Appendix A

Higher-Order Approximation

A.1 Five-Point Formulation

In this case, the field is expanded on either side of the interface in terms of the field at the interface using Taylor's series expansion, that is:

$$\psi_{+1} = \psi_{0^+} + h_2\psi'_{0^+} + \frac{h_2^2}{2!}\psi''_{0^+} + \frac{h_2^3}{3!}\psi'''_{0^+} + \frac{h_2^4}{4!}\psi''''_{0^+} + ... \quad (A.1)$$

$$\psi_{-1} = \psi_{0^-} - h_1\psi'_{0^-} + \frac{h_1^2}{2!}\psi''_{0^-} - \frac{h_1^3}{3!}\psi'''_{0^-} + \frac{h_1^4}{4!}\psi''''_{0^-} - ... \quad (A.2)$$

$$\psi_{+2} = \psi_{0^+} + 2h_2\psi'_{0^+} + \frac{(2h_2)^2}{2!}\psi''_{0^+} + \frac{(2h_2)^3}{3!}\psi'''_{0^+} + \frac{(2h_2)^4}{4!}\psi''''_{0^+} + ... \quad (A.3)$$

$$\psi_{-2} = \psi_{0^-} - 2h_1\psi'_{0^-} + \frac{(2h_1)^2}{2!}\psi''_{0^-} - \frac{(2h_1)^3}{3!}\psi'''_{0^-} + \frac{(2h_1)^4}{4!}\psi''''_{0^-} - ... \quad (A.4)$$

Using the interface conditions 3.26-3.30 and expressing the fields ψ_{+1} and ψ_{+2} in terms of the 0^- side derivatives of ψ, we obtain [58]:

$$\psi_{+1} = \left(1 + \frac{h_2^2\zeta_{12}}{2} + \frac{h_2^4\zeta_{12}^2}{24}\right)\psi_0 + \rho_{21}\left(h_2 + \frac{h_2^3\zeta_{12}}{6}\right)\psi'_{0^-}$$

$$+\left(\frac{h_2^2}{2}+\frac{h_2^4\zeta_{12}}{12}\right)\psi_{0^-}^{''}+\frac{h_2^3\rho_{21}}{6}\psi_{0^-}^{'''}+\frac{h_2^4}{24}\psi_{0^-}^{''''}+... \tag{A.5}$$

$$\psi_{+2}=\left(1+2h_2^2\zeta_{12}+\frac{2h_2^4\zeta_{12}^2}{3}\right)\psi_0+\rho_{21}\left(2h_2+\frac{4h_2^3\zeta_{12}}{3}\right)\psi_{0^-}^{'}$$

$$+\left(2h_2^2+\frac{4h_2^4\zeta_{12}}{3}\right)\psi_{0^-}^{''}+\frac{4h_2^3\rho_{21}}{3}\psi_{0^-}^{'''}+\frac{2h_2^4}{3}\psi_{0^-}^{''''}+... \tag{A.6}$$

Equations A.2, A.4, A.5 and A.6 can be put in matrix form, that is:

$$\begin{bmatrix} \psi_{+1}-a\cdot\psi_0 \\ \psi_{+2}-b\cdot\psi_0 \\ \psi_{-1}-c\cdot\psi_0 \\ \psi_{-2}-d\cdot\psi_0 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi_{0^-}^{'} \\ \psi_{0^-}^{''} \\ \psi_{0^-}^{'''} \\ \psi_{0^-}^{''''} \end{bmatrix}$$

where a, b, c and d are the coefficients of ψ_0 in the previous equations. Inverting the above matrix equation to find the unknowns:

$$\begin{bmatrix} \psi_{0^-}^{'} \\ \psi_{0^-}^{''} \\ \psi_{0^-}^{'''} \\ \psi_{0^-}^{''''} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix} \begin{bmatrix} \psi_{+1}-a\cdot\psi_0 \\ \psi_{+2}-b\cdot\psi_0 \\ \psi_{-1}-c\cdot\psi_0 \\ \psi_{-2}-d\cdot\psi_0 \end{bmatrix}$$

