Appendix C. Derivation of the Numerical Integration Formulae

C.1. Derivation of the Numerical Integration of $dy(x)/dx = f(x)$

For a given analytical or tabulated function $f(x)$, the left column in Table 3.1 shows how to determine $y(x)$ numerically, where $dy(x)/dx = f(x)$. In this section, we will show how to obtain the integration rules listed in the left column of Table 3.1 for the given accuracy. Based on Taylor's series expansion, we have

$$y_{i+1} = y_i + hf_i + \frac{h^2}{2!} f_i' + \frac{h^3}{3!} f_i^{(2)} + \frac{h^4}{4!} f_i^{(3)} + \frac{h^5}{5!} f_i^{(4)} + \frac{h^6}{6!} f_i^{(5)} + ... \tag{C.1}$$

C.1.1. The first-order numerical integration

Obviously, the first-order numerical integration should be

$$y_{i+1} = y_i + hf_i + O(h^2) \tag{C.2}$$

C.1.2. The second-order numerical integration (Trapezoidal rule)

Let the second-order numerical integration be

$$y_{i+1} = y_i + h(af_i + bf_{i+1}) + O(h^3) \tag{C.3}$$

Since

$$f_{i+1} = f_i + hf_i' + O(h^2) \tag{C.4}$$

Substituting Eq. (C.4) into Eq. (C.3) to eliminate f_{i+1}, it yields

$$y_{i+1} = y_i + h\{af_i + b[f_i + hf_i' + O(h^2)]\} + O(h^3)$$

or

$$y_{i+1} = y_i + h(a+b)f_i + bh^2 f_i' + O(h^3) \tag{C.5}$$

Comparing the coefficients in Eqs. (C.1) and (C.5), it yields $a + b = 1$ and $b = 1/2$. Hence, $a = 1/2$. As a result, we obtain the well-known Trapezoidal rule,

$$y_{i+1} = y_i + h(\frac{f_i + f_{i+1}}{2}) + O(h^3) \tag{C.6}$$

C.1.3. The fourth-order numerical integration (Simpson's rule)

Let a fourth-order numerical integration be

$$y_{i+1} = y_i + h(a\, f_i + b\, f_{i+(1/2)} + c\, f_{i+1}) + O(h^5) \tag{C.7}$$

Since

$$f_{i+(1/2)} = f_i + \frac{h}{2} f_i' + \frac{(h/2)^2}{2!} f_i^{(2)} + \frac{(h/2)^3}{3!} f_i^{(3)} + O(h^4) \tag{C.8}$$

$$f_{i+1} = f_i + h f_i' + \frac{h^2}{2!} f_i^{(2)} + \frac{h^3}{3!} f_i^{(3)} + O(h^4) \tag{C.9}$$

Substituting Eqs. (C.8) and (C.9) into Eq. (C.7) to eliminate $f_{i+(1/2)}$ and f_{i+1}, respectively, it yields

$$\begin{aligned} y_{i+1} = y_i + h\{a f_i + b[f_i + \frac{h}{2} f_i' + \frac{(h/2)^2}{2!} f_i^{(2)} + \frac{(h/2)^3}{3!} f_i^{(3)} + O(h^4)] \\ + c[f_i + h f_i' + \frac{h^2}{2!} f_i^{(2)} + \frac{h^3}{3!} f_i^{(3)} + O(h^4)]\} + O(h^5) \end{aligned}$$

or

$$y_{i+1} = y_i + h(a+b+c) f_i + h^2(\frac{1}{2}b + c) f' + h^3(\frac{1}{2^2 2!}b + \frac{1}{2!}c) f_i^{(2)} + h^4(\frac{1}{2^3 3!}b + \frac{1}{3!}c) f_i^{(3)} + O(h^5) \tag{C.10}$$

Comparing the coefficients in Eqs. (C.1) and (C.10), it yields

$$a + b + c = 1 \tag{C.11}$$

$$\frac{1}{2}b + c = \frac{1}{2!} \tag{C.12}$$

$$\frac{1}{2^2 2!}b + \frac{1}{2!}c = \frac{1}{3!} \tag{C.13}$$

where Eqs. (C.12) and (C.13) can be rewritten as

$$\begin{bmatrix} 1 & 2^1 \\ 1 & 2^2 \end{bmatrix} \begin{bmatrix} b \\ c \end{bmatrix} = \begin{bmatrix} 1!2^1/2! \\ 2!2^2/3! \end{bmatrix} \tag{C.14}$$

Solving Eq. (C.14), it yields $b = 4/6$, $c = 1/6$. Substituting these results into Eq. (C.11), it yields $a = 1/6$. It is interesting to note that the following equation is satisfied

$$\frac{1}{2^3 3!}b+\frac{1}{3!}c=\frac{1}{4!}$$

Thus, the following Simpson rule is indeed a fourth-order-accuracy integration form

$$y_{i+1}=y_i+h(\frac{1}{6}f_i+\frac{4}{6}f_{i+(1/2)}+\frac{1}{6}f_{i+1})+O(h^5) \tag{C.15}$$

C.1.4. The Simpson's 3/8 rule (a fourth-order numerical integration)

Let a fourth-order numerical integration be

$$y_{i+1}=y_i+h(a\,f_i+b\,f_{i+(1/3)}+c\,f_{i+(2/3)}+d\,f_{i+1})+O(h^5) \tag{C.16}$$

Since

$$f_{i+(1/3)}=f_i+\frac{h}{3}f_i'+\frac{(h/3)^2}{2!}f_i^{(2)}+\frac{(h/3)^3}{3!}f_i^{(3)}+O(h^4) \tag{C.17}$$

$$f_{i+(2/3)}=f_i+\frac{2h}{3}f_i'+\frac{(2h/3)^2}{2!}f_i^{(2)}+\frac{(2h/3)^3}{3!}f_i^{(3)}+O(h^4) \tag{C.18}$$

$$f_{i+1}=f_i+hf_i'+\frac{h^2}{2!}f_i^{(2)}+\frac{h^3}{3!}f_i^{(3)}+O(h^4) \tag{C.19}$$

