta,k}\partial_\eta f_{\gamma,k}\right) f_{\delta,k}\partial_{\gamma\delta}^2 f_{\beta,k}\right) + \mathcal{O}\left(\Delta t\right)^4.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
x_{\beta,k+1} =& x_{\beta,k} + \Delta t\left(A_{\beta,1} + \cdots + A_{\beta,4}\right) f_{\beta,k} + (\Delta t)^2\left(\frac{A_{\beta,2}}{B_2} + \frac{A_{\beta,3}}{B_3} + \frac{A_{\beta,4}}{B_4}\right)\left(\partial_t f_{\beta,k} + \sum_\gamma f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^3}{2!}\left(\frac{A_{\beta,2}}{B_2^2} + \frac{A_{\beta,3}}{B_3^2} + \frac{A_{\beta,4}}{B_4^2}\right)\left(\partial_{tt}^2 f_{\beta,k} + 2\sum_\gamma f_{\gamma,k}\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial_{\gamma\delta}^2 f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^4}{3!}\left(\frac{A_{\beta,2}}{B_2^3} + \frac{A_{\beta,3}}{B_3^3} + \frac{A_{\beta,4}}{B_4^3}\right)\left(\partial_{ttt}^3 f_{\beta,k} + 3\sum_\gamma f_{\gamma,k}\partial_{tt\gamma}^3 f_{\beta,k} + 3\sum_{\gamma,\delta} f_{\gamma,k}f_{\delta,k}\partial_{t\gamma\delta}^3 f_{\beta,k}\right. \\
&\left.+ \sum_{\eta,\gamma,\delta} f_{\gamma,k}f_{\eta,k}f_{\delta,k}\partial_{\eta\gamma\delta}^3 f_{\beta,k}\right) + (\Delta t)^3\left(\frac{A_{\beta,3}}{B_2B_3} + \frac{A_{\beta,4}}{B_3B_4}\right)\left(\sum_\gamma \partial_t f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\gamma,\delta} f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \frac{(\Delta t)^4}{2!}\left(\frac{A_{\beta,3}}{B_2^2B_3} + \frac{A_{\beta,4}}{B_3^2B_4}\right)\left(\sum_\gamma \partial_{tt}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k} + 2\sum_{\delta,\gamma} f_{\delta,k}\partial_{t\delta}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\eta,k}f_{\delta,k}\partial_{\eta\delta}^2 f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ (\Delta t)^4\left(\frac{A_{\beta,3}}{B_2B_3^2} + \frac{A_{\beta,4}}{B_3B_4^2}\right)\left(\sum_\gamma \partial_t f_{\gamma,k}\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\delta,\gamma} f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_{t\gamma}^2 f_{\beta,k} + \sum_{\gamma,\delta} f_{\delta,k}\partial_t f_{\gamma,k}\partial_{\gamma\delta}^2 f_{\beta,k}\right. \\
&\left.+ \sum_{\eta,\delta,\gamma} f_{\eta,k}f_{\delta,k}\partial_\eta f_{\gamma,k}\partial_{\gamma\delta}^2 f_{\beta,k}\right) + \frac{(\Delta t)^4 A_{\beta,4}}{B_2B_3B_4}\left(\sum_{\delta,\gamma} \partial_t f_{\delta,k}\partial_\delta f_{\gamma,k}\partial_\gamma f_{\beta,k} + \sum_{\eta,\delta,\gamma} f_{\delta,k}\partial_\delta f_{\eta,k}\partial_\eta f_{\gamma,k}\partial_\gamma f_{\beta,k}\right) \\
&+ \mathcal{O}\left(f_{\beta,k}^{(4)}\left(\Delta t\right)^5\right),
\end{aligned}
$$