From which we have:

$$\begin{aligned}\psi_{0^-}^{''} \;&=\; b_{22}\psi_{+2}+b_{21}\psi_{+1}-(a\cdot b_{21}+b\cdot b_{22}+c\cdot b_{23}+d\cdot b_{24})\psi_0+ \\ &\quad b_{23}\psi_{-1}+b_{24}\psi_{-2}\end{aligned} \tag{A.7}$$

This relation gives $\psi_i^{''}$ approximation at an interface in terms of the field samples

ψ_{i+2} , ψ_{i+1} , ψ_i , ψ_{i-1} and ψ_{i-2}. In this relation, the discontinuity in $\psi^{'}$, $\psi^{''}$, $\psi^{'''}$ and $\psi^{''''}$ at an index or mesh discontinuity are appropriately included. In regions of uniform index and mesh, this reduces to the familiar 5-point approximation, that is:

$$\psi^{''}_{0^-} \approx \frac{1}{12h^2}(-\psi_{+2} + 16\psi_{+1} - 30\psi_0 + 16\psi_{-1} - \psi_{-2}) \tag{A.8}$$

By using this five-point approximation, we get a penta-diagonal matrix of the form [36]:

$$\frac{1}{12h^2}\begin{bmatrix} -30 & 16 & -1 & & & & & \\ 16 & -30 & 16 & -1 & & & \mathcal{O} & \\ -1 & 16 & -30 & 16 & -1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & -1 & 16 & -30 & 16 & -1 \\ & \mathcal{O} & & & -1 & 16 & -30 & 16 \\ & & & & & -1 & 16 & -30 \end{bmatrix}$$

It is necessary to find the 5-point second-derivative formula at one sampling point *ahead* and one sampling point *before* the interface. In this derivation, it is assumed that the minimum number of samples in one layer is 3. With reference to figure 3.2, $\psi^{''}_0$ is to be expressed in terms of ψ_{-1} , ψ_0 , ψ_{+1} , ψ_{+2} and ψ_{+3}. Expanding the field samples on either side of the interface in terms of ψ_0:

$$\psi_{+1} = \psi_{0^+} + h_2\psi^{'}_{0^+} + \frac{h_2^2}{2!}\psi^{''}_{0^+} + \frac{h_2^3}{3!}\psi^{'''}_{0^+} + \frac{h_2^4}{4!}\psi^{''''}_{0^+} + ... \tag{A.9}$$

$$\psi_{+2} = \psi_{0^+} + 2h_2\psi^{'}_{0^+} + \frac{(2h_2)^2}{2!}\psi^{''}_{0^+} + \frac{(2h_2)^3}{3!}\psi^{'''}_{0^+} + \frac{(2h_2)^4}{4!}\psi^{''''}_{0^+} + ... \tag{A.10}$$

$$\psi_{+3} = \psi_{0+} + 3h_2\psi'_{0+} + \frac{(3h_2)^2}{2!}\psi''_{0+} + \frac{(3h_2)^3}{3!}\psi'''_{0+} + \frac{(3h_2)^4}{4!}\psi''''_{0+} + ... \quad (A.11)$$

$$\psi_{-1} = \psi_{0-} - h_1\psi'_{0-} + \frac{h_1^2}{2!}\psi''_{0-} - \frac{h_1^3}{3!}\psi'''_{0-} + \frac{h_1^4}{4!}\psi''''_{0-} - ... \quad (A.12)$$

Using the interface conditions 3.26-3.30, we express ψ_{0-} derivatives in terms of ψ_{0+} derivatives in equation A.12:

$$\psi_{-1} = \psi_0\left(1 - \frac{h_1^2}{2}\zeta_{12} + \frac{h_1^4}{24}\zeta_{12}^2\right) + \psi'_{0+}\left(\frac{-h_1}{\rho_{21}} + \frac{h_1^3}{6\rho_{21}}\zeta_{12}\right) + \psi''_{0+}\left(\frac{h_1^2}{2} - \frac{h_1^4}{12}\zeta_{12}\right) - \frac{h_1^3}{6\rho_{21}}\psi'''_{0+} + \frac{h_1^4}{24}\psi''''_{0+} \quad (A.13)$$

