Appendix B. Higher-Order Finite Differences

B.1. Central-Finite-Difference Expressions of a Function's Derivative With Uniform Grid Distribution

Let us consider a tabulate function $f_i = f(x_i)$ in a simulation system with uniform grid distribution x_i. We wish to express the *k*th derivatives of the tabulate function at $x = x_i$ based on the function at the nearby grids. Namely, for the central difference, the *k*th derivatives of the tabulate function at $x = x_i$, i.e., $f^{(k)}(x_i) = f_i^{(k)}$, can be written as

$$f_i^{(k)} = \frac{1}{h^k}\left(\sum_{j=-n}^{+n} a_j f_{i+j}\right) + O[h^{m+1} f_i^{(m+k+1)}] \tag{B.1}$$

where h is the grid size and we have assumed that the accuracy of this scheme is on the order of h^m, where m is a function of k and n and will be determined later. For $x_{i+j} = x_i + jh$, the Taylor's series expansion of $f_{i+j} = f(x_{i+j}) = f(x_i + jh)$ with respect to $x = x_i$ can be written as

$$f_{i+j} = f_i + (jh) f_i' + \frac{(jh)^2}{2!} f_i'' + \frac{(jh)^3}{3!} f_i^{(3)} + ... + \frac{(jh)^{(k)}}{k!} f_i^{(k)} + ... \tag{B.2}$$

Substituting Eq. (B.2) into the first term on the right of Eq. (B.1), it yields

$$\begin{aligned}
f_i^{(k)} = \frac{1}{h^k}\{ & [a_0 + (a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) + (a_{+3} + a_{-3}) + ... + (a_{+n} + a_{-n})] f_i \\
& + [(a_{+1} - a_{-1}) + (a_{+2} - a_{-2}) \cdot 2 + (a_{+3} - a_{-3}) \cdot 3 + ... + (a_{+n} - a_{-n}) \cdot n] f_i' \cdot h \\
& + [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^2 + (a_{+3} + a_{-3}) \cdot 3^2 + ... + (a_{+n} + a_{-n}) \cdot n^2] f_i'' \cdot \frac{h^2}{2} \\
& + [(a_{+1} - a_{-1}) + (a_{+2} - a_{-2}) \cdot 2^3 + (a_{+3} - a_{-3}) \cdot 3^3 + ... + (a_{+n} - a_{-n}) \cdot n^3] f_i^{(3)} \cdot \frac{h^3}{3!} \\
& + ... \\
& + [(a_{+1} + (-1)^k a_{-1}) + (a_{+2} + (-1)^k a_{-2}) \cdot 2^k + ... + (a_{+n} + (-1)^k a_{-n}) \cdot n^k] f_i^{(k)} \cdot \frac{h^k}{k!} \\
& + ... \\
& + [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^{2n} + ... + (a_{+n} + a_{-n}) \cdot n^{2n}] f_i^{(2n)} \cdot \frac{h^{2n}}{(2n)!} \\
& + [(a_{+1} - a_{-1}) + (a_{+2} - a_{-2}) \cdot 2^{2n+1} + ... + (a_{+n} - a_{-n}) \cdot n^{2n+1}] f_i^{(2n+1)} \cdot \frac{h^{2n+1}}{(2n+1)!} \\
& + [(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^{2n+2} + ... + (a_{+n} + a_{-n}) \cdot n^{2n+2}] f_i^{(2n+2)} \cdot \frac{h^{2n+2}}{(2n+2)!} \\
& + ... \}
\end{aligned} \tag{B.3}$$

Since we have $2n+1$ unknowns ($a_{-n} \sim a_{+n}$), we need $2n+1$ equations. Comparing the coefficients of f_i, ..., $f_i^{(k)}$, ..., $f_i^{(2n)}$ on two sides of Eq. (B.3), it yields the following $2n+1$ equations. Namely, the coefficients of f_i yields

$$a_0 + (a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) + (a_{+3} + a_{-3}) + ... + (a_{+n} + a_{-n}) = 0 \quad \text{(B.4)}$$

The coefficient of $f_i^{(k)}$ yields

$$(a_{+1} + (-1)^k a_{-1}) + (a_{+2} + (-1)^k a_{-2}) \cdot 2^k + ... + (a_{+n} + (-1)^k a_{-n}) \cdot n^k = k!$$

Namely, for an even number k, it yields

$$(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^k + (a_{+3} + a_{-3}) \cdot 3^k + ... + (a_{+n} + a_{-n}) \cdot n^k = k! \quad \text{(B.5)}$$

For an odd number k, it yields

$$(a_{+1} - a_{-1}) + (a_{+2} - a_{-2}) \cdot 2^k + (a_{+3} - a_{-3}) \cdot 3^k + ... + (a_{+n} - a_{-n}) \cdot n^k = k! \quad \text{(B.6)}$$

The coefficients of $f_i^{(j)}$ with $j \neq k$ and $1 \leq j \leq 2n$ yields total $2n-1$ equations of the following form

$$(a_{+1} + (-1)^j a_{-1}) + (a_{+2} + (-1)^j a_{-2}) \cdot 2^j + ... + (a_{+n} + (-1)^j a_{-n}) \cdot n^j = 0$$

Namely, for an even number j, it yields

$$(a_{+1} + a_{-1}) + (a_{+2} + a_{-2}) \cdot 2^j + (a_{+3} + a_{-3}) \cdot 3^j + ... + (a_{+n} + a_{-n}) \cdot n^j = 0 \quad \text{(B.7)}$$

For an odd number j, it yields

$$(a_{+1} - a_{-1}) + (a_{+2} - a_{-2}) \cdot 2^j + (a_{+3} - a_{-3}) \cdot 3^j + ... + (a_{+n} - a_{-n}) \cdot n^j = 0 \quad \text{(B.8)}$$

B.1.1. Determine $f_i^{(k)}$ for an even number k

For an even number k, the governing equations are Eqs. (B.4), (B.5), (B.7) and (B.8). Since Eq. (B.5), we cannot set $a_j + a_{-j} = 0$, but we can set $a_j - a_{-j} = 0$. As a result, the Eq. (B.8) is automatically fulfilled and the coefficient of $f_i^{(2n+1)}$ in the Eq. (B.3) is equal to zero. Thus, the finite difference expression of

$$f_i^{(k)} = \frac{1}{h^k}\left(\sum_{j=-n}^{+n} a_j f_{i+j}\right)$$

will have a residue (or a discretization error) on the order of $O[h^{2n+2-k} f_i^{(2n+2)}]$. Thus, the order of accuracy of the expression of $f_i^{(k)}$ in Eq. (B.1) is $m = 2n+1-k$ if k is an even number.

For $a_j - a_{-j} = 0$, we have $a_j + a_{-j} = 2a_j$, and Eqs. (B.4), (B.5), (B.7) and (B.8) can be rewritten as

$$a_0 = -2(a_{+1} + a_{+2} + a_{+3} + ... + a_{+n}) \tag{B.9}$$

$$\begin{pmatrix} 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ 1 & 2^4 & 3^4 & \cdots & \cdots & n^4 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & n^{2n} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!/2 \\ 0 \\ \vdots \end{pmatrix} \tag{B.10}$$

The matrix on the left is a Vandermonde matrix. Eq. (B.1) can be rewritten as

$$f_i^{(k)} = \frac{1}{h^k}[-2(a_1 + ... + a_n)f_0 + a_1(f_{i+1} + f_{i-1}) + ... + a_n(f_{i+n} + f_{i-n})] + O[\frac{n^{2n+2}}{(2n+2)!} h^{2n+2-k} f_i^{(2n+2)}] \tag{B.11}$$

where k is an even number and $a_1 \sim a_n$ are given by Eq. (B.10).

Remarks: Note that for $0 = a_3 = a_5 = a_6 = a_7 = a_9 = ...$, we have

$$\begin{pmatrix} 1 & 2^2 & 4^2 & 8^2 & \cdots & n^2 \\ 1 & 2^4 & 4^4 & 8^4 & \cdots & n^4 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 4^k & 8^k & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_4 \\ a_8 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!/2 \\ 0 \\ \vdots \end{pmatrix}$$

We can recover the coefficients of the Richardson's formula (Maron and Lopez, 1991). It means that the expression of $f_i^{(k)}$ in the finite-difference scheme is not unique. In deed, for $k >> 1$ and with very small grid size, the Richardson's formula is better than the one obtained in this section, because we need a wide range of spatial information to conclude the higher order derivatives. A detailed discussion on Richardson's formula can be found in the Appendix D.

B.1.2. Determine $f_i^{(k)}$ for an odd number k

For an odd number k, the governing equations are Eqs. (B.4), (B.6), (B.7) and (B.8). Since Eq. (B6), we cannot set $a_j - a_{-j} = 0$, but we can set $a_j + a_{-j} = 0$. As a result, the condition given in Eq. (B.7) is automatically fulfilled and the coefficient of $f_i^{(2n+1)}$ in the Eq. (B.3) is NOT equal to zero. Thus, the finite difference expression of

$$f_i^{(k)} = \frac{1}{h^k}(\sum_{j=-n}^{+n} a_j f_{i+j})$$

will have a residue (or a discretization error) on the order of $O[h^{2n+1-k} f_i^{(2n+1)}]$. Thus, the order of accuracy of the expression of $f_i^{(k)}$ in Eq. (B.1) is $m = 2n - k$ if k is an odd number.

For $a_j + a_{-j} = 0$, we have $a_j - a_{-j} = 2a_j$, and Eqs. (B.4), (B6), (B.7) and (B.8) can be rewritten as

$$a_0 = 0 \tag{B.12}$$

$$\begin{pmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^3 & 3^3 & \cdots & \cdots & n^3 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & n^{2n-1} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!/2 \\ 0 \\ \vdots \end{pmatrix} \tag{B.13}$$

Eq. (B.1) can be rewritten as

$$f_i^{(k)} = \frac{1}{h^k}[a_1(f_{i+1} - f_{i-1}) + ... + a_n(f_{i+n} - f_{i-n})] + O[\frac{n^{2n+1}}{(2n+1)!} h^{2n+1-k} f_i^{(2n+1)}] \tag{B.14}$$

where k is an odd number and $a_1 \sim a_n$ are given by Eq. (B.13).

For simplicity, we shall set $i = 0$ in the following discussion. A few examples are given below. More examples can be found in Table B.1.

Case 1A

If $f_0^{(1)} = \frac{1}{h}[a_1(f_1 - f_{-1}) + O(h^3 f_0^{(3)})]$ then

$$(a_1) = \frac{1}{2}(1^1)^{-1}(1!) = \frac{1}{2}$$

That is, $f_0^{(1)} = \frac{1}{2h}(f_1 - f_{-1}) + O(h^2 f_0^{(3)})$

Case 1B

If $f_0^{(2)} = \frac{1}{h^2}[a_1(f_1 + f_{-1}) - 2a_1 f_0 + O(h^4 f_0^{(4)})]$ then

$$(a_1) = \frac{1}{2}(1^2)^{-1}(2!) = 1$$

That is, $f_0^{(2)} = \frac{1}{h^2}(f_1 - 2f_0 + f_{-1}) + O(h^2 f_0^{(4)})$

Case 2A

If $f_0^{(1)} = \frac{1}{h}[a_1(f_1 - f_{-1}) + a_2(f_2 - f_{-2}) + O(h^5 f_0^{(5)})]$, then

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1^1 & 2^1 \\ 1^3 & 2^3 \end{pmatrix}^{-1}\begin{pmatrix} 1! \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4/3 & -1/3 \\ -1/6 & 1/6 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2/3 \\ -1/12 \end{pmatrix}$$

That is, $f_0^{(1)} = \frac{1}{h}(-\frac{1}{12}f_2 + \frac{2}{3}f_1 - \frac{2}{3}f_{-1} + \frac{1}{12}f_{-2}) + O(h^4 f_0^{(5)})$

Case 2B

If $f_0^{(2)} = \frac{1}{h^2}[a_1(f_1 + f_{-1}) - 2(a_1 + a_2)f_0 + a_2(f_2 + f_{-2}) + O(h^6 f_0^{(6)})]$, then

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1^2 & 2^2 \\ 1^4 & 2^4 \end{pmatrix}^{-1}\begin{pmatrix} 2! \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4/3 & -1/3 \\ -1/12 & 1/12 \end{pmatrix}\begin{pmatrix} 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 4/3 \\ -1/12 \end{pmatrix}$$

That is, $f_0^{(2)} = \frac{1}{h^2}(-\frac{1}{12}f_2 + \frac{4}{3}f_1 - \frac{5}{2}f_0 + \frac{4}{3}f_{-1} - \frac{1}{12}f_{-2}) + O(h^4 f_0^{(6)})$

Case 2C

If $f_0^{(3)} = \frac{1}{h^3}[a_1(f_1 - f_{-1}) + a_2(f_2 - f_{-2}) + O(h^5 f_0^{(5)})]$, then