Substituting Eqs. (C.17), (C.18), and (C.19) into Eq. (C.16), then comparing the coefficients in the resulting equation with the coefficients in equation (C.1), it yields

$$a+b+c+d=1 \tag{C.20}$$

$$\begin{bmatrix} 1 & 2^1 & 3^1 \\ 1 & 2^2 & 3^2 \\ 1 & 2^3 & 3^3 \end{bmatrix}\begin{bmatrix} b \\ c \\ d \end{bmatrix}=\begin{bmatrix} 1!3^1/2! \\ 2!3^2/3! \\ 3!3^3/4! \end{bmatrix} \tag{C.21}$$

Solving Eq. (C.21), it yields $b=3/8$, $c=3/8$, $d=1/8$. Substituting these results into Eq. (C.20), it yields $a=1/8$. We have obtained the Simpson's 3/8 law

$$y_{i+1}=y_i+h(\frac{1}{8}f_i+\frac{3}{8}f_{i+(1/3)}+\frac{3}{8}f_{i+(2/3)}+\frac{1}{8}f_{i+1})+O(h^5) \tag{C.22}$$

C.1.5. The sixth-order numerical integration

Let a sixth-order numerical integration be

$$y_{i+1} = y_i + h(a\, f_i + b\, f_{i+(1/4)} + c\, f_{i+(1/2)} + d\, f_{i+(3/4)} + e\, f_{i+1}) + O(h^7) \tag{C.23}$$

Since

$$f_{i+(1/4)} = f_i + \frac{h}{2} f_i' + \frac{(h/4)^2}{2!} f_i^{(2)} + \frac{(h/4)^3}{3!} f_i^{(3)} + \frac{(h/4)^4}{4!} f_i^{(4)} + \frac{(h/4)^5}{5!} f_i^{(5)} + O(h^6) \tag{C.24}$$

$$f_{i+(1/2)} = f_i + \frac{h}{2} f_i' + \frac{(h/2)^2}{2!} f_i^{(2)} + \frac{(h/2)^3}{3!} f_i^{(3)} + \frac{(h/2)^4}{4!} f_i^{(4)} + \frac{(h/2)^5}{5!} f_i^{(5)} + O(h^6) \tag{C.25}$$

$$f_{i+(1/2)} = f_i + \frac{3h}{4} f_i' + \frac{(3h/4)^2}{2!} f_i^{(2)} + \frac{(3h/4)^3}{3!} f_i^{(3)} + \frac{(3h/4)^4}{4!} f_i^{(4)} + \frac{(3h/4)^5}{5!} f_i^{(5)} + O(h^6) \tag{C.26}$$

$$f_{i+1} = f_i + h f_i' + \frac{h^2}{2!} f_i^{(2)} + \frac{h^3}{3!} f_i^{(3)} + \frac{h^4}{4!} f_i^{(4)} + \frac{h^5}{5!} f_i^{(5)} + O(h^6) \tag{C.27}$$

Substituting Eqs. (C.24), (C.25), and (C.26) into Eq. (C.23), then comparing the coefficients in the resulting equation with the coefficients in equation (C.1), it yields

$$a + b + c + d + e = 1 \tag{C.28}$$

$$\begin{bmatrix} 1 & 2^1 & 3^1 & 4^1 \\ 1 & 2^2 & 3^2 & 4^2 \\ 1 & 2^3 & 3^3 & 4^3 \\ 1 & 2^4 & 3^4 & 4^4 \end{bmatrix} \begin{bmatrix} b \\ c \\ d \\ e \end{bmatrix} = \begin{bmatrix} 1!4^1/2! \\ 2!4^2/3! \\ 3!4^3/4! \\ 4!4^4/5! \end{bmatrix} \tag{C.29}$$

Solving Eq. (C.29), it yields $b = 32/90$, $c = 12/90$, $d = 32/90$, $e = 7/90$. Substituting these results into Eq. (C.28), it yields $a = 7/90$. Note that the following equation is also satisfied

$$\begin{bmatrix} 1 & 2^5 & 3^5 & 4^5 \end{bmatrix} \begin{bmatrix} b \\ c \\ d \\ e \end{bmatrix} = \begin{bmatrix} 5!4^5/6! \end{bmatrix}$$

Thus, we have obtained the sixth-order integration formula

$$y_{i+1} = y_i + h(\frac{7}{90} f_i + \frac{32}{90} f_{i+(1/4)} + \frac{12}{90} f_{i+(1/2)} + \frac{32}{90} f_{i+(3/4)} + \frac{7}{90} f_{i+1}) + O(h^7) \tag{C.30}$$

C.1.6. Summary of the higher-order numerical integration

In summary, we can obtain the higher-order numerical integration of $dy(x)/dx = f(x)$ based on the procedures discussed in this Section C.1.

C.2. Derivation of the Runge-Kutta Method (This section has been revised on 2016-03-20.)

For $dy(t)/dt = f[t, y(t)]$, the right column in Table 3.1 shows numerical method to obtain $y(t)$, for a given initial value of $y_0 = y(t=0)$. Based on the Taylor's series expansion, we have

$$y^{n+1} = y^n + \frac{\Delta t}{1!}(f)_{t=t^n} + \frac{(\Delta t)^2}{2!}(\frac{df}{dt})_{t=t^n} + \frac{(\Delta t)^3}{3!}(\frac{d^2 f}{dt^2})_{t=t^n} + \frac{(\Delta t)^4}{4!}(\frac{d^3 f}{dt^3})_{t=t^n} + O((\Delta t)^5 f^{(4)}) \tag{C.31}$$

Since

$$\frac{d}{dt} f = (\frac{\partial}{\partial t} + f \frac{\partial}{\partial y}) f$$

Eq. (C.31) can be rewritten as

$$\begin{aligned} y^{n+1} = y^n + \Delta t(f)_{t=t^n} &+ \frac{(\Delta t)^2}{2}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n} + \frac{(\Delta t)^3}{6}[\frac{\partial}{\partial t}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}) + f\frac{\partial}{\partial y}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})]_{t=t^n} \\ &+ \frac{(\Delta t)^4}{24}\{\frac{\partial}{\partial t}[\frac{\partial}{\partial t}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}) + f\frac{\partial}{\partial y}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})] \\ &\qquad + f\frac{\partial}{\partial y}[\frac{\partial}{\partial t}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}) + f\frac{\partial}{\partial y}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})]\}_{t=t^n} + O((\Delta t)^5 f^{(4)}) \end{aligned} \tag{C.32}$$