In matrix form:

$$\begin{bmatrix} \psi_{+1} - \psi_0 \\ \psi_{+2} - \psi_0 \\ \psi_{+3} - \psi_0 \\ \psi_{-1} - a\cdot\psi_0 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi'_{0+} \\ \psi''_{0+} \\ \psi'''_{0+} \\ \psi''''_{0+} \end{bmatrix}$$

where a is the coefficient of ψ_0 in equation A.13. Inverting the above matrix equation, we have [58]:

$$\begin{bmatrix} \psi'_{0+} \\ \psi''_{0+} \\ \psi'''_{0+} \\ \psi''''_{0+} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix} \begin{bmatrix} \psi_{+1} - \psi_0 \\ \psi_{+2} - \psi_0 \\ \psi_{+3} - \psi_0 \\ \psi_{-1} - a\cdot\psi_0 \end{bmatrix}$$

Differentiating equation A.9 twice with respect to x:

$$\psi''_{+1} = \psi''_{0+} + h_2\psi'''_{0+} + \frac{h_2^2}{2}\psi''''_{0+} + ... \quad (A.14)$$

Putting the values of ψ''_{0+} , ψ'''_{0+} and ψ''''_{0+} in the above equation and simplifying, we have [58]:

$$\begin{aligned}\psi''_{+1} = \quad & \psi_{+3}(b_{23} + h_2 b_{33} + 0.5h_2^2 b_{43}) + \psi_{+2}(b_{22} + h_2 b_{32} + 0.5h_2^2 b_{42}) + \\ & \psi_{+1}(b_{21} + h_2 b_{31} + 0.5h_2^2 b_{41}) - \psi_0(p_1 + h_2 p_2 + 0.5h_2^2 p_3) \\ & \psi_{-1}(b_{24} + h_2 b_{34} + 0.5h_2^2 b_{44}) \end{aligned} \tag{A.15}$$

where

$p_1 = b_{21} + b_{22} + b_{23} + a \cdot b_{24}$

$p_2 = b_{31} + b_{32} + b_{33} + a \cdot b_{34}$

$p_3 = b_{41} + b_{42} + b_{43} + a \cdot b_{44}$

This relation gives the five-point second-derivative approximation at one sample point ahead of an index or mesh discontinuity. The relation at one sample point before the interface can obtained by interchanging $h_2 \rightleftharpoons -h_1$, $\psi_{+2} \rightleftharpoons \psi_0$, $\psi_{+3} \rightleftharpoons \psi_{-1}$ and $n_1^2 \rightleftharpoons n_2^2$ [58].

A.2 Seven-Point Formulation

A similar procedure is adopted to find the 7-point second-derivative approximation with appropriate interface conditions.

$$\begin{aligned}\psi_{+1} &= \psi_{0+} + h_2\psi'_{0+} + \frac{h_2^2}{2!}\psi''_{0+} + \frac{h_2^3}{3!}\psi'''_{0+} + \frac{h_2^4}{4!}\psi''''_{0+} + \\ & \quad \frac{h_5^4}{5!}\psi'''''_{0+} + \frac{h_2^6}{6!}\psi''''''_{0+} + ... \end{aligned} \tag{A.16}$$

$$\psi_{+2} = \psi_{0+} + 2h_2\psi'_{0+} + \frac{(2h_2)^2}{2!}\psi''_{0+} + \frac{(2h_2)^3}{3!}\psi'''_{0+} + \frac{(2h_2)^4}{4!}\psi''''_{0+}$$

$$+\frac{(2h_2)^5}{5!}\psi_{0+}^{'''''}+\frac{(2h_2)^6}{6!}\psi_{0+}^{''''''}+... \quad (A.17)$$