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1^1 & 2^1 \\ 1^3 & 2^3 \end{pmatrix}^{-1}\begin{pmatrix} 0 \\ 3! \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4/3 & -1/3 \\ -1/6 & 1/6 \end{pmatrix}\begin{pmatrix} 0 \\ 6 \end{pmatrix} = \begin{pmatrix} -1 \\ +1/2 \end{pmatrix}$$

That is, $f_0^{(3)} = \frac{1}{h^3}(\frac{1}{2}f_2 - f_1 + f_{-1} - \frac{1}{2}f_{-2}) + O(h^2 f_0^{(5)})$

Case 2D

If $f_0^{(4)} = \frac{1}{h^4}[a_1(f_1 + f_{-1}) - 2(a_1 + a_2)f_0 + a_2(f_2 + f_{-2}) + O(h^6 f_0^{(6)})]$, then

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1^2 & 2^2 \\ 1^4 & 2^4 \end{pmatrix}^{-1}\begin{pmatrix} 0 \\ 4! \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4/3 & -1/3 \\ -1/12 & 1/12 \end{pmatrix}\begin{pmatrix} 0 \\ 24 \end{pmatrix} = \begin{pmatrix} -4 \\ 1 \end{pmatrix}$$

That is, $f_0^{(4)} = \frac{1}{h^4}(f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}) + O(h^2 f_0^{(6)})$

Case 3A

If $f_0^{(1)} = \frac{1}{h}[a_1(f_1 - f_{-1}) + a_2(f_2 - f_{-2}) + a_3(f_3 - f_{-3}) + O(h^7 f_0^{(7)})]$, then

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1^1 & 2^1 & 3^1 \\ 1^3 & 2^3 & 3^3 \\ 1^5 & 2^5 & 3^5 \end{pmatrix}^{-1}\begin{pmatrix} 1! \\ 0 \\ 0 \end{pmatrix}$$

$$= (\frac{1}{2})\frac{1}{120}\begin{pmatrix} 180 & -65 & 5 \\ -36 & 40 & -4 \\ 4 & -5 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{240}\begin{pmatrix} 180 \\ -36 \\ 4 \end{pmatrix} = \begin{pmatrix} 3/4 \\ -3/20 \\ 1/60 \end{pmatrix},$$

That is $f_0^{(1)} = \frac{1}{h}(+\frac{1}{60}f_3 - \frac{3}{20}f_2 + \frac{3}{4}f_1 - \frac{3}{4}f_{-1} + \frac{3}{20}f_{-2} - \frac{1}{60}f_{-3}) + O(h^6 f_0^{(7)})$

B.2. Higher-Order Finite Differences With Non-Equal Spacing Grid Distribution

Let us consider a tabulate function $f_i = f(x_i)$ in a simulation system with non-uniform grid distribution x_i. We wish to express the *k*th derivatives of the tabulate function at $x = x_i$ based on the function at the nearby grids. We can assume a polynomial with lowest power that passing through the given tabulate function at the given nearby grids and then evaluate the derivatives from this fitting polynomial. Two examples are given below.

Example 1

Let

$$f(x) = \frac{(x - x_{-1})(x - x_1)}{(x_0 - x_{-1})(x_0 - x_1)}f_0 + \frac{(x - x_0)(x - x_1)}{(x_{-1} - x_0)(x_{-1} - x_1)}f_{-1} + \frac{(x - x_{-1})(x - x_0)}{(x_{+1} - x_{-1})(x_{+1} - x_0)}f_{+1} \quad \text{(B.15)}$$

One can obtain $f_0^{(1)}, f_0^{(2)},$ form Eq. (B.15). For example, the first order $f_0^{(1)}$ is

$$f_0^{(1)} = [\frac{1}{(x_0 - x_{-1})} + \frac{1}{(x_0 - x_1)}]f_0 + \frac{(x_0 - x_1)}{(x_{-1} - x_0)(x_{-1} - x_1)}f_{-1} + \frac{(x_0 - x_{-1})}{(x_{+1} - x_{-1})(x_{+1} - x_0)}f_{+1} \quad \text{(B.16)}$$

For equal-spacing grid distribution, the derivatives $f_0^{(1)}$ and $f_0^{(2)}$ obtained form Eq. (B.15) should be the same as those shown in Case 1A and 1B, respectively.

Example 2

Let

$$f(x)=$$

$$=\frac{(x-x_{-2})(x-x_{-1})(x-x_1)(x-x_2)}{(x_0-x_{-2})(x_0-x_{-1})(x_0-x_1)(x_0-x_2)}f_0$$
$$+\frac{(x-x_{-1})(x-x_0)(x-x_1)(x-x_2)}{(x_{-2}-x_{-1})(x_{-2}-x_0)(x_{-2}-x_1)(x_{-2}-x_2)}f_{-2}+\frac{(x-x_{-2})(x-x_0)(x-x_1)(x-x_2)}{(x_{-1}-x_{-2})(x_{-1}-x_0)(x_{-1}-x_1)(x_{-1}-x_2)}f_{-1}$$
$$+\frac{(x-x_{-2})(x-x_{-1})(x-x_0)(x-x_2)}{(x_{+1}-x_{-2})(x_{+1}-x_{-1})(x_{+1}-x_0)(x_{+1}-x_2)}f_{+1}+\frac{(x-x_{-2})(x-x_{-1})(x-x_0)(x-x_1)}{(x_{+2}-x_{-2})(x_{+2}-x_{-1})(x_{+2}-x_0)(x_{+2}-x_1)}f_{+2}$$

(B.17)

One can obtain $f_0^{(1)}, f_0^{(2)}, f_0^{(3)}, f_0^{(4)}$, form Eq. (B.17). For example, the third order $f_0^{(1)}$ is

$$f_0^{(1)}=[\frac{1}{(x_0-x_{-2})}+\frac{1}{(x_0-x_{-1})}+\frac{1}{(x_0-x_1)}+\frac{1}{(x_0-x_2)}]f_0$$
$$+\frac{(x_0-x_{-1})(x_0-x_1)(x_0-x_2)}{(x_{-2}-x_{-1})(x_{-2}-x_0)(x_{-2}-x_1)(x_{-2}-x_2)}f_{-2}+\frac{(x_0-x_{-2})(x_0-x_1)(x_0-x_2)}{(x_{-1}-x_{-2})(x_{-1}-x_0)(x_{-1}-x_1)(x_{-1}-x_2)}f_{-1}$$
$$+\frac{(x_0-x_{-2})(x_0-x_{-1})(x_0-x_2)}{(x_{+1}-x_{-2})(x_{+1}-x_{-1})(x_{+1}-x_0)(x_{+1}-x_2)}f_{+1}+\frac{(x_0-x_{-2})(x_0-x_{-1})(x_0-x_1)}{(x_{+2}-x_{-2})(x_{+2}-x_{-1})(x_{+2}-x_0)(x_{+2}-x_1)}f_{+2}$$

(B.18)

For uniform grid distribution, the derivatives $f_0^{(1)}$, $f_0^{(2)}$, $f_0^{(3)}$, and $f_0^{(4)}$ obtained form Eq. (B.17) should be the same as those shown in Cases 2A, 2B, 2C, and 2D, respectively.

B.3. Summary of the Higher-Order Central-Finite-Differences Expressions

(1) The finite-difference expression of $f_0^{(k)}$ is not unique. For instance, the expression of $f_0^{(k)}$ obtained in the Appendix B and the Appendix D are different for $k>2$.

(2) For uniform grid distribution, the f_0 is not included in the central-finite-difference expressions of the odd-order derivatives.

(3) The results of the central-finite-difference expressions obtained in Section B.1 are summarized in the Table B.1.

(4) The sum of the coefficients is always equal to zero in each expression listed in Table B.1.

B.4. Forward/Backward Finite-Difference Expressions of a Function's Derivative With Uniform Grid Distribution

To determine the derivatives at the boundaries, we can use forward-finite-difference expressions and the backward-finite-difference expressions. Namely, let us consider a tabulate function $f_i = f(x_i)$ in a simulation system with uniform grid distribution x_i. We wish to express the *k*th derivatives of the tabulate function at $x = x_0$ based on the function at the grids with $x > x_0$ (forward difference) or based on the function at the grids with $x < x_0$ (backward difference). The forward/backward finite difference of $f^{(k)}(x_0) = f_0^{(k)}$ in a simulation system with uniform grid distribution can be written as

$$f_0^{(k)} = \frac{1}{h^k}(\sum_{j=0}^{\pm n} a_j f_j) + O[h^{m+1} f_0^{(k+m+1)}] \tag{B.19}$$

where h is the grid size and the accuracy of this scheme is on the order of h^m, where *m* is a function of *k* and *n* and will be determined later. For $x_j = x_0 + jh$, the Taylor's series expansion of $f_j = f(x_j)$ with respect to $x = x_0$ can be written as

$$f_j = f_0 + (jh)f_0' + \frac{(jh)^2}{2!} f_0'' + \frac{(jh)^3}{3!} f_0^{(3)} + ... \tag{B.20}$$

Substituting Eq. (B.20) into Eq. (B.19), it yields

$$\begin{aligned} f_0^{(k)} = \frac{1}{h^k}[&(a_0 + a_{\pm 1} + a_{\pm 2} + a_{\pm 3} + ... + a_{\pm n}) f_0 \\ &+ (a_{\pm 1} + 2a_{\pm 2} + 3a_{\pm 3} + ... + na_{\pm n}) f_0' \cdot (\pm h) \\ &+ (a_{\pm 1} + 2^2 a_{\pm 2} + 3^2 a_{\pm 3} + ... + n^2 a_{\pm n}) f_0'' \cdot \frac{(\pm h)^2}{2} \\ &+ ... \\ &+ (a_{\pm 1} + 2^k a_{\pm 2} + 3^k a_{\pm 3} + ... + n^k a_{\pm n}) f_0^{(k)} \cdot \frac{(\pm h)^k}{k!} \\ &+ ... \\ &+ (a_{\pm 1} + 2^n a_{\pm 2} + 3^n a_{\pm 3} + ... + n^n a_{\pm n}) f_0^{(n)} \cdot \frac{(\pm h)^n}{n!}] + O[\frac{n^{n+1}}{(n+1)!} h^{n+1-k} f_0^{(n+1)}] \end{aligned} \tag{B.21}$$

Since we have $n+1$ unknowns ($a_0 \sim a_{+n}$ for forward difference, or $a_{-n} \sim a_0$ for backward difference), we need $n+1$ equations. Comparing the coefficients of f_0, ..., $f_0^{(k)}$, ..., $f_0^{(n)}$ on two sides of Eq. (B.21), it yields $n+1$ equations. Thus, the last term in Eq. (B.21) is corresponding to the last term in Eq. (B.19). Namely, the finite difference expression of

$$f_0^{(k)} = \frac{1}{h^k}(\sum_{j=0}^{\pm n} a_j f_j)$$

will have a residue (or a discretization error) on the order of $O[h^{n+1-k} f_0^{(n+1)}]$. Thus, the order of accuracy of the expression of $f_0^{(k)}$ in Eq. (B.19) is $m = n - k$.

Comparing the coefficients on two sides of Eq. (B.21), it yields,

$$\begin{pmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ 1 & 2^n & 3^n & & & n^n \end{pmatrix} \begin{pmatrix} a_{\pm 1} \\ a_{\pm 2} \\ a_{\pm 3} \\ \vdots \\ \vdots \\ a_{\pm n} \end{pmatrix} = (\pm 1)^k \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k! \\ \vdots \\ 0 \end{pmatrix} \tag{B.22}$$

and

$$a_0 + a_{\pm 1} + a_{\pm 2} + a_{\pm 3} + \ldots + a_{\pm n} = 0 \tag{B.23}$$

Solving Eqs. (B.22) and (B.23), we can obtain the k th derivatives with m th-order accuracy, where $m = n - k$. The results of $a_0 \sim a_{\pm n}$ are listed in Tables B.2, B.3, and B.4, for $k = 1$, 2, and 3, respectively. Tables B.5 and B.6 show respectively the forward and backward finite differences of k th derivatives with m th-order accuracy, where $k \le 3$ and $m \le 8$.