and comparing the Taylor series, we then have that

$$
A_{\beta,1} + \cdots + A_{\beta,4} = 1,\ \ \frac{A_{\beta,2}}{B_2} + \frac{A_{\beta,3}}{B_3} + \frac{A_{\beta,4}}{B_4} = \frac{1}{2},\ \ \frac{A_{\beta,2}}{B_2^2} + \frac{A_{\beta,3}}{B_3^2} + \frac{A_{\beta,4}}{B_4^2} = \frac{1}{3},
$$

$$\frac{A_{\beta,3}}{B_2B_3}+\frac{A_{\beta,4}}{B_3B_4}=\frac{1}{3!},\ \frac{A_{\beta,2}}{B_2^3}+\frac{A_{\beta,3}}{B_3^3}+\frac{A_{\beta,4}}{B_4^3}=\frac{1}{4},\ \frac{A_{\beta,3}}{B_2^2B_3}+\frac{A_{\beta,4}}{B_3^2B_4}=\frac{2!}{4!},$$

$$\frac{A_{\beta,3}}{B_2B_3^2}+\frac{A_{\beta,4}}{B_3B_4^2}=\frac{3}{4!}\text{ and }\frac{A_{\beta,4}}{B_2B_3B_4}=\frac{1}{4!}.$$

Unlike the cases of 2nd and 3rd order, the solution in 4th order is unique and equals

$$2A_{\beta,1}=2A_{\beta,4}=A_{\beta,2}=A_{\beta,3}=\frac{1}{3}\text{ and }B_2=B_3=2B_4=2.$$

In other words,

$$x_{\beta,k+1}=x_{\beta,k}+\frac{\Delta t}{6}\left(F_{\beta,k,1}+2F_{\beta,k,2}+2F_{\beta,k,3}+F_{\beta,k,4}\right),$$

where

$$F_{\beta,k,1}=f_{\beta,k},\ F_{\beta,k,2}=f_\beta\left(\left\{x_{\gamma,k}+\frac{\Delta t}{2}f_{\gamma,k}\right\},t_k+\frac{\Delta t}{2}\right),$$

$$F_{\beta,k,3}=f_\beta\left(\left\{x_{\gamma,k}+\frac{\Delta t}{2}F_{\gamma,k,2}\right\},t_k+\frac{\Delta t}{2}\right)\text{ and }F_{\beta,k,4}=f_\beta\left(\left\{x_{\gamma,k}+\Delta tF_{\gamma,k,3}\right\},t_k+\Delta t\right).$$

IV. DOUBLE PENDULUM

Let us apply the 4th order approximation to the case of a double pendulum.

We need the equations of motion. The positions are $\mathbf{r}_1=\ell_1\hat{r}_1$. Then, $\dot{\mathbf{r}}_1=\ell_1\dot{\theta}_1\hat{\theta}_1$ and $\ddot{\mathbf{r}}_1=\ell_1\left(\ddot{\theta}_1\hat{\theta}_1-\dot{\theta}_1^2\hat{r}_1\right)$. Thus,

$$m_1\ell_1\left(\ddot{\theta}_1\hat{\theta}_1-\dot{\theta}_1^2\hat{r}_1\right)=-T_1\hat{r}_1+T_2\hat{r}_2-m_1g\hat{y},$$
$$m_2\left[\ell_1\left(\ddot{\theta}_1\hat{\theta}_1-\dot{\theta}_1^2\hat{r}_1\right)+\ell_2\left(\ddot{\theta}_2\hat{\theta}_2-\dot{\theta}_2^2\hat{r}_2\right)\right]=-T_2\hat{r}_2-m_2g\hat{y}.$$