C.2.1. The Second-Order Runge-Kutta Method

Let us assume a second-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_2] + O((\Delta t)^3 f^{(2)}) \tag{C.33}$$

where

$$f_1 = f(t^n, y^n) \tag{C.34}$$

$$f_2 = f(t^n + \Delta t, y^n + \Delta t f_1) \tag{C.35}$$

Since the 2-dimensional Taylor's series expansion of $f(t+\Delta t, y+\Delta y)$ can be written as

$$f(t+\Delta t, y+\Delta y) = f(t,y) + (\Delta t\frac{\partial}{\partial t} + \Delta y\frac{\partial}{\partial y})f(t,y) + \frac{1}{2!}(\Delta t\frac{\partial}{\partial t} + \Delta y\frac{\partial}{\partial y})^2 f(t,y) + ... + \frac{1}{k!}(\Delta t\frac{\partial}{\partial t} + \Delta y\frac{\partial}{\partial y})^k f(t,y) + ... \quad (C.36)$$

Let $(f)_{t=t^n} = f(t^n, y^n)$. Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + \Delta t, y^n + \Delta t(f)_{t=t^n})$ into Eq. (C.35), it yields

$$f_2 = (f)_{t=t^n} + \Delta t(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n} + O[(\Delta t)^2 f^{(2)}] \quad (C.37)$$

Substituting Eqs. (C.34) and (C.37) into Eq. (C.33), it yields

$$y^{n+1} = y^n + \Delta t\{a(f)_{t=t^n} + b[(f)_{t=t^n} + \Delta t(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}]\} + O[(\Delta t)^3 f^{(2)}] \quad (C.38)$$

Comparing the coefficients in Eqs. (C.32) and (C.38), it yields $a = b = 1/2$.
Thus, we have obtained the expression of the second-order Runge-Kutta method

$$y^{n+1} = y^n + \Delta t[\frac{1}{2}(f)_{t=t^n} + \frac{1}{2}f(t^n + \Delta t, y^n + \Delta t(f)_{t=t^n})] + O((\Delta t)^3 f^{(2)}) \quad (C.39)$$

The second-order Runge-Kutta method shown in Eq. (C.39) is similar to the Trapezoidal rule of the second-order integration shown in the first column of Table 3.1, but is different from the second-order Runge-Kutta method shown in the second column of Table 3.1. Apparently, the expression of the second-order Runge-Kutta method is not unique.

Let us assume another second-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_3] + O((\Delta t)^3 f^{(2)}) \quad (C.40)$$

where

$$f_1 = f(t^n, y^n) \quad (C.41)$$

$$f_3 = f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2} f_1) \quad (C.42)$$

Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + (\Delta t/2), y^n + (\Delta t/2)(f)_{t=t^n})$ into Eq. (C.42), it yields

$$f_3 = (f)_{t=t^n} + \frac{\Delta t}{2}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n} + O[(\Delta t)^2 f^{(2)}] \quad (C.43)$$

Substituting Eqs. (C.41) and (C.43) into Eq. (C.40), it yields

$$y^{n+1} = y^n + \Delta t\{a(f)_{t=t^n} + b[(f)_{t=t^n} + \frac{\Delta t}{2}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}]\} + O[(\Delta t)^3 f^{(2)}] \quad (C.44)$$

Comparing the coefficients in Eqs. (C.32) and (C.44), it yields $a = 0$ and $b = 1$.

Thus, we have obtained another expression of the second-order Runge-Kutta method

$$y^{n+1} = y^n + \Delta t f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2}(f)_{t=t^n}) + O((\Delta t)^3 f^{(2)}) \quad (C.45)$$

The second-order Runge-Kutta method shown in Eq. (C.45) is the same as the one shown in the second column of Table 3.1. The expression given in Eq. (C.45) is also similar to the second-order Lax-Wendroff scheme discussed in Section 3.1.

C.2.2. The Fourth-Order Runge-Kutta Method

Let us assume a fourth-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_2 + c f_3 + d f_4] + O((\Delta t)^5 f^{(4)}) \quad (C.46)$$

where

$$f_1 = f(t^n, y^n) \quad (C.47)$$

$$f_2 = f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2} f_1) \quad (C.48)$$

$$f_3 = f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2} f_2) \quad (C.49)$$

$$f_4 = f(t^n + \Delta t, y^n + \Delta t f_3) \quad (C.50)$$

Let $(f)_{t=t^n} = f(t^n, y^n)$. Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + (\Delta t/2), y^n + (\Delta t/2)(f)_{t=t^n})$ into Eq. (C.48), it yields

$$\begin{aligned} f_2 = (f)_{t=t^n} &+ \frac{\Delta t}{2}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n} + \frac{1}{2}(\frac{\Delta t}{2})^2(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2})_{t=t^n} \\ &+ \frac{1}{6}(\frac{\Delta t}{2})^3(\frac{\partial^3 f}{\partial t^3} + 3f\frac{\partial^3 f}{\partial t^2\partial y} + 3f^2\frac{\partial^3 f}{\partial t\,\partial y^2} + f^3\frac{\partial^3 f}{\partial y^3})_{t=t^n} \\ &+ \frac{1}{24}(\frac{\Delta t}{2})^4(\frac{\partial^4 f}{\partial t^4} + 4f\frac{\partial^4 f}{\partial t^3\partial y} + 6f^2\frac{\partial^4 f}{\partial t^2\partial y^2} + 4f^3\frac{\partial^4 f}{\partial t\,\partial y^3} + f^4\frac{\partial^4 f}{\partial y^4})_{t=t^n} + O[(\Delta t)^5 f^{(5)}] \end{aligned} \quad (C.51)$$

Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + (\Delta t/2), y^n + (\Delta t/2) f_2)$ into Eq. (C.49), it yields

$$f_3 = (f)_{t=t^n} + \frac{\Delta t}{2}(\frac{\partial f}{\partial t} + f_2 \frac{\partial f}{\partial y})_{t=t^n} + \frac{1}{2}(\frac{\Delta t}{2})^2(\frac{\partial^2 f}{\partial t^2} + 2 f_2 \frac{\partial^2 f}{\partial t\,\partial y} + (f_2)^2 \frac{\partial^2 f}{\partial y^2})_{t=t^n}$$
$$+\frac{1}{6}(\frac{\Delta t}{2})^3(\frac{\partial^3 f}{\partial t^3} + 3 f_2 \frac{\partial^3 f}{\partial t^2\,\partial y} + 3(f_2)^2 \frac{\partial^3 f}{\partial t\,\partial y^2} + (f_2)^3 \frac{\partial^3 f}{\partial y^3})_{t=t^n} \qquad \text{(C.52)}$$
$$+\frac{1}{24}(\frac{\Delta t}{2})^4(\frac{\partial^4 f}{\partial t^4} + 4 f_2 \frac{\partial^4 f}{\partial t^3\,\partial y} + 6(f_2)^2 \frac{\partial^4 f}{\partial t^2\,\partial y^2} + 4(f_2)^3 \frac{\partial^4 f}{\partial t\,\partial y^3} + (f_2)^4 \frac{\partial^4 f}{\partial y^4})_{t=t^n} + O[(\Delta t)^5 f^{(5)}]$$

Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + \Delta t, y^n + \Delta t f_3)$ into Eq. (C.50), it yields

$$f_4 = (f)_{t=t^n} + \Delta t(\frac{\partial f}{\partial t} + f_3 \frac{\partial f}{\partial y})_{t=t^n} + \frac{1}{2}(\Delta t)^2(\frac{\partial^2 f}{\partial t^2} + 2 f_3 \frac{\partial^2 f}{\partial t\,\partial y} + (f_3)^2 \frac{\partial^2 f}{\partial y^2})_{t=t^n}$$
$$+\frac{1}{6}(\Delta t)^3(\frac{\partial^3 f}{\partial t^3} + 3 f_3 \frac{\partial^3 f}{\partial t^2\,\partial y} + 3(f_3)^2 \frac{\partial^3 f}{\partial t\,\partial y^2} + (f_3)^3 \frac{\partial^3 f}{\partial y^3})_{t=t^n} \qquad \text{(C.53)}$$
$$+\frac{1}{24}(\Delta t)^4(\frac{\partial^4 f}{\partial t^4} + 4 f_3 \frac{\partial^4 f}{\partial t^3\,\partial y} + 6(f_3)^2 \frac{\partial^4 f}{\partial t^2\,\partial y^2} + 4(f_3)^3 \frac{\partial^4 f}{\partial t\,\partial y^3} + (f_3)^4 \frac{\partial^4 f}{\partial y^4})_{t=t^n} + O[(\Delta t)^5 f^{(5)}]$$

Substituting Eqs. (C.47), (C.51)-(C.53) into Eq. (C.46), it yields

$$y^{n+1} = y^n + \Delta t[(a+b+c+d)(f)_{t=t^n}]$$
$$+(\Delta t)^2[(\frac{b}{2}+\frac{c}{2}+d)(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}]$$
$$+\frac{(\Delta t)^3}{2}[(\frac{b}{4}+\frac{c}{4}+d)(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2})_{t=t^n} + (\frac{c}{2}+d)(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}(\frac{\partial f}{\partial y})_{t=t^n}]$$
$$+\frac{(\Delta t)^4}{6}[(\frac{b}{8}+\frac{c}{8}+d)(\frac{\partial^3 f}{\partial t^3} + 3f\frac{\partial^3 f}{\partial t^2\,\partial y} + 3f^2\frac{\partial^3 f}{\partial t\,\partial y^2} + f^3\frac{\partial^3 f}{\partial y^3})_{t=t^n}$$
$$+(\frac{3c}{8}+\frac{3d}{4})(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2})_{t=t^n}(\frac{\partial f}{\partial y})_{t=t^n}$$
$$+(\frac{3d}{2})(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}(\frac{\partial f}{\partial y})^2_{t=t^n} \qquad \text{(C.54)}$$
$$+(\frac{3c}{4}+3d)(f)_{t=t^n}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}(\frac{\partial^2 f}{\partial y^2})_{t=t^n}$$
$$+(\frac{3c}{4}+3d)(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n}(\frac{\partial^2 f}{\partial t\,\partial y})_{t=t^n}]$$
$$+\frac{(\Delta t)^5}{24}[(\frac{b}{16}+\frac{c}{16}+d)(\frac{\partial^4 f}{\partial t^4} + 4f\frac{\partial^4 f}{\partial t^3\,\partial y} + 6f^2\frac{\partial^4 f}{\partial t^2\,\partial y^2} + 4f^3\frac{\partial^4 f}{\partial t\,\partial y^3} + f^4\frac{\partial^4 f}{\partial y^4})_{t=t^n} + ...]$$
$$+O((\Delta t)^6 f^{(5)})$$

For easy comparison, we rewrite Eq. (C.32) into the following form

$$
\begin{aligned}
y^{n+1} &= y^n + \Delta t(f)_{t=t^n} + \frac{(\Delta t)^2}{2}\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)_{t=t^n} \\
&+ \frac{(\Delta t)^3}{6}\left[\left(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2}\right) + \left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\left(\frac{\partial f}{\partial y}\right)\right]_{t=t^n} \\
&+ \frac{(\Delta t)^4}{24}\left[\left(\frac{\partial^3 f}{\partial t^3} + 3f\frac{\partial^3 f}{\partial t^2\,\partial y} + 3f^2\frac{\partial^3 f}{\partial t\,\partial y^2} + f^3\frac{\partial^3 f}{\partial y^3}\right)\right. \\
&\qquad + \left(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2}\right)\left(\frac{\partial f}{\partial y}\right) \\
&\qquad + \left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\left(\frac{\partial f}{\partial y}\right)^2 \\
&\qquad + 3(f)\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\left(\frac{\partial^2 f}{\partial y^2}\right) \\
&\qquad \left. + 3\left(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y}\right)\left(\frac{\partial^2 f}{\partial t\,\partial y}\right)\right]_{t=t^n} \\
&+ \frac{(\Delta t)^5}{120}\left[\left(\frac{\partial^4 f}{\partial t^4} + 4f\frac{\partial^4 f}{\partial t^3\,\partial y} + 6f^2\frac{\partial^4 f}{\partial t^2\,\partial y^2} + 4f^3\frac{\partial^4 f}{\partial t\,\partial y^3} + f^4\frac{\partial^4 f}{\partial y^4}\right)_{t=t^n} + \ldots\right] \\
&+ O((\Delta t)^6 f^{(5)})
\end{aligned}
\tag{C.55}
$$