Solving Eqs. (B.22) and (B.23)

Gauss elimination of Equation (B.22) yields

$$L\begin{pmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ 1 & 2^n & 3^n & & & n^n \end{pmatrix} RR^{-1} \begin{pmatrix} a_{\pm 1} \\ a_{\pm 2} \\ a_{\pm 3} \\ \vdots \\ \vdots \\ a_{\pm n} \end{pmatrix} = (\pm 1)^k (k!) L \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

where

$$L = L_{n-1}(L_{n-1}L_{n-2})\cdots(L_{n-1}\cdots L_1)$$

$$L_1 = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 1 & 0 & \cdots & \cdots & \vdots \\ \vdots & -1 & 1 & \ddots & \cdots & \vdots \\ \vdots & \vdots & -1 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}, \quad \cdots \quad L_{n-1} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \cdots & \cdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \ddots & 1 & \ddots & \vdots \\ \vdots & \vdots & \vdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}, \text{ and}$$

$$R^{-1} = \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & 2! & 0 & \cdots & \cdots & \vdots \\ \vdots & \ddots & 3! & \ddots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & n! \end{pmatrix}$$

It can be shown that

$$L\begin{pmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ 1 & 2^n & 3^n & & & n^n \end{pmatrix} R = \begin{pmatrix} 1 & 1 & \frac{1}{2} & \cdots & \frac{1}{(n-2)!} & \frac{1}{(n-1)!} \\ 0 & 1 & 1 & \ddots & \ddots & \frac{1}{(n-2)!} \\ \vdots & 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & \vdots & 0 & \ddots & \ddots & \frac{1}{2} \\ \vdots & \vdots & \vdots & \ddots & \ddots & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}$$

$$R^{-1}\begin{pmatrix} a_{\pm 1} \\ a_{\pm 2} \\ a_{\pm 3} \\ \vdots \\ \vdots \\ a_{\pm n} \end{pmatrix} = \begin{pmatrix} a_{\pm 1} \\ 2!a_{\pm 2} \\ 3!a_{\pm 3} \\ \vdots \\ \vdots \\ n!a_{\pm n} \end{pmatrix} \quad \text{and} \quad L\begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ Y_{out}(k) \\ -Y_{out}(k+1) \\ \vdots \\ (-1)^{n-k} Y_{out}(n) \end{pmatrix}$$

where $Y_{out}(k)$ can be obtained from the following Fortran program.

```
      PROGRAM BACKFD
      DIMENSION IY(10)
      N=10
!-------------------------
      DO II=1,N
!-------
      DO I=1,N
      IY(I)=0
      IF(I.EQ.II) IY(I)=1
      ENDDO
      WRITE(9,*) 'INPUT IY=', IY
```

```
!-------
      DO K=2,N
      DO J=K,N
      DO I=N,J,-1
      IY(I)=IY(I)+IY(I-1)
      ENDDO
      ENDDO
      ENDDO
      WRITE(9,*) 'OUTPUT IY=', IY
!-------
      ENDDO
!-------------------------
      STOP
      END
```

The results are

```
 INPUT IY= 1 0 0 0 0 0 0 0 0 0
 OUTPUT IY= 1 1 2 6 24 120 720 5040 40320 362880
 INPUT IY= 0 1 0 0 0 0 0 0 0 0
 OUTPUT IY= 0 1 3 11 50 274 1764 13068 109584 1026576
 INPUT IY= 0 0 1 0 0 0 0 0 0 0
 OUTPUT IY= 0 0 1 6 35 225 1624 13132 118124 1172700
 INPUT IY= 0 0 0 1 0 0 0 0 0 0
 OUTPUT IY= 0 0 0 1 10 85 735 6769 67284 723680
 INPUT IY= 0 0 0 0 1 0 0 0 0 0
 OUTPUT IY= 0 0 0 0 1 15 175 1960 22449 269325
 INPUT IY= 0 0 0 0 0 1 0 0 0 0
 OUTPUT IY= 0 0 0 0 0 1 21 322 4536 63273
 INPUT IY= 0 0 0 0 0 0 1 0 0 0
 OUTPUT IY= 0 0 0 0 0 0 1 28 546 9450
 INPUT IY= 0 0 0 0 0 0 0 1 0 0
 OUTPUT IY= 0 0 0 0 0 0 0 1 36 870
 INPUT IY= 0 0 0 0 0 0 0 0 1 0
 OUTPUT IY= 0 0 0 0 0 0 0 0 1 45
 INPUT IY= 0 0 0 0 0 0 0 0 0 1
 OUTPUT IY= 0 0 0 0 0 0 0 0 0 1
```

where

```
OUTPUT IY= 1 1 2 6 24 120 720 5040 40320 362880
         = 1 1 2! 3! 4! 5! 6! 7!    8!    9!
```

As an example, entering the following statements into Mathematica, one can easily obtain the coefficients of the backward difference of the 3rd derivatives with 6th-order accuracy.

```
a9=3!*(-118124)/9!
a8=(-9!*a9+3!*13132)/8!
a7=(-8!*a8-9!*a9/2!-3!*1624)/7!
a6=(-7!*a7-8!*a8/2!-9!*a9/3!+3!*225)/6!
a5=(-6!*a6-7!*a7/2!-8!*a8/3!-9!*a9/4!-3!*35)/5!
a4=(-5!*a5-6!*a6/2!-7!*a7/3!-8!*a8/4!-9!*a9/5!+3!*6)/4!
a3=(-4!*a4-5!*a5/2!-6!*a6/3!-7!*a7/4!-8!*a8/5!-9!*a9/6!-3!*1)/3!
a2=(-3!*a3-4!*a4/2!-5!*a5/3!-6!*a6/4!-7!*a7/5!-8!*a8/6!-9!*a9/7!)/2!
a1=(-2*a2-3*a3-4*a4-5*a5-6*a6-7*a7-8*a8-9*a9)
a0=(-a1-a2-a3-a4-a5-a6-a7-a8-a9)
a9 = -29531/15120
a8 =  5469/280
a7 = -12303/140
a6 =  84307/360
a5 = -3273/8
a4 =  19557/40
```

```
a3 = -72569/180
a2 =  62511/280
a1 = -42417/560
a0 =  4523/37
```

Likewise, entering the following statements into Mathematica, one can easily obtain the coefficients of the backward difference of the 2nd derivatives with 6th-order accuracy:

```
a10=0
a9=0
a8=(-9!*a9-10!*a10/2!+2!*13068)/8!
a7=(-8!*a8-9!*a9/2!-10!*a10/3!-2!*1764)/7!
a6=(-7!*a7-8!*a8/2!-9!*a9/3!-10!*a10/4!+2!*274)/6!
a5=(-6!*a6-7!*a7/2!-8!*a8/3!-9!*a9/4!-10!*a10/5!-2!*50)/5!
a4=(-5!*a5-6!*a6/2!-7!*a7/3!-8!*a8/4!-9!*a9/5!-10!*a10/6!+2!*11)/4!
a3=(-4!*a4-5!*a5/2!-6!*a6/3!-7!*a7/4!-8!*a8/5!-9!*a9/6!-10!*a10/7!-2!*3)/3!
a2=(-3!*a3-4!*a4/2!-5!*a5/3!-6!*a6/4!-7!*a7/5!-8!*a8/6!-9!*a9/7!-10!*a10/8!
    +2!*1)/2!
a1=(-2*a2-3*a3-4*a4-5*a5-6*a6-7*a7-8*a8-9*a9-10*a10)
a0=(-a1-a2-a3-a4-a5-a6-a7-a8-a9-a10)
```

or the coefficients of the backward difference of the 2nd derivatives with 8th-order accuracy:

```
a10=2!*1026576/10!
a9=(-10!*a10-2!*109584)/9!
a8=(-9!*a9-10!*a10/2!+2!*13068)/8!
a7=(-8!*a8-9!*a9/2!-10!*a10/3!-2!*1764)/7!
a6=(-7!*a7-8!*a8/2!-9!*a9/3!-10!*a10/4!+2!*274)/6!
a5=(-6!*a6-7!*a7/2!-8!*a8/3!-9!*a9/4!-10!*a10/5!-2!*50)/5!
a4=(-5!*a5-6!*a6/2!-7!*a7/3!-8!*a8/4!-9!*a9/5!-10!*a10/6!+2!*11)/4!
a3=(-4!*a4-5!*a5/2!-6!*a6/3!-7!*a7/4!-8!*a8/5!-9!*a9/6!-10!*a10/7!-2!*3)/3!
a2=(-3!*a3-4!*a4/2!-5!*a5/3!-6!*a6/4!-7!*a7/5!-8!*a8/6!-9!*a9/7!-10!*a10/8!
    +2!*1)/2!
a1=(-2*a2-3*a3-4*a4-5*a5-6*a6-7*a7-8*a8-9*a9-10*a10)
a0=(-a1-a2-a3-a4-a5-a6-a7-a8-a9-a10)
```

B.5. Benchmarks

In this section, we use $f(x)=\sin(2\pi\, x/\lambda)$ as an example to study the differences between the numerical solutions and the analytic solutions of the derivatives of $f(x)$, where λ is the wavelength.

Figure B.1 shows log-log plots of the maximum absolute errors (the thick curves with marks) in the numerical derivatives of $f(x)=\sin(2\pi\, x/\lambda)$, as a function of grid size normalized by the wavelength, for *m* = 1, 3, 5, and *k* = 1, 2, 3, where *m* and *k* denote that we use the *m*-th order central-finite-difference scheme to evaluate the *k*-th order derivative numerically. The discretization errors are estimated and plotted in the thin lines with similar colors as the corresponding numerical errors, where the discretization errors are obtained from the residues given in equations (B.11) and (B.14). The round-off errors are estimated based on the double-precision calculation and plotted in the purple thin line for reference.

The accuracy of central-finite-difference scheme is much higher than the accuracy of forward-finite-difference (or backward-finite-difference) scheme, which is mainly due to the differences in the coefficient of $h^{m+1}f_0^{(m+k+1)}$ in the residues given in Eqs. (B.11), (B.14), and (B.21). Namely, for even number *k*, we can rewrite the residue shown in Eq. (B.11) to the following from (for $i=0$)

$$O[\frac{n^{2n+2}}{(2n+2)!}h^{2n+2-k}f_0^{(2n+2)}]=O[\frac{[(m+k-1)/2]^{(m+k+1)}}{(m+k+1)!}h^{m+1}f_0^{(m+k+1)}] \tag{B.24}$$

Whereas, for odd number *k*, we can rewrite the residue shown in Eq. (B.14) to the following from (for $i=0$)

$$O[\frac{n^{2n+1}}{(2n+1)!}h^{2n+1-k}f_0^{(2n+1)}]=O[\frac{[(m+k)/2]^{m+k+1}}{(m+k+1)!}h^{m+1}f_0^{(m+k+1)}] \tag{B.25}$$

Likewise, we can rewrite the residue shown in Eq. (B.21) to the following from

$$O[\frac{n^{n+1}}{(n+1)!}h^{n+1-k}f_0^{(n+1)}]=O[\frac{(m+k)^{m+k+1}}{(m+k+1)!}h^{m+1}f_0^{(m+k+1)}] \tag{B.26}$$

Thus, for a given set of *m* and *k*, the coefficient in Eq. (B.26) is always greater than the coefficients shown in Eqs. (B.24) and (B.25) by a factor about 2^{m+k+1}.

Figure B.2 shows plots of coefficients of $h^{m+1}f_0^{(m+k+1)}$ in Eqs. (B.24), (B.25), (B.26), and the estimated ratio of the discretization errors in different schemes as a function of *m*+*k*, where CFD denotes central-finite-difference scheme, FFD denotes forward-finite-difference scheme, *m* denotes *m*-th order finite-difference scheme, and *k* denotes the *k*-th order derivatives. We can see that, even for small m+k (m+k < 10), the discretization errors in the forward-finite-difference scheme can be 10 to 1000 (2^3 to 2^{10}) times higher than the corresponding errors obtained in central-finite-difference scheme.

Figure B.3 shows log-log plots of the maximum absolute errors (the thick curves) in the numerical derivatives of $f(x) = \sin(2\pi\, x / \lambda)$, as a function of grid size normalized by wavelength, for m = 2, 3, 4, 5, 6, 7 and k = 1, 2, 3, where m and k denote the m-th order forward-finite-difference scheme and the k-th order derivative. The purple thin line denotes the estimated round-off errors.

According to Figures B.1 and B.3 the best choice of grid size is about 1% of the dominated wavelength or the characteristic length in the system. In addition to the periodic boundary condition, uniform boundary condition, we can also construct a radiation boundary condition by replacing the central-finite-difference scheme by a higher-order forward- and backward-finite-difference scheme when we evaluate respectively the derivatives near the left and right boundaries.