$$\psi_{+3} = \psi_{0+}+3h_2\psi_{0+}^{'}+\frac{(3h_2)^2}{2!}\psi_{0+}^{''}+\frac{(3h_2)^3}{3!}\psi_{0+}^{'''}+\frac{(3h_2)^4}{4!}\psi_{0+}^{''''}$$
$$+\frac{(3h_2)^5}{5!}\psi_{0+}^{'''''}+\frac{(3h_2)^6}{6!}\psi_{0+}^{''''''}+... \quad (A.18)$$

$$\psi_{-1} = \psi_{0-}-h_1\psi_{0-}^{'}+\frac{h_1^2}{2!}\psi_{0-}^{''}-\frac{h_1^3}{3!}\psi_{0-}^{'''}+\frac{h_1^4}{4!}\psi_{0-}^{''''}$$
$$-\frac{h_1^5}{5!}\psi_{0-}^{'''''}+\frac{h_1^6}{6!}\psi_{0-}^{''''''}-... \quad (A.19)$$

$$\psi_{-2} = \psi_{0-}-2h_1\psi_{0-}^{'}+\frac{(2h_1)^2}{2!}\psi_{0-}^{''}-\frac{(2h_1)^3}{3!}\psi_{0-}^{'''}+\frac{(2h_1)^4}{4!}\psi_{0-}^{''''}$$
$$-\frac{(2h_1)^5}{5!}\psi_{0-}^{'''''}+\frac{(2h_1)^6}{6!}\psi_{0-}^{''''''}-... \quad (A.20)$$

$$\psi_{-3} = \psi_{0-}-3h_1\psi_{0-}^{'}+\frac{(3h_1)^2}{2!}\psi_{0-}^{''}-\frac{(3h_1)^3}{3!}\psi_{0-}^{'''}+\frac{(3h_1)^4}{4!}\psi_{0-}^{''''}$$
$$-\frac{(3h_1)^5}{5!}\psi_{0-}^{'''''}+\frac{(3h_1)^6}{6!}\psi_{0-}^{''''''}-... \quad (A.21)$$

Using the interface conditions 3.26-3.32, we express ψ_{0^+} side derivatives in terms of ψ_{0^-} derivatives:

$$\psi_{+1} = \psi_0\left(1+\frac{\zeta_{12}h_2^2}{2!}+\frac{\zeta_{12}^2h_2^4}{4!}+\frac{\zeta_{12}^3h_2^6}{6!}\right)+\rho_{21}\psi_{0-}^{'}\left(h_2+\frac{\zeta_{12}h_2^3}{3!}+\frac{\zeta_{12}^2h_2^5}{5!}\right)$$
$$+\psi_{0-}^{''}\left(\frac{h_2^2}{2!}+\frac{2\zeta_{12}h_2^4}{4!}+\frac{3\zeta_{12}^2h_2^6}{6!}\right)+\rho_{21}\psi_{0-}^{'''}\left(\frac{h_2^3}{3!}+\frac{2\zeta_{12}h_2^5}{5!}\right)$$
$$+\psi_{0-}^{''''}\left(\frac{h_2^4}{4!}+\frac{3\zeta_{12}h_2^6}{6!}\right)+\rho_{21}\psi_{0-}^{'''''}\left(\frac{h_2^5}{5!}\right)+\psi_{0-}^{''''''}\left(\frac{h_2^6}{6!}\right) \quad (A.22)$$

Expressions for ψ_{+2} and ψ_{+3} are obtained by replacing h_2 by $2h_2$ and $3h_2$ in equation A.22 respectively. We then assimilate the final results in the matrix form :

$$\begin{bmatrix} \psi_{+1} - a \cdot \psi_0 \\ \psi_{+2} - b \cdot \psi_0 \\ \psi_{+3} - c \cdot \psi_0 \\ \psi_{-1} - \psi_0 \\ \psi_{-2} - \psi_0 \\ \psi_{-3} - \psi_0 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} \end{bmatrix} \begin{bmatrix} \psi_{0^-}^{'} \\ \psi_{0^-}^{''} \\ \psi_{0^-}^{'''} \\ \psi_{0^-}^{''''} \\ \psi_{0^-}^{'''''} \\ \psi_{0^-}^{''''''} \end{bmatrix}$$