If Eq. (C.54) is equal to Eq. (C.55), the coefficients in Eqs. (C.54) and (C.55) should be identical to each other. Namely,

$$a + b + c + d = 1 \tag{C.56}$$

$$\frac{b}{2} + \frac{c}{2} + d = \frac{1}{2} \tag{C.57}$$

$$\frac{b}{4} + \frac{c}{4} + d = \frac{1}{3} \tag{C.58}$$

$$\frac{c}{2} + d = \frac{1}{3} \tag{C.59}$$

$$\frac{b}{8} + \frac{c}{8} + d = \frac{1}{4} \tag{C.60}$$

$$\frac{3c}{8} + \frac{3d}{4} = \frac{1}{4} \tag{C.61}$$

$$\frac{3d}{2} = \frac{1}{4} \tag{C.62}$$

$$\frac{3c}{4} + 3d = \frac{3}{4} \tag{C.63}$$

$$\frac{b}{16} + \frac{c}{16} + d = \frac{1}{5} \tag{C.64}$$

Solving Eqs. (C.56)-(C.59), we can find a set of solutions $a = d = 1/6$ and $b = c = 1/3$. These solutions also satisfy Eqs. (C.60)-(C.63), but do not satisfy Eq. (C.64). Thus, we have obtained the expression of the fourth-order Runge-Kutta method

$$y^{n+1} = y^n + \Delta t[\frac{1}{6} f_1 + \frac{1}{3} f_2 + \frac{1}{3} f_3 + \frac{1}{6} f_4] + O((\Delta t)^5 f^{(4)}) \tag{C.65}$$

where

$$f_1 = f(t^n, y^n)$$

$$f_2 = f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2} f_1)$$

$$f_3 = f(t^n + \frac{\Delta t}{2}, y^n + \frac{\Delta t}{2} f_2)$$

$$f_4 = f(t^n + \Delta t, y^n + \Delta t f_3)$$

C.2.3. Looking for the Third-Order and Higher-Order Expressions of y^{n+1}

Let us assume a third-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_2 + c f_3] + O((\Delta t)^4 f^{(3)}) \tag{C.66}$$

where

$$f_1 = f(t^n, y^n) \tag{C.67}$$

$$f_2 = f(t^n + \frac{\Delta t}{k}, y^n + \frac{\Delta t}{k} f_1) \tag{C.68}$$

$$f_3 = f(t^n + \frac{\Delta t}{l}, y^n + \frac{\Delta t}{l} f_2) \tag{C.69}$$

Let $(f)_{t=t^n} = f(t^n, y^n)$. Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + (\Delta t / k), y^n + (\Delta t / k)(f)_{t=t^n})$ into Eq. (C.68), it yields

$$f_2 = (f)_{t=t^n} + \frac{\Delta t}{k}(\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial y})_{t=t^n} + \frac{1}{2}(\frac{\Delta t}{k})^2(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t\,\partial y} + f^2\frac{\partial^2 f}{\partial y^2})_{t=t^n} + O[(\Delta t)^3 f^{(3)}] \tag{C.70}$$

Substituting the 2-dimensional Taylor's series expansion of the function $f(t^n + (\Delta t / l), y^n + (\Delta t / l) f_2)$ into Eq. (C.69) yields

$$f_3 = (f)_{t=t^n} + \frac{\Delta t}{l}(\frac{\partial f}{\partial t} + f_2\frac{\partial f}{\partial y})_{t=t^n} + \frac{1}{2}(\frac{\Delta t}{l})^2(\frac{\partial^2 f}{\partial t^2} + 2f_2\frac{\partial^2 f}{\partial t\,\partial y} + (f_2)^2\frac{\partial^2 f}{\partial y^2})_{t=t^n} + O[(\Delta t)^3 f^{(3)}] \tag{C.71}$$

Substituting Eqs. (C.67), (C.70) and (C.71) into Eq. (C.66), it yields

$$
\begin{aligned}
y^{n+1} &= y^n + \Delta t[(a+b+c)(f)_{t=t^n}] \\
&+(\Delta t)^2[(\frac{b}{k}+\frac{c}{l})(\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial y})_{t=t^n}] \\
&+\frac{(\Delta t)^3}{2}[(\frac{b}{k^2}+\frac{c}{l^2})(\frac{\partial^2 f}{\partial t^2}+2f\frac{\partial^2 f}{\partial t\,\partial y}+f^2\frac{\partial^2 f}{\partial y^2})_{t=t^n}] \\
&+(\Delta t)^3[\frac{c}{kl}(\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial y})_{t=t^n}(\frac{\partial f}{\partial y})_{t=t^n}]+O((\Delta t)^4 f^{(3)})
\end{aligned}
\tag{C.72}
$$

For easy comparison, we cast Eq. (C.32) into the following form

$$
\begin{aligned}
y^{n+1} &= y^n + \Delta t(f)_{t=t^n} + \frac{(\Delta t)^2}{2}(\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial y})_{t=t^n} \\
&+\frac{(\Delta t)^3}{6}[(\frac{\partial^2 f}{\partial t^2}+2f\frac{\partial^2 f}{\partial t\,\partial y}+f^2\frac{\partial^2 f}{\partial y^2})+(\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial y})(\frac{\partial f}{\partial y})]_{t=t^n}+O((\Delta t)^4 f^{(3)})
\end{aligned}
\tag{C.73}
$$