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Table B.1. Summary of Central-Finite-Difference Expressions of $f_0^{(k)}$ with Equal Spacing Grid Distribution (Keller and Pereyra, 1978; Fornberg, 1988; 1996)

$f_0^{(k)} = \frac{1}{h^k}[\sum_{l=1}^{+n}(a_{-l}f_{-l} + a_l f_l) + a_0 f_0] + O[h^{m+1} f_0^{(m+k+1)}]$ $f_0^{(k)} = \frac{1}{h^k}[\sum_{l=1}^{+n}(a_{-l}f_{-l} + a_l f_l) + a_0 f_0] + O[h^{2n+2-k} f_0^{(2n+2)}]$		m is an odd number $k + m = 2n + 1$
For an even number k	$\begin{pmatrix} 1 & 2^2 & 3^2 & \cdots & \cdots & n^2 \\ 1 & 2^4 & 3^4 & \cdots & \cdots & n^4 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!/2 \\ 0 \\ \vdots \end{pmatrix}$	$a_{-l} = a_{+l}$ $a_0 = -2\sum_{l=1}^{n} a_l$
$f_0^{(k)} = \frac{1}{h^k}\sum_{l=1}^{+n}(a_{-l}f_{-l} + a_l f_l) + O[h^{m+1} f_0^{(m+k+1)}]$ $f_0^{(k)} = \frac{1}{h^k}\sum_{l=1}^{+n}(a_{-l}f_{-l} + a_l f_l) + O[h^{2n+1-k} f_0^{(2n+1)}]$		m is an odd number $k + m = 2n$
For an odd number k	$\begin{pmatrix} 1 & 2^1 & 3^1 & \cdots & \cdots & n^1 \\ 1 & 2^3 & 3^3 & \cdots & \cdots & n^3 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 2^k & 3^k & \cdots & \cdots & n^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!/2 \\ 0 \\ \vdots \end{pmatrix}$	$a_{-l} = -a_{+l}$ $a_0 = 0$

$f_0^{(k)} = \frac{1}{h^k}\sum_{l=1}^{+n}[a_{-(l-0.5)}f_{-(l-0.5)} + a_{l-0.5}f_{l-0.5}] + O[h^{2n+1-k} f_0^{(2n+1)}]$		
For an odd number k	$\begin{pmatrix} 1 & 3^1 & 5^1 & \cdots & \cdots & (2n-1)^1 \\ 1 & 3^3 & 5^3 & \cdots & \cdots & (2n-1)^3 \\ \vdots & & & \cdots & \cdots & \vdots \\ 1 & 3^k & 5^k & \cdots & \cdots & (2n-1)^k \\ \vdots & & & & & \vdots \\ \vdots & \vdots & & & & (2n-1)^{2n-1} \end{pmatrix} \begin{pmatrix} a_{0.5} \\ a_{1.5} \\ a_{2.5} \\ \vdots \\ \vdots \\ a_{n-0.5} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ k!2^{k-1} \\ 0 \\ \vdots \end{pmatrix}$	$a_{-(l-0.5)} = -a_{(l-0.5)}$

First-Order Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{1}{2}f_{-1} + \frac{1}{2}f_{+1}) + O(h^2 f_0^{(3)})$ $f_0^{(1)} = \frac{1}{h}(-f_{-0.5} + f_{+0.5}) + O(h^2 f_0^{(3)})$
$f_0^{(2)} = \frac{1}{h^2}(f_{-1} - 2f_0 + f_{+1}) + O(h^2 f_0^{(4)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{1}{2}f_{-2} + f_{-1} - f_{+1} + \frac{1}{2}f_{+2}) + O(h^2 f_0^{(5)})$
$f_0^{(4)} = \frac{1}{h^4}(+f_{-2} - 4f_{-1} + 6f_0 - 4f_{+1} + f_{+2}) + O(h^2 f_0^{(6)})$
$f_0^{(5)} = \frac{1}{h^5}(-\frac{1}{2}f_{-3} + 2f_{-2} - \frac{5}{2}f_{-1} + \frac{5}{2}f_{+1} - 2f_{+2} + \frac{1}{2}f_{+3}) + O(h^2 f_0^{(7)})$
$f_0^{(6)} = \frac{1}{h^6}(+f_{-3} - 6f_{-2} + 15f_{-1} - 20f_0 + 15f_{+1} - 6f_{+2} + f_{+3}) + O(h^2 f_0^{(8)})$
$f_0^{(7)} = \frac{1}{h^7}(-\frac{1}{2}f_{-4} + 3f_{-3} - 7f_{-2} + 7f_{-1} - 7f_{+1} + 7f_{+2} - 3f_{+3} + \frac{1}{2}f_{+4})$ $+ O(h^2 f_0^{(9)})$
$f_0^{(8)} = \frac{1}{h^8}(+f_{-4} - 8f_{-3} + 28f_{-2} - 56f_{-1} + 70f_0$ $- 56f_{+1} + 28f_{+2} - 8f_{+3} + f_{+4}) + O(h^2 f_0^{(10)})$
$f_0^{(9)} = \frac{1}{h^9}(-\frac{1}{2}f_{-5} + 4f_{-4} - \frac{27}{2}f_{-3} + 24f_{-2} - 21f_{-1}$ $+ 21f_{+1} - 24f_{+2} + \frac{27}{2}f_{+3} - 4f_{+4} + \frac{1}{2}f_{+5}) + O(h^2 f_0^{(11)})$
$f_0^{(10)} = \frac{1}{h^{10}}(+f_{-5} - 10f_{-4} + 45f_{-3} - 120f_{-2} + 210f_{-1} - 252f_0$ $+ 210f_{+1} - 120f_{+2} + 45f_{+3} - 10f_{+4} + f_{+5}) + O(h^2 f_0^{(12)})$

Third-Order Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{1}{12}f_{-2} - \frac{2}{3}f_{-1} + \frac{2}{3}f_{+1} - \frac{1}{12}f_{+2}) + O(h^4 f_0^{(5)})$ $f_0^{(1)} = \frac{1}{h}(+\frac{1}{24}f_{-1.5} - \frac{9}{8}f_{-0.5} + \frac{9}{8}f_{+0.5} - \frac{1}{24}f_{+1.5}) + O(h^4 f_0^{(5)})$
$f_0^{(2)} = \frac{1}{h^2}(-\frac{1}{12}f_{-2} + \frac{4}{3}f_{-1} - \frac{5}{2}f_0 + \frac{4}{3}f_{+1} - \frac{1}{12}f_{+2}) + O(h^4 f_0^{(6)})$
$f_0^{(3)} = \frac{1}{h^3}(+\frac{1}{8}f_{-3} - f_{-2} + \frac{13}{8}f_{-1} - \frac{13}{8}f_{+1} + f_{+2} - \frac{1}{8}f_{+3}) + O(h^4 f_0^{(7)})$
$f_0^{(4)} = \frac{1}{h^4}(-\frac{1}{6}f_{-3} + 2f_{-2} - \frac{13}{2}f_{-1} + \frac{28}{3}f_0 - \frac{13}{2}f_{+1} + 2f_{+2} - \frac{1}{6}f_{+3})$ $+O(h^4 f_0^{(8)})$
$f_0^{(5)} = \frac{1}{h^5}(+\frac{1}{6}f_{-4} - \frac{3}{2}f_{-3} + \frac{13}{3}f_{-2} - \frac{29}{6}f_{-1} + \frac{29}{6}f_{+1} - \frac{13}{3}f_{+2} + \frac{3}{2}f_{+3} - \frac{1}{6}f_{+4})$ $+O(h^4 f_0^{(9)})$
$f_0^{(6)} = \frac{1}{h^6}(-\frac{1}{4}f_{-4} + 3f_{-3} - 13f_{-2} + 29f_{-1} - \frac{75}{2}f_0 + 29f_{+1} - 13f_{+2} + 3f_{+3} - \frac{1}{4}f_{+4})$ $+O(h^4 f_0^{(10)})$
$f_0^{(7)} = \frac{1}{h^7}(+\frac{5}{24}f_{-5} - \frac{13}{6}f_{-4} + \frac{69}{8}f_{-3} - 17f_{-2} + \frac{63}{4}f_{-1}$ $-\frac{63}{4}f_{+1} + 17f_{+2} - \frac{69}{8}f_{+3} + \frac{13}{6}f_{+4} - \frac{5}{24}f_{+5}) + O(h^4 f_0^{(11)})$
$f_0^{(8)} = \frac{1}{h^8}(-\frac{1}{3}f_{-5} + \frac{13}{3}f_{-4} - 23f_{-3} + 68f_{-2} - 126f_{-1} + 154f_0$ $-126f_{+1} + 68f_{+2} - 23f_{+3} + \frac{13}{3}f_{+4} - \frac{1}{3}f_{+5}) + O(h^4 f_0^{(12)})$
$f_0^{(9)} = \frac{1}{h^9}(+\frac{1}{4}f_{-6} - 3f_{-5} + 15f_{-4} - 41f_{-3} + \frac{261}{4}f_{-2} - 54f_{-1}$ $+54f_{+1} - \frac{261}{4}f_{+2} + 41f_{+3} - 15f_{+4} + 3f_{+5} - \frac{1}{4}f_{+6}) + O(h^4 f_0^{(13)})$
$f_0^{(10)} = \frac{1}{h^{10}}(-\frac{5}{12}f_{-6} + 6f_{-5} - \frac{75}{2}f_{-4} + \frac{410}{3}f_{-3} - \frac{1305}{4}f_{-2} + 540f_{-1} - 637f_0$ $+540f_{+1} - \frac{1305}{4}f_{+2} + \frac{410}{3}f_{+3} - \frac{75}{2}f_{+4} + 6f_{+5} - \frac{5}{12}f_{+6}) + O(h^4 f_0^{(14)})$

Fifth-Order Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{1}{60}f_{-3} + \frac{3}{20}f_{-2} - \frac{3}{4}f_{-1} + \frac{3}{4}f_{+1} - \frac{3}{20}f_{+2} + \frac{1}{60}f_{+3}) + O(h^6 f_0^{(7)})$ $f_0^{(1)} = \frac{1}{h}[\frac{75}{64}(f_{+0.5} - f_{-0.5}) - \frac{25}{64 \cdot 6}(f_{+1.5} - f_{-1.5}) + \frac{3}{64 \cdot 10}(f_{+2.5} - f_{-2.5})] + O(h^6 f_0^{(7)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{1}{90}f_{-3} - \frac{3}{20}f_{-2} + \frac{3}{2}f_{-1} - \frac{49}{18}f_0 + \frac{3}{2}f_{+1} - \frac{3}{20}f_{+2} + \frac{1}{90}f_{+3})$ $+ O(h^6 f_0^{(8)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{7}{240}f_{-4} + \frac{3}{10}f_{-3} - \frac{169}{120}f_{-2} + \frac{61}{30}f_{-1}$ $- \frac{61}{30}f_{+1} + \frac{169}{120}f_{+2} - \frac{3}{10}f_{+3} + \frac{7}{240}f_{+4}) + O(h^6 f_0^{(9)})$
$f_0^{(4)} = \frac{1}{h^4}(+\frac{7}{240}f_{-4} - \frac{2}{5}f_{-3} + \frac{169}{60}f_{-2} - \frac{122}{15}f_{-1} + \frac{91}{8}f_0$ $- \frac{122}{15}f_{+1} + \frac{169}{60}f_{+2} - \frac{2}{5}f_{+3} + \frac{7}{240}f_{+4}) + O(h^6 f_0^{(10)})$
$f_0^{(5)} = \frac{1}{h^5}(-\frac{13}{288}f_{-5} + \frac{19}{36}f_{-4} - \frac{87}{32}f_{-3} + \frac{13}{2}f_{-2} - \frac{323}{48}f_{-1}$ $+ \frac{323}{48}f_{+1} - \frac{13}{2}f_{+2} + \frac{87}{32}f_{+3} - \frac{19}{36}f_{+4} + \frac{13}{288}f_{+5}) + O(h^6 f_0^{(11)})$
$f_0^{(6)} = \frac{1}{h^6}(+\frac{13}{240}f_{-5} - \frac{19}{24}f_{-4} + \frac{87}{16}f_{-3} - \frac{39}{2}f_{-2} + \frac{323}{8}f_{-1} - \frac{1023}{20}f_0$ $+ \frac{323}{8}f_{+1} - \frac{39}{2}f_{+2} + \frac{87}{16}f_{+3} - \frac{19}{24}f_{+4} + \frac{13}{240}f_{+5}) + O(h^6 f_0^{(12)})$
$f_0^{(7)} = \frac{1}{h^7}(-\frac{31}{480}f_{-6} + \frac{41}{48}f_{-5} - \frac{601}{120}f_{-4} + \frac{755}{48}f_{-3} - \frac{885}{32}f_{-2} + \frac{971}{40}f_{-1}$ $- \frac{971}{40}f_{+1} + \frac{885}{32}f_{+2} - \frac{755}{48}f_{+3} + \frac{601}{120}f_{+4} - \frac{41}{48}f_{+5} + \frac{31}{480}f_{+6})$ $+ O(h^6 f_0^{(13)})$
$f_0^{(8)} = \frac{1}{h^8}(+\frac{31}{360}f_{-6} - \frac{41}{30}f_{-5} + \frac{601}{60}f_{-4} - \frac{755}{18}f_{-3} + \frac{885}{8}f_{-2} - \frac{971}{5}f_{-1} + \frac{7007}{30}f_0$ $- \frac{971}{5}f_{+1} + \frac{885}{8}f_{+2} - \frac{755}{18}f_{+3} + \frac{601}{60}f_{+4} - \frac{41}{30}f_{+5} + \frac{31}{360}f_{+6})$ $+ O(h^6 f_0^{(14)})$

$$f_0^{(9)} = \frac{1}{h^9}\left(-\frac{7}{80}f_{-7} + \frac{13}{10}f_{-6} - \frac{139}{16}f_{-5} + \frac{166}{5}f_{-4} - \frac{6283}{80}f_{-3}\right.$$
$$+\frac{1153}{10}f_{-2} - \frac{7323}{80}f_{-1} + \frac{7323}{80}f_{+1} - \frac{1153}{10}f_{+2}$$
$$\left.+\frac{6283}{80}f_{+3} - \frac{166}{5}f_{+4} + \frac{139}{16}f_{+5} - \frac{13}{10}f_{+6} + \frac{7}{80}f_{+7}\right) + O(h^6 f_0^{(15)})$$

$$f_0^{(10)} = \frac{1}{h^{10}}\left(+\frac{1}{8}f_{-7} - \frac{13}{6}f_{-6} + \frac{139}{8}f_{-5} - 83f_{-4} + \frac{6283}{24}f_{-3}\right.$$
$$-\frac{1153}{2}f_{-2} + \frac{7323}{80}f_{-1} - 1066f_0 + \frac{7323}{80}f_{+1} - \frac{1153}{2}f_{+2}$$
$$\left.+\frac{6283}{24}f_{+3} - 83f_{+4} + \frac{139}{8}f_{+5} - \frac{13}{6}f_{+6} + \frac{1}{8}f_{+7}\right) + O(h^6 f_0^{(16)})$$