where a, b and c are the coefficients of corresponding ψ_0 terms in the previous equation. Inverting the above matrix equation, we have [36]:

$$\begin{bmatrix} \psi_{0^-}^{'} \\ \psi_{0^-}^{''} \\ \psi_{0^-}^{'''} \\ \psi_{0^-}^{''''} \\ \psi_{0^-}^{'''''} \\ \psi_{0^-}^{''''''} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{36} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{46} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{56} \\ b_{61} & b_{62} & b_{63} & b_{64} & b_{65} & b_{66} \end{bmatrix} \begin{bmatrix} \psi_{+1} - a \cdot \psi_0 \\ \psi_{+2} - b \cdot \psi_0 \\ \psi_{+3} - c \cdot \psi_0 \\ \psi_{-1} - \psi_0 \\ \psi_{-2} - \psi_0 \\ \psi_{-3} - \psi_0 \end{bmatrix}$$

From which we have [36]:

$$\begin{aligned} \psi_{0^-}^{''} &= b_{23}\psi_{+3} + b_{22}\psi_{+2} + b_{21}\psi_{+1} - (a \cdot b_{21} + b \cdot b_{22} + c \cdot b_{23} + b_{24} + b_{25} + b_{26})\psi_0 \\ &\quad + b_{24}\psi_{-1} + b_{25}\psi_{-2} + b_{26}\psi_{-3} \end{aligned} \tag{A.23}$$

This relation gives approximation of $\psi_i^{''}$ at an interface point. In the regions of uniform index and uniform mesh, this relation reduces to the 7-point approximation of the form:

$$\psi''_{0^-} \approx \frac{1}{180h^2}(2\psi_{+3} - 27\psi_{+2} + 270\psi_{+1} - 490\psi_0 + 270\psi_{-1} - 27\psi_{-2} + 2\psi_{-3}) \quad \text{(A.24)}$$

By using this seven-point approximations, we get a hepta-diagonal matrix of the form [36]:

$$\frac{1}{180h^2}\begin{bmatrix} -490 & 270 & -27 & 2 & & & & & & \\ 270 & -490 & 270 & -27 & 2 & & & & \mathcal{O} & \\ -27 & 270 & -490 & 270 & -27 & 2 & & & & \\ 2 & -27 & 270 & -490 & 270 & -27 & 2 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 2 & -27 & 270 & -490 & 270 & -27 & 2 \\ & & & & 2 & -27 & 270 & -490 & 270 & -27 \\ & \mathcal{O} & & & & 2 & -27 & 270 & -490 & 270 \\ & & & & & & 2 & -27 & 270 & -490 \end{bmatrix}$$

To find the second-derivative formula at one sampling point before the interface, the procedure is similar to that followed in the previous section. With reference to the figure 3.2, ψ''_0 is to be expressed in terms of ψ_{-1} , ψ_{-2} , ψ_{-3} , ψ_{-4} , ψ_{+1} and ψ_{+2}. Expanding the field samples on either side of the interface in terms of ψ_0:

$$\psi_{-1} = \psi_{0^-} - h_1\psi'_{0^-} + ... + \frac{h_1^6}{6!}\psi''''''_{0^-} + ... \quad \text{(A.25)}$$

$$\psi_{-2} = \psi_{0^-} - 2h_1\psi'_{0^-} + ... + \frac{(-2h_1)^6}{6!}\psi''''''_{0^-} + ... \quad \text{(A.26)}$$

$$\psi_{-3} = \psi_{0-} - 3h_1\psi_{0-}^{'} + ... + \frac{(-3h_1)^6}{6!}\psi_{0-}^{''''''} + ... \tag{A.27}$$

$$\psi_{-4} = \psi_{0-} - 4h_1\psi_{0-}^{'} + ... + \frac{(-4h_1)^6}{6!}\psi_{0-}^{''''''} + ... \tag{A.28}$$

$$\psi_{+1} = \psi_{0+} + h_2\psi_{0+}^{'} + ... + \frac{h_2^6}{6!}\psi_{0+}^{''''''} + ... \tag{A.29}$$

$$\psi_{+2} = \psi_{0+} + 2h_2\psi_{0+}^{'} + ... + \frac{(2h_2)^6}{6!}\psi_{0+}^{''''''} + ... \tag{A.30}$$