If Eq. (C.72) is equal to Eq. (C.73), the coefficients in Eqs. (C.72) and (C.73) should be identical to each other. Namely,

$$a+b+c=1 \tag{C.74}$$

$$\frac{b}{k}+\frac{c}{l}=\frac{1}{2} \tag{C.75}$$

$$\frac{b}{k^2}+\frac{c}{l^2}=\frac{1}{3} \tag{C.76}$$

$$\frac{c}{kl}=\frac{1}{6} \tag{C.77}$$

Solving Eqs. (C.56)-(C.59), we can find a set of solutions $a=1/4$, $b=0$, $c=3/4$, $k=3$, and $l=3/2$. Thus, we have obtained an expression of the third-order Runge-Kutta method

$$y^{n+1} = y^n + \Delta t[\frac{1}{4}f_1+\frac{3}{4}f_3]+O((\Delta t)^4 f^{(3)}) \tag{C.78}$$

where

$$f_1 = f(t^n, y^n)$$

$$f_2 = f(t^n+\frac{\Delta t}{3}, y^n+\frac{\Delta t}{3}f_1)$$

$$f_3 = f(t^n+\frac{2}{3}\Delta t, y^n+\frac{2}{3}\Delta t\, f_2)$$

Exercise C.1 Find a general expression of the second-order expression of y^{n+1}

Let us assume a second-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_2] + O((\Delta t)^3 f^{(2)}) \tag{C.79}$$

where

$$f_1 = f(t^n, y^n) \tag{C.80}$$

$$f_2 = f(t^n + \frac{\Delta t}{k}, y^n + \frac{\Delta t}{k} f_1) \tag{C.81}$$

Please find possible solutions of a, b, and k.

Answer: Substituting Eqs. (C.80) and (C.70) into Eq. (C.79), it yields

$$a + b = 1 \tag{C.82}$$

$$\frac{b}{k} = \frac{1}{2} \tag{C.83}$$

Possible solutions include:

Type 1 solutions: $\{a = b = 1/2,\ k = 1\}$, which resemble the Trapezoidal rule.

Type 2 solutions: $\{a = 0,\ b = 1,\ k = 2\}$, which resemble the second-order Lax-Wendroff scheme.

General solutions: $\{b = k/2,\ a = 1-(k/2)$, for all real number $k\}$.

Exercise C.2 Find a fifth-order expression of y^{n+1}

Let us assume a sixth-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a f_1 + b f_2 + c f_3 + d f_4 + g f_5] + O((\Delta t)^6 f^{(5)}) \tag{C.84}$$

where

$$f_1 = f(t^n, y^n) \tag{C.85}$$

$$f_2 = f(t^n + \frac{\Delta t}{j}, y^n + \frac{\Delta t}{j} f_1) \tag{C.86}$$

$$f_3 = f(t^n + \frac{\Delta t}{k}, y^n + \frac{\Delta t}{k} f_2) \tag{C.87}$$

$$f_4 = f(t^n + \frac{\Delta t}{l}, y^n + \frac{\Delta t}{l} f_3) \tag{C.88}$$

$$f_5 = f(t^n + \frac{\Delta t}{m}, y^n + \frac{\Delta t}{m} f_4) \tag{C.89}$$

Please find possible solutions of a, b, c, d, g, and j, k, l, m.

Exercise C.3 Find a sixth-order expression of y^{n+1}

Let us assume a sixth-order expression of y^{n+1}

$$y^{n+1} = y^n + \Delta t[a\, f_1 + b\, f_2 + c\, f_3 + d\, f_4 + g\, f_5 + h\, f_6] + O((\Delta t)^7 f^{(6)}) \tag{C.90}$$

where

$$f_1 = f(t^n, y^n) \tag{C.91}$$

$$f_2 = f(t^n + \frac{\Delta t}{j}, y^n + \frac{\Delta t}{j} f_1) \tag{C.92}$$

$$f_3 = f(t^n + \frac{\Delta t}{k}, y^n + \frac{\Delta t}{k} f_2) \tag{C.93}$$

$$f_4 = f(t^n + \frac{\Delta t}{l}, y^n + \frac{\Delta t}{l} f_3) \tag{C.94}$$

$$f_5 = f(t^n + \frac{\Delta t}{m}, y^n + \frac{\Delta t}{m} f_4) \tag{C.95}$$

$$f_6 = f(t^n + \frac{\Delta t}{p}, y^n + \frac{\Delta t}{p} f_5) \tag{C.96}$$

Please find possible solutions of a, b, c, d, g, h, and j, k, l, m, p.

C.3. Derivation of the Adams' Formulae

Let $dy/dt = f(y,t)$, $y^n = y(t = n\Delta t)$, and $[f^{(k)}]^n = [d^k f / dt^k]_{t=n\Delta t}$. The Taylor series expansion of y^{n+1} is given by

$$y^{n+1} = y^n + hf^n + \frac{h^2}{2!}[f^{(1)}]^n + \frac{h^3}{3!}[f^{(2)}]^n + \frac{h^4}{4!}[f^{(3)}]^n + ... + \frac{h^m}{m!}[f^{(m-1)}]^n + O(h^{m+1} f^{(m)}) \tag{C.97}$$

For Adams' open formula, the m-th order expression of y^{n+1} can be written as

$$y^{n+1} = y^n + h[a_0 f^n + a_{-1} f^{n-1} + +a_{-2} f^{n-2} + a_{-3} f^{n-3} + ... + a_{-(m-1)} f^{n-(m-1)}] + O(h^{m+1}) \tag{C.98}$$

For Adams close formula, the m-th order expression of y^{n+1} can be written as

$$y^{n+1} = y^n + h[b_{+1} f^{n+1} + b_0 f^n + b_{-1} f^{n-1} + b_{-2} f^{n-2} + ... + b_{-(m-2)} f^{n-(m-2)}] + O(h^{m+1}) \tag{C.99}$$