Seventh-Order Finite Differences
$f_0^{(1)}=\frac{1}{h}(+\frac{1}{280}f_{-4}-\frac{4}{105}f_{-3}+\frac{1}{5}f_{-2}-\frac{4}{5}f_{-1}+\frac{4}{5}f_{+1}-\frac{1}{5}f_{+2}+\frac{4}{105}f_{+3}-\frac{1}{280}f_{+4}) +O(h^8 f_0^{(9)})$
$f_0^{(2)}=\frac{1}{h^2}(-\frac{1}{560}f_{-4}+\frac{8}{315}f_{-3}-\frac{1}{5}f_{-2}+\frac{8}{5}f_{-1}-\frac{205}{72}f_0 +\frac{8}{5}f_{+1}-\frac{1}{5}f_{+2}+\frac{8}{315}f_{+3}-\frac{1}{560}f_{+4})+O(h^8 f_0^{(10)})$
$f_0^{(3)}=\frac{1}{h^3}(+\frac{41}{6048}f_{-5}-\frac{1261}{15120}f_{-4}+\frac{541}{1120}f_{-3}-\frac{4369}{2520}f_{-2}+\frac{1669}{720}f_{-1} -\frac{1669}{720}f_{+1}+\frac{4369}{2520}f_{+2}-\frac{541}{1120}f_{+3}+\frac{1261}{15120}f_{+4}-\frac{41}{6048}f_{+5})+O(h^8 f_0^{(11)})$
$f_0^{(4)}=\frac{1}{h^4}(-\frac{41}{7560}f_{-5}+\frac{1261}{15120}f_{-4}-\frac{541}{840}f_{-3}+\frac{4369}{1260}f_{-2}-\frac{1669}{180}f_{-1}+\frac{1529}{120}f_0 -\frac{1669}{180}f_{+1}+\frac{4369}{1260}f_{+2}-\frac{541}{840}f_{+3}+\frac{1261}{15120}f_{+4}-\frac{41}{7560}f_{+5})+O(h^8 f_0^{(12)})$
$f_0^{(5)}=\frac{1}{h^5}(+\frac{139}{12096}f_{-6}-\frac{121}{756}f_{-5}+\frac{3125}{3024}f_{-4}-\frac{3011}{756}f_{-3} +\frac{33853}{4032}f_{-2}-\frac{1039}{126}f_{-1}+\frac{1039}{126}f_{+1}-\frac{33853}{4032}f_{+2} +\frac{3011}{756}f_{+3}-\frac{3125}{3024}f_{+4}+\frac{121}{756}f_{+5}-\frac{139}{12096}f_{+6})+O(h^8 f_0^{(13)})$
$f_0^{(6)}=\frac{1}{h^6}(-\frac{139}{12096}f_{-6}+\frac{121}{630}f_{-5}-\frac{3125}{2016}f_{-4}+\frac{3011}{378}f_{-3} -\frac{33853}{1344}f_{-2}+\frac{1039}{21}f_{-1}-\frac{44473}{720}f_0+\frac{1039}{21}f_{+1}-\frac{33853}{1344}f_{+2} +\frac{3011}{378}f_{+3}-\frac{3125}{2016}f_{+4}+\frac{121}{630}f_{+5}-\frac{139}{12096}f_{+6})+O(h^8 f_0^{(14)})$
$f_0^{(7)}=\frac{1}{h^7}(+\frac{311}{17280}f_{-7}-\frac{101}{360}f_{-6}+\frac{6995}{3456}f_{-5}-\frac{2363}{270}f_{-4}+\frac{135075}{5760}f_{-3} -\frac{40987}{1080}f_{-2}+\frac{184297}{5760}f_{-1}-\frac{184297}{5760}f_{+1}+\frac{40987}{1080}f_{+2} -\frac{135075}{5760}f_{+3}+\frac{2363}{270}f_{+4}-\frac{6995}{3456}f_{+5}+\frac{101}{360}f_{+6}-\frac{311}{17280}f_{+7}) +O(h^8 f_0^{(15)})$

$$f_0^{(8)} = \frac{1}{h^8}(-\frac{311}{15120}f_{-7} + \frac{101}{270}f_{-6} - \frac{1399}{432}f_{-5} + \frac{2363}{135}f_{-4} - \frac{135075}{2160}f_{-3} + \frac{40987}{270}f_{-2} - \frac{184297}{720}f_{-1} + \frac{19162}{63}f_0 - \frac{184297}{720}f_{+1} + \frac{40987}{270}f_{+2} - \frac{135075}{2160}f_{+3} + \frac{2363}{135}f_{+4} - \frac{1399}{432}f_{+5} + \frac{101}{270}f_{+6} - \frac{311}{15120}f_{+7}) + O(h^8 f_0^{(16)})$$

$$f_0^{(9)} = \frac{1}{h^9}(+\frac{67}{2520}f_{-8} - \frac{331}{720}f_{-7} + \frac{517}{140}f_{-6} - \frac{2591}{144}f_{-5} + \frac{10331}{180}f_{-4} - \frac{9767}{80}f_{-3} + \frac{6067}{36}f_{-2} - \frac{652969}{5040}f_{-1} + \frac{652969}{5040}f_{+1} - \frac{6067}{36}f_{+2} + \frac{9767}{80}f_{+3} - \frac{10331}{180}f_{+4} + \frac{2591}{144}f_{+5} - \frac{517}{140}f_{+6} + \frac{331}{720}f_{+7} - \frac{67}{2520}f_{+8}) + O(h^8 f_0^{(17)})$$

$$f_0^{(10)} = \frac{1}{h^{10}}(-\frac{67}{2520}f_{-8} + \frac{331}{504}f_{-7} - \frac{517}{84}f_{-6} + \frac{2591}{72}f_{-5} - \frac{10331}{72}f_{-4} + \frac{9767}{24}f_{-3} - \frac{30335}{36}f_{-2} + \frac{652969}{504}f_{-1} - \frac{167297}{112}f_0 + \frac{652969}{504}f_{+1} - \frac{30335}{36}f_{+2} + \frac{9767}{24}f_{+3} - \frac{10331}{72}f_{+4} + \frac{2591}{72}f_{+5} - \frac{517}{84}f_{+6} + \frac{331}{504}f_{+7} - \frac{67}{2520}f_{+8}) + O(h^8 f_0^{(18)})$$

Ninth-Order Finite Differences
$f_0^{(1)}=\frac{1}{h}(-\frac{1}{1260}f_{-5}+\frac{5}{504}f_{-4}-\frac{5}{84}f_{-3}+\frac{5}{21}f_{-2}-\frac{5}{6}f_{-1}$ $+\frac{5}{6}f_{+1}-\frac{5}{21}f_{+2}+\frac{5}{84}f_{+3}-\frac{5}{504}f_{+4}+\frac{1}{1260}f_{+5})+O(h^{10}f_0^{(11)})$
$f_0^{(2)}=\frac{1}{h^2}(+\frac{1}{3150}f_{-5}-\frac{5}{1008}f_{-4}+\frac{5}{126}f_{-3}-\frac{5}{21}f_{-2}+\frac{5}{3}f_{-1}-\frac{5269}{1800}f_0$ $+\frac{5}{3}f_{+1}-\frac{5}{21}f_{+2}+\frac{5}{126}f_{+3}-\frac{5}{1008}f_{+4}+\frac{1}{3150}f_{+5})+O(h^{10}f_0^{(12)})$
$f_0^{(3)}=\frac{1}{h^3}(-\frac{479}{302400}f_{-6}+\frac{19}{840}f_{-5}-\frac{643}{4200}f_{-4}+\frac{4969}{7560}f_{-3}-\frac{4469}{2240}f_{-2}+\frac{1769}{700}f_{-1}$ $-\frac{1769}{700}f_{+1}+\frac{4469}{2240}f_{+2}-\frac{4969}{7560}f_{+3}+\frac{643}{4200}f_{+4}-\frac{19}{840}f_{+5}+\frac{479}{302400}f_{+6})$ $+O(h^{10}f_0^{(13)})$
$f_0^{(4)}=\frac{1}{h^4}(+\frac{479}{453600}f_{-6}-\frac{19}{1050}f_{-5}+\frac{643}{4200}f_{-4}-\frac{4969}{5670}f_{-3}$ $+\frac{4469}{1120}f_{-2}-\frac{1769}{175}f_{-1}+\frac{37037}{2700}f_0-\frac{1769}{175}f_{+1}+\frac{4469}{1120}f_{+2}$ $-\frac{4969}{5670}f_{+3}+\frac{643}{4200}f_{+4}-\frac{19}{1050}f_{+5}+\frac{479}{453600}f_{+6})+O(h^{10}f_0^{(14)})$
$f_0^{(5)}=\frac{1}{h^5}(-\frac{37}{12960}f_{-7}+\frac{2767}{60480}f_{-6}-\frac{6271}{18144}f_{-5}+\frac{73811}{45360}f_{-4}-\frac{157477}{30240}f_{-3}$ $+\frac{1819681}{181440}f_{-2}-\frac{286397}{30240}f_{-1}+\frac{286397}{30240}f_{+1}-\frac{1819681}{181440}f_{+2}$ $+\frac{157477}{30240}f_{+3}-\frac{73811}{45360}f_{+4}+\frac{6271}{18144}f_{+5}-\frac{2767}{60480}f_{+6}+\frac{37}{12960}f_{+7})$ $+O(h^{10}f_0^{(15)})$
$f_0^{(6)}=\frac{1}{h^6}(+\frac{37}{15120}f_{-7}-\frac{2767}{60480}f_{-6}+\frac{6271}{15120}f_{-5}-\frac{73811}{30240}f_{-4}+\frac{157477}{15120}f_{-3}$ $-\frac{1819681}{60480}f_{-2}+\frac{286397}{5040}f_{-1}-\frac{353639}{5040}f_0+\frac{286397}{5040}f_{+1}-\frac{1819681}{60480}f_{+2}$ $+\frac{157477}{15120}f_{+3}-\frac{73811}{30240}f_{+4}+\frac{6271}{15120}f_{+5}-\frac{2767}{60480}f_{+6}+\frac{37}{15120}f_{+7})$ $+O(h^{10}f_0^{(16)})$

$$f_0^{(7)} = \frac{1}{h^7}(-\frac{2473}{518400}f_{-8} + \frac{2747}{32400}f_{-7} - \frac{1363}{1920}f_{-6}$$
$$+\frac{4787}{1296}f_{-5} - \frac{678739}{51840}f_{-4} + \frac{37517}{1200}f_{-3} - \frac{12312353}{259200}f_{-2}$$
$$+\frac{251539}{64080}f_{-1} - \frac{251539}{64080}f_{+1}$$
$$+\frac{12312353}{259200}f_{+2} - \frac{37517}{1200}f_{+3} + \frac{678739}{51840}f_{+4} - \frac{4787}{1296}f_{+5}$$
$$+\frac{1363}{1920}f_{+6} - \frac{2747}{32400}f_{+7} + \frac{2473}{518400}f_{+8}) + O(h^{10}f_0^{(17)})$$