From the later one multiplying by $\hat{\theta}_2\cdot$, then

$$\ell_1\left(\ddot{\theta}_1\cos\Delta\theta+\dot{\theta}_1^2\sin\Delta\theta\right)+\ell_2\ddot{\theta}_2=-g\sin\theta_2, \tag{4}$$

with $\Delta\theta=\theta_2-\theta_1$. Likewise, summing the former and the latter

$$\left(m_1+m_2\right)\ell_1\left(\ddot{\theta}_1\hat{\theta}_1-\dot{\theta}_1^2\hat{r}_1\right)+m_2\ell_2\left(\ddot{\theta}_2\hat{\theta}_2-\dot{\theta}_2^2\hat{r}_2\right)=-T_1\hat{r}_1-\left(m_1+m_2\right)g\hat{y},$$

and multiplying by $\hat{\theta}_1\cdot$, then

$$\left(m_1+m_2\right)\ell_1\ddot{\theta}_1+m_2\ell_2\left(\ddot{\theta}_2\cos\Delta\theta-\dot{\theta}_2^2\sin\Delta\theta\right)=-\left(m_1+m_2\right)g\sin\theta_1,$$
$$\ell_1\ddot{\theta}_1+\frac{m_2}{m_1+m_2}\ell_2\left(\ddot{\theta}_2\cos\Delta\theta-\dot{\theta}_2^2\sin\Delta\theta\right)=-g\sin\theta_1. \tag{5}$$

Now, we just need to manipulate Eqs. (4) and (5) in order to isolate for $\ddot{\theta}_{1,2}$. Thus,

$$\ell_1\ddot{\theta}_1\left(\cos^2\Delta\theta-\frac{m_1+m_2}{m_2}\right)+\ell_1\dot{\theta}_1^2\sin\Delta\theta\cos\Delta\theta+\ell_2\dot{\theta}_2^2\sin\Delta\theta=\frac{m_1+m_2}{m_2}g\sin\theta_1-g\sin\theta_2\cos\Delta\theta,$$
$$\ell_1\dot{\theta}_1^2\sin\Delta\theta+\ell_2\ddot{\theta}_2\left(1-\frac{m_2}{m_1+m_2}\cos^2\Delta\theta\right)+\frac{m_2}{m_1+m_2}\ell_2\dot{\theta}_2^2\sin\Delta\theta\cos\Delta\theta=-g\sin\theta_2+g\sin\theta_1\cos\Delta\theta,$$

and then

$$\ddot{\theta}_1 = \frac{\sin\Delta\theta\left(\dot{\theta}_1^2\cos\Delta\theta + \frac{\ell_2}{\ell_1}\dot{\theta}_2^2\right) + \frac{g}{\ell_1}\left(\sin\theta_2\cos\Delta\theta - \frac{m_1+m_2}{m_2}\sin\theta_1\right)}{\frac{m_1+m_2}{m_2}\left(1 - \frac{m_2}{m_1+m_2}\cos^2\Delta\theta\right)},$$

$$\ddot{\theta}_2 = \frac{-\sin\Delta\theta\left(\dot{\theta}_1^2 + \frac{m_2}{m_1+m_2}\frac{\ell_2}{\ell_1}\dot{\theta}_2^2\cos\Delta\theta\right) + \frac{g}{\ell_1}\left(\sin\theta_1\cos\Delta\theta - \sin\theta_2\right)}{\frac{\ell_2}{\ell_1}\left(1 - \frac{m_2}{m_1+m_2}\cos^2\Delta\theta\right)}.$$

Now, let us define some dimensionless quantities: $\tau = \omega_0 t$, where $\omega_0^2 = \frac{g}{\ell_1}$. Then $\ddot{\theta} = \frac{\mathrm{d}^2}{\mathrm{d}t^2}\theta = \omega_0^2\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\theta \to \frac{g}{\ell_1}\ddot{\theta}$ and $\dot{\theta}^2 \to \frac{g}{\ell_1}\dot{\theta}^2$. With respect to mass, let $\mu = \frac{m_2}{m_1+m_2}$. With respect to length, then let $\lambda = \frac{\ell_2}{\ell_1}$. Then,