The Taylor series expansions of $f^{n+1}, f^{n-1}, .., f^{n-(m-1)}$ are given below:

$$f^{n+1} = f^n + h[f^{(1)}]^n + \frac{h^2}{2!}[f^{(2)}]^n + \frac{h^3}{3!}[f^{(3)}]^n + \frac{h^4}{4!}[f^{(4)}]^n + ... + \frac{h^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \tag{C.100}$$

$$f^{n-1} = f^n - h[f^{(1)}]^n + \frac{h^2}{2!}[f^{(2)}]^n - \frac{h^3}{3!}[f^{(3)}]^n + \frac{h^4}{4!}[f^{(4)}]^n + ... + \frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \tag{C.101}$$

$$f^{n-2} = f^n - 2h[f^{(1)}]^n + 2^2 \frac{h^2}{2!}[f^{(2)}]^n - 2^3 \frac{h^3}{3!}[f^{(3)}]^n + ... + \frac{(-2h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \tag{C.102}$$

$$f^{n-3} = f^n - 3h[f^{(1)}]^n + 3^2 \frac{h^2}{2!}[f^{(2)}]^n - 3^3 \frac{h^3}{3!}[f^{(3)}]^n + ... + \frac{(-3h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \tag{C.103}$$

… … …

$$\begin{aligned} f^{n-(m-2)} = f^n &- (m-2)h[f^{(1)}]^n + (m-2)^2 \frac{h^2}{2!}[f^{(2)}]^n - (m-2)^3 \frac{h^3}{3!}[f^{(3)}]^n \\ &+ ... + (m-2)^{m-1} \frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.104}$$

$$f^{n-(m-1)} = f^n - (m-1)h[f^{(1)}]^n + (m-1)^2 \frac{h^2}{2!}[f^{(2)}]^n - (m-1)^3 \frac{h^3}{3!}[f^{(3)}]^n + ... + (m-1)^{m-1} \frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \tag{C.105}$$

Substituting Eqs. (C.101)~(C.105) into Eq. (C.98), and then comparing the coefficients of $[f^{(k)}]^n$ with the Eq. (C.97) it yields

$$a_0 + a_{-1} + a_{-2} + a_{-3} + ... + a_{-(m-1)} = 1 \tag{C.106}$$

$$\begin{bmatrix} 1 & 2 & 3 & \cdots & (m-1) \\ 1 & 2^2 & 3^2 & \cdots & (m-1)^2 \\ 1 & 2^3 & 3^3 & \cdots & (m-1)^3 \\ \vdots & & \vdots & & \vdots \\ 1 & 2^{m-1} & 3^{m-1} & \cdots & (m-1)^{m-1} \end{bmatrix} \begin{bmatrix} a_{-1} \\ a_{-2} \\ a_{-3} \\ \vdots \\ a_{-(m-1)} \end{bmatrix} = \begin{bmatrix} -1/2 \\ +1/3 \\ -1/4 \\ \vdots \\ (-1)^{m-1}/m \end{bmatrix} \tag{C.107}$$

Substituting Eqs. (C.100)~(C.104) into Eq. (C.99), and then comparing the coefficients of $[f^{(k)}]^n$ with the Eq. (C.97) it yields

$$b_{+1} + b_0 + b_{-1} + b_{-2} + ... + b_{-(m-2)} = 1 \tag{C.108}$$

$$\begin{bmatrix} 1 & -1 & -2 & \cdots & -(m-2) \\ 1 & +1 & +2^2 & \cdots & +(m-2)^2 \\ 1 & -1 & -2^3 & \cdots & -(m-2)^3 \\ \vdots & & & \vdots & \vdots \\ 1 & (-1)^{m-1} & (-2)^{m-1} & \cdots & (-m+2)^{m-1} \end{bmatrix} \begin{bmatrix} b_{+1} \\ b_{-1} \\ b_{-2} \\ \vdots \\ b_{-(m-2)} \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/3 \\ 1/4 \\ \vdots \\ 1/m \end{bmatrix} \tag{C.109}$$

Solutions of Eqs. (C.106) and (C.107) yield the Adams' open formulae as the ones shown in Table C.2. Solutions of Eqs. (C.108) and (C.109) yield the Adams' close formulae as the ones shown in Table C.3. Note that a different way to show the derivations of the Adams' open and close formulae can be found in the textbook by *Hildebrand* (1976).

Table C.2. The *n*th order Adams' Open Formulae (also called Adams-Bashforth Formulae)

Order of Accuracy	Solving $dy/dt = f$ or $\partial y/\partial t = f$ explicitly with $h = \Delta t$
1st	$y^{n+1} = y^n + h[f^n] + O(h^2 f^{(1)})$
2nd	$y^{n+1} = y^n + h[\frac{3}{2}f^n - \frac{1}{2}f^{n-1}] + O(h^3 f^{(2)})$
3rd	$y^{n+1} = y^n + h[\frac{23}{12}f^n - \frac{16}{12}f^{n-1} + \frac{5}{12}f^{n-2}] + O(h^4 f^{(3)})$
4th	$y^{n+1} = y^n + h[\frac{55}{24}f^n - \frac{59}{24}f^{n-1} + \frac{37}{24}f^{n-2} - \frac{9}{24}f^{n-3}] + O(h^5 f^{(4)})$
5th	$y^{n+1} = y^n$ $+ h[\frac{1901}{720}f^n - \frac{2774}{720}f^{n-1} + \frac{2616}{720}f^{n-2} - \frac{1274}{720}f^{n-3} + \frac{251}{720}f^{n-4}] + O(h^6 f^{(5)})$
6th	$y^{n+1} = y^n$ $+ h[\frac{4277}{1440}f^n - \frac{7923}{1440}f^{n-1} + \frac{9982}{1440}f^{n-2} - \frac{7298}{1440}f^{n-3} + \frac{2877}{1440}f^{n-4} - \frac{475}{1440}f^{n-5}]$ $+ O(h^7 f^{(6)})$

Table C.3. The *n*th order Adams' Close Formulae (also called Adams-Moulton Formulae)