$$f_0^{(8)} = \frac{1}{h^8}(+\frac{2473}{518400}f_{-8} - \frac{2747}{28350}f_{-7} + \frac{1363}{1440}f_{-6}$$
$$-\frac{4787}{810}f_{-5} + \frac{678739}{25920}f_{-4} - \frac{37517}{450}f_{-3} + \frac{12312353}{64800}f_{-2}$$
$$-\frac{251539}{810}f_{-1} + \frac{4913051}{13440}f_0 - \frac{251539}{810}f_{+1}$$
$$+\frac{12312353}{64800}f_{+2} - \frac{37517}{450}f_{+3} + \frac{678739}{25920}f_{+4} - \frac{4787}{810}f_{+5}$$
$$+\frac{1363}{1440}f_{+6} - \frac{2747}{28350}f_{+7} + \frac{2473}{518400}f_{+8}) + O(h^{10}f_0^{(18)})$$

$$f_0^{(9)} = \frac{1}{h^9}(-\frac{2021}{268800}f_{-9} + \frac{7403}{50400}f_{-8} - \frac{156031}{115200}f_{-7}$$
$$+\frac{65377}{8400}f_{-6} - \frac{248167}{8064}f_{-5} + \frac{309691}{3600}f_{-4} - \frac{1618681}{9600}f_{-3}$$
$$+\frac{5586823}{25200}f_{-2} - \frac{66976673}{403200}f_{-1} + \frac{66976673}{403200}f_{+1} - \frac{5586823}{25200}f_{+2}$$
$$+\frac{1618681}{9600}f_{+3} - \frac{309691}{3600}f_{+4} + \frac{248167}{8064}f_{+5} - \frac{65377}{8400}f_{+6}$$
$$+\frac{156031}{115200}f_{+7} - \frac{7403}{50400}f_{+8} + \frac{2021}{268800}f_{+9}) + O(h^{10}f_0^{(19)})$$

$$
\begin{aligned}
f_0^{(10)} = \frac{1}{h^{10}}(&+\frac{2021}{241920}f_{-9} - \frac{7403}{40320}f_{-8} + \frac{156031}{80640}f_{-7} \\
&- \frac{65377}{5040}f_{-6} + \frac{248167}{4032}f_{-5} - \frac{309691}{1400}f_{-4} + \frac{1618681}{2880}f_{-3} \\
-\frac{5586823}{5040}f_{-2} &+ \frac{66976673}{40320}f_{-1} - \frac{22981127}{12096}f_{0} + \frac{66976673}{40320}f_{+1} - \frac{5586823}{5040}f_{+2} \\
&+ \frac{1618681}{2880}f_{+3} - \frac{309691}{1400}f_{+4} + \frac{248167}{4032}f_{+5} - \frac{65377}{5040}f_{+6} \\
&+ \frac{156031}{80640}f_{+7} - \frac{7403}{40320}f_{+8} + \frac{2021}{241920}f_{+9}) + O(h^{10} f_0^{(10)})
\end{aligned}
$$

References of Table B.1

http://www-solar.mcs.st-and.ac.uk/~mhd_hpc/talks/high-order.pdf

Fornberg, B. (1996), ‘A practical guide to pseudospectral methods’, Cambridge University Press.

Fornberg, B. (1988), Generation of finite differences formulas on arbitrary spaced grids, *Mathematics of Computation, 51,* 699-706

Keller, H. B., and V. Pereyra (1978), Symbolic generation of finite differences formulas, *Mathematics of Computation, 32,* 955-971

Table B.2. Coefficients of $f_0^{(1)}$ in the Forward and Backward Finite Difference

<table>
<tr><td>m-th order forward FD</td><td>$-a_0$</td><td>$+a_{+1}$</td><td>$-a_{+2}$</td><td>$+a_{+3}$</td><td>$-a_{+4}$</td><td>$+a_{+5}$</td><td>$-a_{+6}$</td><td>$+a_{+7}$</td><td>$-a_{+8}$</td><td>$+a_{+9}$</td><td>$-a_{+10}$</td></tr>
<tr><td>m-th order backward FD</td><td>$+a_0$</td><td>$-a_{-1}$</td><td>$+a_{-2}$</td><td>$-a_{-3}$</td><td>$+a_{-4}$</td><td>$-a_{-5}$</td><td>$+a_{-6}$</td><td>$-a_{-7}$</td><td>$+a_{-8}$</td><td>$-a_{-9}$</td><td>$+a_{-10}$</td></tr>
<tr><td>1st</td><td>3/
2</td><td>2</td><td>1
/2</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>2nd</td><td>11/
6</td><td>3</td><td>3
/2</td><td>1
/3</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>3rd</td><td>25/
12</td><td>4</td><td>6
/2 |3</td><td>4
/3</td><td>1
/4</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>4th</td><td>137/
60</td><td>5</td><td>10
/2 |5</td><td>10
/3</td><td>5
/4</td><td>1
/5</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>5th</td><td>49/
20</td><td>6</td><td>15
/2</td><td>20
/3</td><td>15
/4</td><td>6
/5</td><td>1
/6</td><td></td><td></td><td></td><td></td></tr>
<tr><td>6th</td><td>363/
140</td><td>7</td><td>21
/2</td><td>35
/3</td><td>35
/4</td><td>21
/5</td><td>7
/6</td><td>1
/7</td><td></td><td></td><td></td></tr>
<tr><td>7th</td><td>761/
280</td><td>8</td><td>28
/2 |14</td><td>56
/3</td><td>70 |35
/4 |/2</td><td>56
/5</td><td>28|14
/6 |/3</td><td>8
/7</td><td>1
/8</td><td></td><td></td></tr>
<tr><td>8th</td><td>7129/
2520</td><td>9</td><td>36
/2 |18</td><td>84
/3 |28</td><td>126|63
/4 |2</td><td>126
/5</td><td>84
/6 |14</td><td>36
/7</td><td>9
/8</td><td>1
/9</td><td></td></tr>
<tr><td>9th</td><td>7381/
2520</td><td>10</td><td>45
/2</td><td>120
/3 |40</td><td>210 |105
/4 |2</td><td>252
/5</td><td>210
/6 |35</td><td>120
/7</td><td>45
/8</td><td>10
/9</td><td>1
/10</td></tr>
</table>

A regular pattern has been found in this table. Namely, the numerator of $a_{\pm 1}, a_{\pm 2}, ..., a_{\pm n}$ in this table can be obtained by removing the first column of the following well-known table.

```
1   2   1
1   3   3   1
1   4   6   4  1
1   5  10  10  5  1
```

....

where the first term should be obtained from $a_0 + a_{+1} + ... + a_{+n} = 0$ for the forward finite difference, or from $a_0 + a_{-1} + ... + a_{-n} = 0$ for the backward finite difference , where $n = m + 1$ and $a_{\pm 1}, a_{\pm 2}, ..., a_{\pm n}$ satisfy Eq. (B.22) with $k = 1$.

Table B.3. Coefficients of $f_0^{(2)}$ in the Forward and Backward Finite Difference

m-th order forward FD	$+a_0$	$-a_{+1}$	$+a_{+2}$	$-a_{+3}$	$+a_{+4}$	$-a_{+5}$	$+a_{+6}$	$-a_{+7}$	$+a_{+8}$	$-a_{+9}$	$+a_{+10}$
m-th order backward FD	$+a_0$	$-a_{-1}$	$+a_{-2}$	$-a_{-3}$	$+a_{-4}$	$-a_{-5}$	$+a_{-6}$	$-a_{-7}$	$+a_{-8}$	$-a_{-9}$	$+a_{-10}$
1st	2	5	4	1							
2nd	35/12	26/3	19/2	14/3	11/12						
3rd	15/4	77/6	107/6	13	61/12	5/6					
4th	203/45	87/5	117/4	254/9	33/2	27/5	137/180				
5th	469/90	223/10	879/20	949/18	41	201/10	1019/180	7/10			
6th	29531/5040	962/35	621/10	4006/45	691/8	282/5	2143/90	206/35	363/560		
7th	6515/1008	4609 140	5869/70	6289/45	6499/40	265/2	6709/90	967/35	3407/560	761/1260	
8th	177133/25200	4861/126	6121/56	13082/63	6751/24	6877/25	6961/36	2006/21	3533/112	263/42	7129/12600

where the first term should be obtained from $a_0 + a_{+1} + ... + a_{+n} = 0$ for the forward finite difference, or from $a_0 + a_{-1} + ... + a_{-n} = 0$ for the backward finite difference , where $n = m + 2$ and $a_{\pm 1}, a_{\pm 2}, ..., a_{\pm n}$ satisfy Eq. (B.22) with $k = 2$.

Table B.4. Coefficients of $f_0^{(3)}$ in the Forward and Backward Finite Difference

m-th order forward FD	$-a_0$	$+a_{+1}$	$-a_{+2}$	$+a_{+3}$	$-a_{+4}$	$+a_{+5}$	$-a_{+6}$	$+a_{+7}$	$-a_{+8}$	$+a_{+9}$	$-a_{+10}$
m-th order backward FD	$+a_0$	$-a_{-1}$	$+a_{-2}$	$-a_{-3}$	$+a_{-4}$	$-a_{-5}$	$+a_{-6}$	$-a_{-7}$	$+a_{-8}$	$-a_{-9}$	$+a_{-10}$
1st	5/2	9	12	7	3/2						
2nd	17/4	71/4	59/2	49/2	41/4	7/4					
3rd	49/8	29	461/8	62	307/8	13	15/8				
4th	967/120	638/15	3929/40	389/3	2545/24	268/5	1849/120	29/15			
5th	801/80	349/6	18353/120	2391/10	1457/6	4891/30	561/8	527/30	469/240		
6th	4523/378	42417/560	62511/280	72569/180	19557/40	3273/8	84307/360	12303/140	5469/280	29531/15120	
7th	84095/6048	79913/840	347769/1120	400579/630	71689/80	3591/4	461789/720	22439/70	119601/1120	161353/7560	1303/672

where the first term should be obtained from $a_0 + a_{+1} + ... + a_{+n} = 0$ for the forward finite difference, or from $a_0 + a_{-1} + ... + a_{-n} = 0$ for the backward finite difference , where $n = m + 3$ and $a_{\pm 1}, a_{\pm 2}, ..., a_{\pm n}$ satisfy Eq. (B.22) with $k = 3$.

Table B.5. Forward-Finite-Difference Expressions of $f_0^{(k)}$

First-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{3}{2}f_0 + 2f_{+1} - \frac{1}{2}f_{+2}) + O(h^2 f_0^{(3)})$
$f_0^{(2)} = \frac{1}{h^2}(+2f_0 - 5f_{+1} + 4f_{+2} - f_{+3}) + O(h^2 f_0^{(4)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{5}{2}f_0 + 9f_{+1} - 12f_{+2} + 7f_{+3} - \frac{3}{2}f_{+4}) + O(h^2 f_0^{(5)})$
Second-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{11}{6}f_0 + 3f_{+1} - \frac{3}{2}f_{+2} + \frac{1}{3}f_{+3}) + O(h^3 f_0^{(4)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{35}{12}f_0 - \frac{26}{3}f_{+1} + \frac{19}{2}f_{+2} - \frac{14}{3}f_{+3} + \frac{11}{12}f_{+4}) + O(h^3 f_0^{(5)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{17}{4}f_0 + \frac{71}{4}f_{+1} - \frac{59}{2}f_{+2} + \frac{49}{2}f_{+3} - \frac{41}{4}f_{+4} + \frac{7}{4}f_{+5}) + O(h^3 f_0^{(6)})$
Third-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{25}{12}f_0 + 4f_{+1} - 3f_{+2} + \frac{4}{3}f_{+3} - \frac{1}{4}f_{+4}) + O(h^4 f_0^{(5)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{15}{4}f_0 - \frac{77}{6}f_{+1} + \frac{107}{6}f_{+2} - 13f_{+3} + \frac{61}{12}f_{+4} - \frac{5}{6}f_{+5}) + O(h^4 f_0^{(6)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{49}{8}f_0 + 29f_{+1} - \frac{461}{8}f_{+2} + 62f_{+3} - \frac{307}{8}f_{+4} + 13f_{+5} - \frac{15}{8}f_{+6}) + O(h^4 f_0^{(7)})$
Fourth-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{137}{60}f_0 + 5f_{+1} - 5f_{+2} + \frac{10}{3}f_{+3} - \frac{5}{4}f_{+4} + \frac{1}{5}f_{+5}) + O(h^5 f_0^{(6)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{203}{45}f_0 - \frac{87}{5}f_{+1} + \frac{117}{4}f_{+2} - \frac{254}{9}f_{+3} + \frac{33}{2}f_{+4} - \frac{27}{5}f_{+5} + \frac{137}{180}f_{+6}) + O(h^5 f_0^{(7)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{967}{120}f_0 + \frac{638}{15}f_{+1} - \frac{3929}{40}f_{+2} + \frac{389}{3}f_{+3} - \frac{2545}{24}f_{+4} + \frac{268}{5}f_{+5} - \frac{1849}{120}f_{+6} + \frac{29}{15}f_{+7}) + O(h^5 f_0^{(8)})$
Fifth-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{49}{20}f_0 + 6f_{+1} - \frac{15}{2}f_{+2} + \frac{20}{3}f_{+3} - \frac{15}{4}f_{+4} + \frac{6}{5}f_{+5} - \frac{1}{6}f_{+6}) + O(h^6 f_0^{(7)})$