Replacing all $\psi_{0+}^{(n)}$ derivatives with $\psi_{0-}^{(n)}$ derivatives in the above equations. After simplifying, we obtain:

$$\begin{aligned}\psi_{+1} = \quad & \psi_0\left(1 + \frac{\zeta_{12}h_2^2}{2!} + \frac{\zeta_{12}^2h_2^4}{4!} + \frac{\zeta_{12}^3h_2^6}{6!}\right) + \rho_{21}\psi_{0-}^{'}\left(h_2 + \frac{\zeta_{12}h_2^3}{3!} + \frac{\zeta_{12}^2h_2^5}{5!}\right) \\ & +\psi_{0-}^{''}\left(\frac{h_2^2}{2!} + \frac{2\zeta_{12}h_2^4}{4!} + \frac{3\zeta_{12}^2h_2^6}{6!}\right) + \rho_{21}\psi_{0-}^{'''}\left(\frac{h_2^3}{3!} + \frac{2\zeta_{12}h_2^5}{5!}\right) \\ & +\psi_{0-}^{''''}\left(\frac{h_2^4}{4!} + \frac{3\zeta_{12}h_2^6}{6!}\right) + \rho_{21}\psi_{0-}^{'''''}\left(\frac{h_2^5}{5!}\right) + \psi_{+1-}^{''''''}\left(\frac{h_2^6}{6!}\right)\end{aligned} \tag{A.31}$$

For ψ_{+2}, replace h_2 by $2h_2$ in equation A.31. Assimilated the above equations in matrix form:

$$\begin{bmatrix} \psi_{+1} - a\cdot\psi_0 \\ \psi_{+2} - b\cdot\psi_0 \\ \psi_{-1} - \psi_0 \\ \psi_{-2} - \psi_0 \\ \psi_{-3} - \psi_0 \\ \psi_{-4} - \psi_0 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} \end{bmatrix} \begin{bmatrix} \psi_{0-}^{'} \\ \psi_{0-}^{''} \\ \psi_{0-}^{'''} \\ \psi_{0-}^{''''} \\ \psi_{0-}^{'''''} \\ \psi_{0-}^{''''''} \end{bmatrix}$$

where a and b are the coefficients of the corresponding ψ_0 terms. Inverting the above matrix equation, we obtain:

$$\begin{bmatrix} \psi'_{0^-} \\ \psi''_{0^-} \\ \psi'''_{0^-} \\ \psi''''_{0^-} \\ \psi'''''_{0^-} \\ \psi''''''_{0^-} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & b_{36} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & b_{46} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} & b_{56} \\ b_{61} & b_{62} & b_{63} & b_{64} & b_{65} & b_{66} \end{bmatrix} \begin{bmatrix} \psi_{+1} - a \cdot \psi_0 \\ \psi_{+2} - b \cdot \psi_0 \\ \psi_{-1} - \psi_0 \\ \psi_{-2} - \psi_0 \\ \psi_{-3} - \psi_0 \\ \psi_{-4} - \psi_0 \end{bmatrix}$$

Differentiating Taylor's series expansion A.25 of ψ_{-1} twice with respect to x, we have:

$$\psi''_{-1} = \psi''_{0^-} - h_1\psi'''_{0^-} + \frac{h_1^2}{2!}\psi''''_{0^-} - \frac{h_1^3}{3!}\psi'''''_{0^-} + \frac{h_1^4}{4!}\psi''''''_{0^-} - +... \tag{A.32}$$