$$\begin{aligned}
\dot{\theta}_1 &= \omega_1 = f_1\left(\theta_1, \theta_2, \omega_1, \omega_2\right), \\
\dot{\theta}_2 &= \omega_2 = f_2\left(\theta_1, \theta_2, \omega_1, \omega_2\right), \\
\dot{\omega}_1 &= \frac{\mu\sin\left(\theta_2-\theta_1\right)\left(\omega_1^2\cos\left(\theta_2-\theta_1\right) + \lambda\omega_2^2\right) + \mu\sin\theta_2\cos\left(\theta_2-\theta_1\right) - \sin\theta_1}{1-\mu\cos^2\left(\theta_2-\theta_1\right)} = f_3\left(\theta_1, \theta_2, \omega_1, \omega_2\right), \\
\dot{\omega}_2 &= \frac{-\sin\left(\theta_2-\theta_1\right)\left(\omega_1^2 + \mu\lambda\omega_2^2\cos\left(\theta_2-\theta_1\right)\right) + \sin\theta_1\cos\left(\theta_2-\theta_1\right) - \sin\theta_2}{\lambda\left(1-\mu\cos^2\left(\theta_2-\theta_1\right)\right)} = f_4\left(\theta_1, \theta_2, \omega_1, \omega_2\right).
\end{aligned}$$

In this case, the energy

$$\begin{aligned}
E &= \frac{m_1\dot{r}_1^2}{2} + \frac{m_2\dot{r}_2^2}{2} + m_1 g y_1 + m_2 g y_2 \\
&= \frac{\left(m_1+m_2\right)\ell_1^2\dot{\theta}_1^2 + m_2\ell_2^2\dot{\theta}_2^2}{2} + m_2\ell_1\ell_2\dot{\theta}_1\dot{\theta}_2\cos\Delta\theta - g\left[\left(m_1+m_2\right)\ell_1\cos\theta_1 + m_2\ell_2\cos\theta_2\right],
\end{aligned}$$

becomes

$$\varepsilon = \frac{E}{\left(m_1+m_2\right)g\ell_1} = \frac{\dot{\theta}_1^2 + \mu\lambda^2\dot{\theta}_2^2}{2} + \mu\lambda\dot{\theta}_1\dot{\theta}_2\cos\Delta\theta - \left(\cos\theta_1 + \mu\lambda\cos\theta_2\right),$$

where the time derivative is with respect to the dimensionless time $\tau = \omega_0 t$.

Now we need to apply the method:

$$\begin{aligned}
\theta_{1,k+1} &= \theta_{1,k} + \frac{\Delta t}{6}\left(F_{1,k,1} + 2F_{1,k,2} + 2F_{1,k,3} + F_{1,k,4}\right), \\
\theta_{2,k+1} &= \theta_{2,k} + \frac{\Delta t}{6}\left(F_{2,k,1} + 2F_{2,k,2} + 2F_{2,k,3} + F_{2,k,4}\right), \\
\omega_{1,k+1} &= \theta_{1,k} + \frac{\Delta t}{6}\left(F_{3,k,1} + 2F_{3,k,2} + 2F_{3,k,3} + F_{3,k,4}\right), \\
\omega_{2,k+1} &= \theta_{2,k} + \frac{\Delta t}{6}\left(F_{4,k,1} + 2F_{4,k,2} + 2F_{4,k,3} + F_{4,k,4}\right),
\end{aligned}$$