$f_0^{(2)} = \frac{1}{h^2}(+\frac{469}{90}f_0 - \frac{223}{10}f_{+1} + \frac{879}{20}f_{+2} - \frac{949}{18}f_{+3} + 41f_{+4} - \frac{201}{10}f_{+5} + \frac{1019}{180}f_{+6} - \frac{7}{10}f_{+7}) + O(h^6 f_0^{(8)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{801}{80}f_0 + \frac{349}{6}f_{+1} - \frac{18353}{120}f_{+2} + \frac{2391}{10}f_{+3} - \frac{1457}{6}f_{+4} + \frac{4891}{30}f_{+5} - \frac{561}{8}f_{+6} + \frac{527}{30}f_{+7} - \frac{469}{240}f_{+8}) + O(h^6 f_0^{(9)})$
Sixth-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{363}{140}f_0 + 7f_{+1} - \frac{21}{2}f_{+2} + \frac{35}{3}f_{+3} - \frac{35}{4}f_{+4} + \frac{21}{5}f_{+5} - \frac{7}{6}f_{+6} + \frac{1}{7}f_{+7}) + O(h^7 f_0^{(8)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{29531}{5040}f_0 - \frac{962}{35}f_{+1} + \frac{621}{10}f_{+2} - \frac{4006}{45}f_{+3} + \frac{691}{8}f_{+4} - \frac{282}{5}f_{+5} + \frac{2143}{90}f_{+6} - \frac{206}{35}f_{+7} + \frac{363}{560}f_{+8}) + O(h^7 f_0^{(9)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{4523}{378}f_0 + \frac{42417}{560}f_{+1} - \frac{62511}{280}f_{+2} + \frac{72569}{180}f_{+3} - \frac{19557}{40}f_{+4} + \frac{3273}{8}f_{+5} - \frac{84307}{360}f_{+6} + \frac{12303}{140}f_{+7} - \frac{5469}{280}f_{+8} + \frac{29531}{15120}f_{+9}) + O(h^7 f_0^{(10)})$
Seventh-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{761}{280}f_0 + 8f_{+1} - 14f_{+2} + \frac{56}{3}f_{+3} - \frac{35}{2}f_{+4} + \frac{56}{5}f_{+5} - \frac{14}{3}f_{+6} + \frac{8}{7}f_{+7} - \frac{1}{8}f_{+8}) + O(h^8 f_0^{(9)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{6515}{1008}f_0 - \frac{4609}{140}f_{+1} + \frac{5869}{70}f_{+2} - \frac{6289}{45}f_{+3} + \frac{6499}{40}f_{+4} - \frac{265}{2}f_{+5} + \frac{6709}{90}f_{+6} - \frac{967}{35}f_{+7} + \frac{3407}{560}f_{+8} - \frac{761}{1260}f_{+9}) + O(h^8 f_0^{(10)})$
$f_0^{(3)} = \frac{1}{h^3}(-\frac{84095}{6048}f_0 + \frac{79913}{840}f_{+1} - \frac{347769}{1120}f_{+2} + \frac{400579}{630}f_{+3} - \frac{71689}{80}f_{+4} + \frac{3591}{4}f_{+5} - \frac{461789}{720}f_{+6} + \frac{22439}{70}f_{+7} - \frac{119601}{1120}f_{+8} + \frac{161353}{7560}f_{+9} - \frac{1303}{672}f_{+10}) + O(h^8 f_0^{(11)})$
Eighth-Order Forward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(-\frac{7129}{2520}f_0 + 9f_{+1} - 18f_{+2} + 28f_{+3} - \frac{63}{2}f_{+4} + \frac{126}{5}f_{+5} - 14f_{+6} + \frac{36}{7}f_{+7} - \frac{9}{8}f_{+8} + \frac{1}{9}f_{+9}) + O(h^9 f_0^{(10)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{177133}{25200}f_0 - \frac{4861}{126}f_{+1} + \frac{6121}{56}f_{+2} - \frac{13082}{63}f_{+3} + \frac{6751}{24}f_{+4} - \frac{6877}{25}f_{+5} + \frac{6961}{36}f_{+6} - \frac{2006}{21}f_{+7} + \frac{3533}{112}f_{+8} - \frac{263}{42}f_{+9} + \frac{7129}{12600}f_{+10}) + O(h^9 f_0^{(11)})$

Table B.6. Backward-Finite-Difference Expressions of $f_0^{(k)}$

First-Order Backward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{3}{2}f_0 - 2f_{-1} + \frac{1}{2}f_{-2}) + O(h^2 f_0^{(3)})$
$f_0^{(2)} = \frac{1}{h^2}(+2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}) + O(h^2 f_0^{(4)})$
$f_0^{(3)} = \frac{1}{h^3}(+\frac{5}{2}f_0 - 9f_{-1} + 12f_{-2} - 7f_{-3} + \frac{3}{2}f_{-4}) + O(h^2 f_0^{(5)})$
Second-Order Backward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{11}{6}f_0 - 3f_{-1} + \frac{3}{2}f_{-2} - \frac{1}{3}f_{-3}) + O(h^3 f_0^{(4)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{35}{12}f_0 - \frac{26}{3}f_{-1} + \frac{19}{2}f_{-2} - \frac{14}{3}f_{-3} + \frac{11}{12}f_{-4}) + O(h^3 f_0^{(5)})$
$f_0^{(3)} = \frac{1}{h^3}(+\frac{17}{4}f_0 - \frac{71}{4}f_{-1} + \frac{59}{2}f_{-2} - \frac{49}{2}f_{-3} + \frac{41}{4}f_{-4} - \frac{7}{4}f_{-5}) + O(h^3 f_0^{(6)})$
Third-Order Backward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{25}{12}f_0 - 4f_{-1} + 3f_{-2} - \frac{4}{3}f_{-3} + \frac{1}{4}f_{-4}) + O(h^4 f_0^{(5)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{15}{4}f_0 - \frac{77}{6}f_{-1} + \frac{107}{6}f_{-2} - 13f_{-3} + \frac{61}{12}f_{-4} - \frac{5}{6}f_{-5}) + O(h^4 f_0^{(6)})$
$f_0^{(3)} = \frac{1}{h^3}(+\frac{49}{8}f_0 - 29f_{-1} + \frac{461}{8}f_{-2} - 62f_{-3} + \frac{307}{8}f_{-4} - 13f_{-5} + \frac{15}{8}f_{-6}) + O(h^4 f_0^{(7)})$
Fourth-Order Backward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{137}{60}f_0 - 5f_{-1} + 5f_{-2} - \frac{10}{3}f_{-3} + \frac{5}{4}f_{-4} - \frac{1}{5}f_{-5}) + O(h^5 f_0^{(6)})$
$f_0^{(2)} = \frac{1}{h^2}(+\frac{203}{45}f_0 - \frac{87}{5}f_{-1} + \frac{117}{4}f_{-2} - \frac{254}{9}f_{-3} + \frac{33}{2}f_{-4} - \frac{27}{5}f_{-5} + \frac{137}{180}f_{-6}) + O(h^5 f_0^{(7)})$
$f_0^{(3)} = \frac{1}{h^3}(+\frac{967}{120}f_0 - \frac{638}{15}f_{-1} + \frac{3929}{40}f_{-2} - \frac{389}{3}f_{-3} + \frac{2545}{24}f_{-4} - \frac{268}{5}f_{-5}$ $+ \frac{1849}{120}f_{-6} - \frac{29}{15}f_{-7}) + O(h^5 f_0^{(8)})$
Fifth-Order Backward-Finite Differences
$f_0^{(1)} = \frac{1}{h}(+\frac{49}{20}f_0 - 6f_{-1} + \frac{15}{2}f_{-2} - \frac{20}{3}f_{-3} + \frac{15}{4}f_{-4} - \frac{6}{5}f_{-5} + \frac{1}{6}f_{-6}) + O(h^6 f_0^{(7)})$

$$f_0^{(2)} = \frac{1}{h^2}(+\frac{469}{90}f_0 - \frac{223}{10}f_{-1} + \frac{879}{20}f_{-2} - \frac{949}{18}f_{-3} + 41f_{-4} - \frac{201}{10}f_{-5} + \frac{1019}{180}f_{-6} - \frac{7}{10}f_{-7}) + O(h^6 f_0^{(8)})$$

$$f_0^{(3)} = \frac{1}{h^3}(+\frac{801}{80}f_0 - \frac{349}{6}f_{-1} + \frac{18353}{120}f_{-2} - \frac{2391}{10}f_{-3} + \frac{1457}{6}f_{-4} - \frac{4891}{30}f_{-5} + \frac{561}{8}f_{-6} - \frac{527}{30}f_{-7} + \frac{469}{240}f_{-8}) + O(h^6 f_0^{(9)})$$

Sixth-Order Backward-Finite Differences

$$f_0^{(1)} = \frac{1}{h}(+\frac{363}{140}f_0 - 7f_{-1} + \frac{21}{2}f_{-2} - \frac{35}{3}f_{-3} + \frac{35}{4}f_{-4} - \frac{21}{5}f_{-5} + \frac{7}{6}f_{-6} - \frac{1}{7}f_{-7}) + O(h^7 f_0^{(8)})$$

$$f_0^{(2)} = \frac{1}{h^2}(+\frac{29531}{5040}f_0 - \frac{962}{35}f_{-1} + \frac{621}{10}f_{-2} - \frac{4006}{45}f_{-3} + \frac{691}{8}f_{-4} - \frac{282}{5}f_{-5} + \frac{2143}{90}f_{-6} - \frac{206}{35}f_{-7} + \frac{363}{560}f_{-8}) + O(h^7 f_0^{(9)})$$

$$f_0^{(3)} = \frac{1}{h^3}(+\frac{4523}{378}f_0 - \frac{42417}{560}f_{-1} + \frac{62511}{280}f_{-2} - \frac{72569}{180}f_{-3} + \frac{19557}{40}f_{-4} - \frac{3273}{8}f_{-5} + \frac{84307}{360}f_{-6} - \frac{12303}{140}f_{-7} + \frac{5469}{280}f_{-8} - \frac{29531}{15120}f_{-9}) + O(h^7 f_0^{(10)})$$

Seventh-Order Backward-Finite Differences

$$f_0^{(1)} = \frac{1}{h}(+\frac{761}{280}f_0 - 8f_{-1} + 14f_{-2} - \frac{56}{3}f_{-3} + \frac{35}{2}f_{-4} - \frac{56}{5}f_{-5} + \frac{14}{3}f_{-6} - \frac{8}{7}f_{-7} + \frac{1}{8}f_{-8}) + O(h^8 f_0^{(9)})$$

$$f_0^{(2)} = \frac{1}{h^2}(+\frac{6515}{1008}f_0 - \frac{4609}{140}f_{-1} + \frac{5869}{70}f_{-2} - \frac{6289}{45}f_{-3} + \frac{6499}{40}f_{-4} - \frac{265}{2}f_{-5} + \frac{6709}{90}f_{-6} - \frac{967}{35}f_{-7} + \frac{3407}{560}f_{-8} - \frac{761}{1260}f_{-9}) + O(h^8 f_0^{(10)})$$

$$f_0^{(3)} = \frac{1}{h^3}(+\frac{84095}{6048}f_0 - \frac{79913}{840}f_{-1} + \frac{347769}{1120}f_{-2} - \frac{400579}{630}f_{-3} + \frac{71689}{80}f_{-4} - \frac{3591}{4}f_{-5} + \frac{461789}{720}f_{-6} - \frac{22439}{70}f_{-7} + \frac{119601}{1120}f_{-8} - \frac{161353}{7560}f_{-9} + \frac{1303}{672}f_{-10}) + O(h^8 f_0^{(11)})$$

Eighth-Order Forward-Finite Differences

$$f_0^{(1)} = \frac{1}{h}(+\frac{7129}{2520}f_0 - 9f_{-1} + 18f_{-2} - 28f_{-3} + \frac{63}{2}f_{-4} - \frac{126}{5}f_{-5} + 14f_{-6} - \frac{36}{7}f_{-7} + \frac{9}{8}f_{-8} - \frac{1}{9}f_{-9}) + O(h^9 f_0^{(10)})$$

$$f_0^{(2)} = \frac{1}{h^2}(+\frac{177133}{25200}f_0 - \frac{4861}{126}f_{-1} + \frac{6121}{56}f_{-2} - \frac{13082}{63}f_{-3} + \frac{6751}{24}f_{-4} - \frac{6877}{25}f_{-5} + \frac{6961}{36}f_{-6} - \frac{2006}{21}f_{-7} + \frac{3533}{112}f_{-8} - \frac{263}{42}f_{-9} + \frac{7129}{12600}f_{-10}) + O(h^9 f_0^{(11)})$$