Order of Accuracy	Solving $dy/dt = f$ or $\partial y/\partial t = f$ implicitly with $h = \Delta t$
1st	$y^{n+1} = y^n + h[f^{n+1}] + O(h^2 f^{(1)})$
2nd	$y^{n+1} = y^n + h[\frac{1}{2}f^{n+1} + \frac{1}{2}f^n] + O(h^3 f^{(2)})$
3rd	$y^{n+1} = y^n + h[\frac{5}{12}f^{n+1} + \frac{8}{12}f^n - \frac{1}{12}f^{n-1}] + O(h^4 f^{(3)})$
4th	$y^{n+1} = y^n + h[\frac{9}{24}f^{n+1} + \frac{19}{24}f^n - \frac{5}{24}f^{n-1} + \frac{1}{24}f^{n-2}] + O(h^5 f^{(4)})$
5th	$y^{n+1} = y^n$ $+ h[\frac{251}{720}f^{n+1} + \frac{646}{720}f^n - \frac{264}{720}f^{n-1} + \frac{106}{720}f^{n-2} - \frac{19}{720}f^{n-3}] + O(h^6 f^{(5)})$
6th	$y^{n+1} = y^n$ $+ h[\frac{475}{1440}f^{n+1} + \frac{1427}{1440}f^n - \frac{798}{1440}f^{n-1} + \frac{482}{1440}f^{n-2} - \frac{173}{1440}f^{n-3} + \frac{27}{1440}f^{n-4}]$ $+ O(h^7 f^{(6)})$

C.4. Derivation of the Open Formulae at half time steps

For open formula, the m-th order expression of y^{n+1} can be written as

$$\begin{aligned} y^{n+1} = y^n + h[&a_{0.5} f^{n+0.5} + a_{-0.5} f^{n-0.5} + + a_{-1.5} f^{n-1.5} + a_{-2.5} f^{n-2.5} \\ &+ ... + a_{-(m-0.5)} f^{n-(m-0.5)}] + O(h^{m+1}) \end{aligned} \tag{C.110}$$

The Taylor series expansions of $f^{n+0.5}, f^{n-0.5}, ..., f^{n-(m-0.5)}$ are given below:

$$\begin{aligned} f^{n+0.5} = f^n &+ \frac{h}{2}[f^{(1)}]^n + \frac{1}{2^2}\frac{h^2}{2!}[f^{(2)}]^n + \frac{1}{2^3}\frac{h^3}{3!}[f^{(3)}]^n + \frac{1}{2^4}\frac{h^4}{4!}[f^{(4)}]^n \\ &+ ... + \frac{1}{2^{m-1}}\frac{h^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.111}$$

$$\begin{aligned} f^{n-0.5} = f^n &- \frac{h}{2}[f^{(1)}]^n + \frac{1}{2^2}\frac{h^2}{2!}[f^{(2)}]^n - \frac{1}{2^3}\frac{h^3}{3!}[f^{(3)}]^n + \frac{1}{2^4}\frac{h^4}{4!}[f^{(4)}]^n \\ &+ ... + \frac{1}{2^{m-1}}\frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.112}$$

$$\begin{aligned} f^{n-1.5} = f^n &- \frac{3}{2}h[f^{(1)}]^n + \frac{3^2}{2^2}\frac{h^2}{2!}[f^{(2)}]^n - \frac{3^3}{2^3}\frac{h^3}{3!}[f^{(3)}]^n + \frac{3^4}{2^4}\frac{h^4}{4!}[f^{(4)}]^n \\ &+ ... + \frac{3^{m-1}}{2^{m-1}}\frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.113}$$

$$\begin{aligned} f^{n-2.5} = f^n &- \frac{5}{2}h[f^{(1)}]^n + \frac{5^2}{2^2}\frac{h^2}{2!}[f^{(2)}]^n - \frac{5^3}{2^3}\frac{h^3}{3!}[f^{(3)}]^n + \frac{5^4}{2^4}\frac{h^4}{4!}[f^{(4)}]^n \\ &+ ... + \frac{5^{m-1}}{2^{m-1}}\frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.114}$$

… … …

$$\begin{aligned} f^{n-(m-0.5)} = f^n &- (m-0.5)h[f^{(1)}]^n + (m-0.5)^2\frac{h^2}{2!}[f^{(2)}]^n - (m-0.5)^3\frac{h^3}{3!}[f^{(3)}]^n \\ &+ ... + (m-0.5)^{m-1}\frac{(-h)^{m-1}}{(m-1)!}[f^{(m-1)}]^n + O(h^m f^{(m)}) \end{aligned} \tag{C.115}$$

Substituting Eqs. (C.111)~(C.115) into Eq. (C.110), and then comparing the coefficients of $[f^{(k)}]^n$

with the Eq. (C.97) it yields

$$\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1/2 & -1/2 & -3/2 & -5/2 & \cdots & -(m-0.5) \\ 1/2^2 & 1/2^2 & 3^2/2^2 & 5^2/2^2 & \cdots & (m-0.5)^2 \\ 1/2^3 & -1/2^3 & -3^3/2^3 & -5^3/2^3 & \cdots & -(m-0.5)^3 \\ \vdots & \cdots & \cdots & \cdots & \cdots & \vdots \\ 1/2^{m-1} & (-1/2)^{m-1} & (-3/2)^{m-1} & (-5/2)^{m-1} & \cdots & [-(m-0.5)]^{m-1} \end{bmatrix} \begin{bmatrix} a_{0.5} \\ a_{-0.5} \\ a_{-1.5} \\ a_{-2.5} \\ \vdots \\ a_{-(m-0.5)} \end{bmatrix} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ \vdots \\ 1/m \end{bmatrix}$$

(C.116)

Solutions of Eqs. (C.116) are shown in Table C.4.

Table C.4. The *n*th order Open Formulae at half time steps

Order of Accuracy	Solving $dy/dt = f$ or $\partial y/\partial t = f$ explicitly with $h = \Delta t$
2nd	$y^{n+1} = y^n + h[1 f^{n+0.5} - 0 f^{n-0.5}] + O(h^3 f^{(2)})$
3rd	$y^{n+1} = y^n + h[\frac{25}{24} f^{n+0.5} - \frac{2}{24} f^{n-0.5} + \frac{1}{24} f^{n-1.5}] + O(h^4 f^{(3)})$
4th	$y^{n+1} = y^n + h[\frac{26}{24} f^{n+0.5} - \frac{5}{24} f^{n-0.5} + \frac{4}{24} f^{n-1.5} - \frac{1}{24} f^{n-2.5}] + O(h^5 f^{(4)})$

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