where

$$
\begin{aligned}
F_{1,k,1} &= f_{1,k} = \omega_{1,k}, \\
F_{2,k,1} &= f_{2,k} = \omega_{2,k}, \\
F_{3,k,1} &= f_{3,k} = \frac{\mu \sin \Delta\theta_k \left(\omega_{1,k}^2 \cos \Delta\theta_k + \lambda \omega_2^2\right) + \mu \sin \theta_{2,k} \cos \Delta\theta_k - \sin \theta_{1,k}}{1 - \mu \cos^2 \Delta\theta_k} = f_3\left(\theta_{1,k}, \theta_{2,k}, \omega_{1,k}, \omega_{2,k}\right), \\
F_{4,k,1} &= f_{4,k} = \frac{-\sin \Delta\theta_k \left(\omega_{1,k}^2 + \mu\lambda \omega_{2,k}^2 \cos \Delta\theta_k\right) + \sin \theta_{1,k} \cos \Delta\theta_k - \sin \theta_{2,k}}{\lambda\left(1 - \mu \cos^2 \Delta\theta_k\right)} = f_4\left(\theta_{1,k}, \theta_{2,k}, \omega_{1,k}, \omega_{2,k}\right), \\
F_{1,k,2} &= f_1\left(\left\{x_{\gamma,k} + \frac{\Delta t}{2} F_{\gamma,k,1}\right\}, t_k + \frac{\Delta t}{2}\right) = \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,1}, \\
F_{2,k,2} &= f_2\left(\left\{x_{\gamma,k} + \frac{\Delta t}{2} F_{\gamma,k,1}\right\}, t_k + \frac{\Delta t}{2}\right) = \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,1}, \\
F_{3,k,2} &= f_3\left(\theta_{1,k} + \frac{\Delta t}{2} F_{1,k,1}, \theta_{2,k} + \frac{\Delta t}{2} F_{2,k,1}, \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,1}, \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,1}\right), \\
F_{4,k,2} &= f_4\left(\theta_{1,k} + \frac{\Delta t}{2} F_{1,k,1}, \theta_{2,k} + \frac{\Delta t}{2} F_{2,k,1}, \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,1}, \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,1}\right), \\
F_{1,k,3} &= f_1\left(\left\{x_{\gamma,k} + \frac{\Delta t}{2} F_{\gamma,k,2}\right\}, t_k + \frac{\Delta t}{2}\right) = \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,2}, \\
F_{2,k,3} &= f_2\left(\left\{x_{\gamma,k} + \frac{\Delta t}{2} F_{\gamma,k,2}\right\}, t_k + \frac{\Delta t}{2}\right) = \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,2}, \\
F_{3,k,3} &= f_3\left(\theta_{1,k} + \frac{\Delta t}{2} F_{1,k,2}, \theta_{2,k} + \frac{\Delta t}{2} F_{2,k,2}, \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,2}, \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,2}\right), \\
F_{4,k,3} &= f_4\left(\theta_{1,k} + \frac{\Delta t}{2} F_{1,k,2}, \theta_{2,k} + \frac{\Delta t}{2} F_{2,k,2}, \omega_{1,k} + \frac{\Delta t}{2} F_{3,k,2}, \omega_{2,k} + \frac{\Delta t}{2} F_{4,k,2}\right), \\
F_{1,k,4} &= f_1\left(\left\{x_{\gamma,k} + \Delta t F_{\gamma,k,2}\right\}, t_k + \Delta t\right) = \omega_{1,k} + \Delta t F_{3,k,3}, \\
F_{2,k,4} &= f_2\left(\left\{x_{\gamma,k} + \Delta t F_{\gamma,k,2}\right\}, t_k + \frac{\Delta t}{2}\right) = \omega_{2,k} + \Delta t F_{4,k,3}, \\
F_{3,k,4} &= f_3\left(\theta_{1,k} + \Delta t F_{1,k,3}, \theta_{2,k} + \Delta t F_{2,k,3}, \omega_{1,k} + \Delta t F_{3,k,3}, \omega_{2,k} + \Delta t F_{4,k,3}\right), \\
F_{4,k,4} &= f_4\left(\theta_{1,k} + \Delta t F_{1,k,3}, \theta_{2,k} + \Delta t F_{2,k,3}, \omega_{1,k} + \Delta t F_{3,k,3}, \omega_{2,k} + \Delta t F_{4,k,3}\right).
\end{aligned}
$$