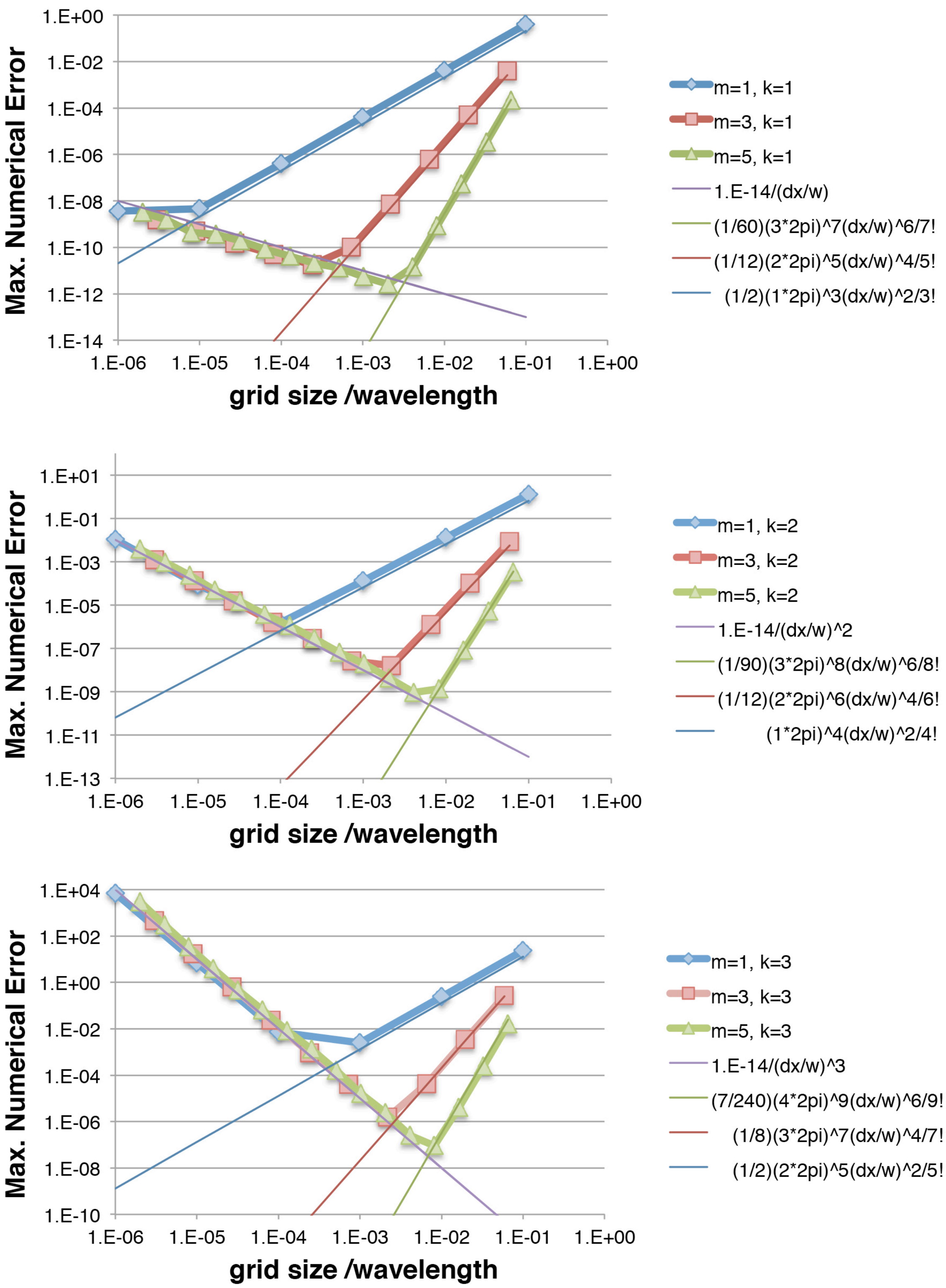
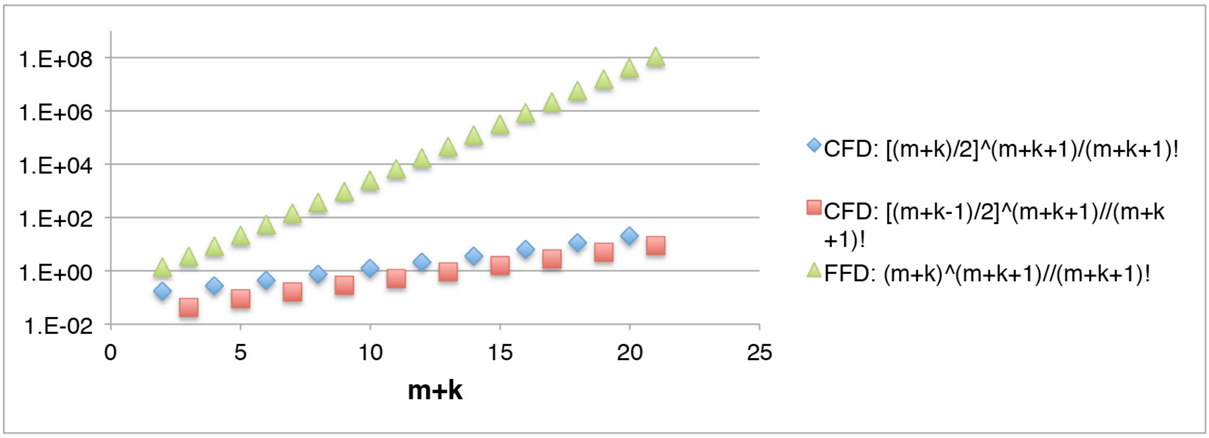


Figure B.1. Log-log plots of the maximum absolute errors (the thick curves with marks) in the numerical derivatives of $f(x) = \sin(2\pi\, x / \lambda)$, as a function of grid size normalized by the wavelength, for m = 1, 3, 5, and k = 1, 2, 3, where m and k denote the m-th order central-finite-difference scheme and the k-th order derivatives. The discretization errors are estimated and plotted in the thin lines with similar colors as the corresponding numerical errors. The round-off errors are estimated and plotted in the purple thin line.



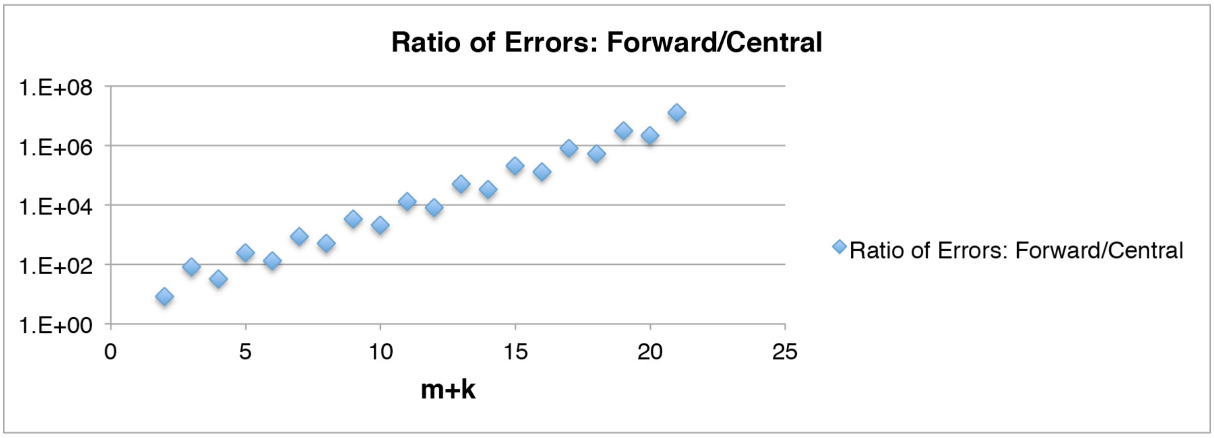


Figure B.2. Plots of the coefficients of $h^{m+1} f_0^{(m+k+1)}$ in Eqs. (8.24), (8.25), (8.26), and the estimated ratio of the discretization errors in different schemes as a function of *m*+*k*, where CFD denotes central-finite-difference scheme, FFD denotes forward-finite-difference scheme, *m* denotes *m*-th order finite-difference scheme, and *k* denotes the *k*-th order derivatives. We can see that, even for small *m*+*k* ($m+k < 10$), the discretization errors in the FFD can be 10 to 1000 (2^3 to 2^{10}) times higher than the corresponding errors in CFD. Namely, the accuracy of the central-finite-difference scheme is much higher than the accuracy of the forward-finite-difference (or backward-finite-difference) scheme.

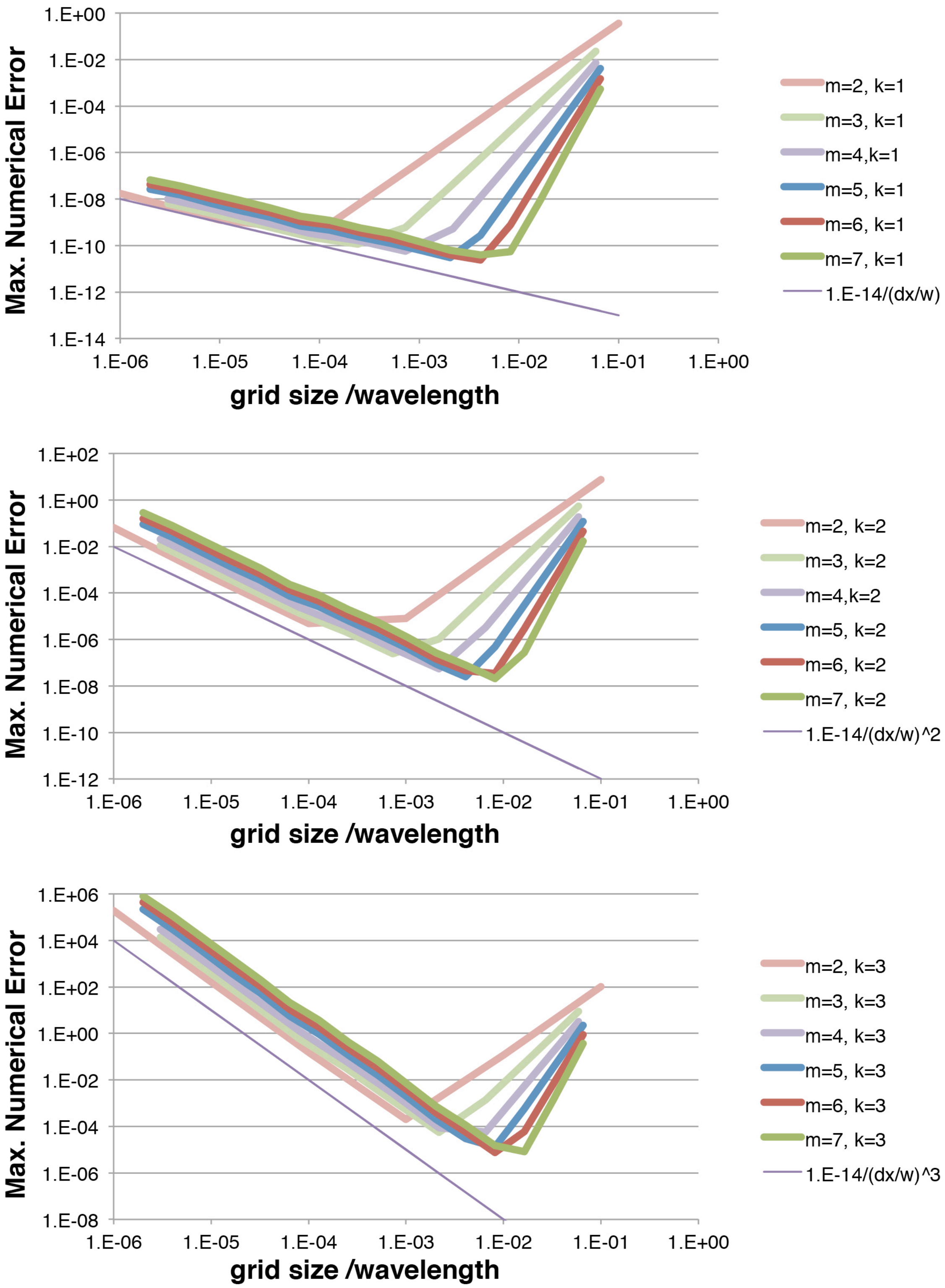


Figure B.3. Log-log plots of the maximum absolute errors (the thick curves) in the numerical derivatives of $f(x) = \sin(2\pi\, x/\lambda)$, as a function of grid size normalized by the wavelength, for m = 2, 3, 4, 5, 6, 7 and k = 1, 2, 3, where m and k denote the m-th order forward-finite-difference scheme and the k-th order derivatives. The round-off errors are estimated and plotted in the purple thin line.