Putting the values of ψ''_{0^-} , ψ'''_{0^-} , ψ''''_{0^-} , ψ'''''_{0^-} and ψ''''''_{0^-} in equation A.32 and simplifying, we obtain:

$$\begin{aligned} \psi''_{-1} = \quad & \psi_{-4}\left(b_{26} - h_1 b_{36} + \frac{h_1^2}{2!}b_{46} - \frac{h_1^3}{3!}b_{56} + \frac{h_1^4}{4!}b_{66}\right) + \\ & \psi_{-3}\left(b_{25} - h_1 b_{35} + \frac{h_1^2}{2!}b_{45} - \frac{h_1^3}{3!}b_{55} + \frac{h_1^4}{4!}b_{65}\right) + \\ & \psi_{-2}\left(b_{24} - h_1 b_{34} + \frac{h_1^2}{2!}b_{44} - \frac{h_1^3}{3!}b_{54} + \frac{h_1^4}{4!}b_{64}\right) + \\ & \psi_{-1}\left(b_{23} - h_1 b_{33} + \frac{h_1^2}{2!}b_{43} - \frac{h_1^3}{3!}b_{53} + \frac{h_1^4}{4!}b_{63}\right) + \\ & \psi_{0}\left(p_1 - h_1 p_2 + \frac{h_1^2}{2!}p_3 - \frac{h_1^3}{3!}p_4 + \frac{h_1^4}{4!}p_5\right) + \\ & \psi_{+1}\left(b_{21} - h_1 b_{31} + \frac{h_1^2}{2!}b_{41} - \frac{h_1^3}{3!}b_{51} + \frac{h_1^4}{4!}b_{61}\right) + \end{aligned}$$

$$\psi_{+2}\left(b_{22}-h_1b_{32}+\frac{h_1^2}{2!}b_{42}-\frac{h_1^3}{3!}b_{52}+\frac{h_1^4}{4!}b_{62}\right) \tag{A.33}$$

where $p_1 = a\cdot b_{21}+b\cdot b_{22}+b_{23}+b_{24}+b_{25}+b_{26}$, $p_2 = a\cdot b_{31}+b\cdot b_{32}+b_{33}+b_{34}+b_{35}+b_{36}$, $p_3 = a\cdot b_{41}+b\cdot b_{42}+b_{43}+b_{44}+b_{45}+b_{46}$, $p_4 = a\cdot b_{51}+b\cdot b_{52}+b_{53}+b_{54}+b_{55}+b_{56}$ and $p_5 = a\cdot b_{61}+b\cdot b_{62}+b_{63}+b_{64}+b_{65}+b_{66}$. This relation gives the seven-point second derivative approximation at one sample point before the interface. The relation at one sample point ahead of the interface is obtained by interchanging $h_2 \rightleftharpoons -h_1$, $\psi_0 \rightleftharpoons \psi_{-2}$, $\psi_{+1} \rightleftharpoons \psi_{-3}$, $\psi_{+2} \rightleftharpoons \psi_{-4}$ and $n_1^2 \rightleftharpoons n_2^2$.

A similar procedure is followed to find the second-derivative formula at two sample points before the interface. With reference to figure 3.2, expanding the field on either sides of the interface in terms of ψ_0:

$$\psi_{-1} = \psi_{0^-} - h_1\psi'_{0^-} + ... + \frac{h_1^6}{6!}\psi''''''_{0^-} + ... \tag{A.34}$$

$$\psi_{-2} = \psi_{0^-} - 2h_1\psi'_{0^-} + ... + \frac{(2h_1)^6}{6!}\psi''''''_{0^-} + ... \tag{A.35}$$

$$\psi_{-3} = \psi_{0^-} - 3h_1\psi'_{0^-} + ... + \frac{(3h_1)^6}{6!}\psi''''''_{0^-} + ... \tag{A.36}$$

$$\psi_{-4} = \psi_{0^-} - 4h_1\psi'_{0^-} + ... + \frac{(4h_1)^6}{6!}\psi''''''_{0^-} + ... \tag{A.37}$$

$$\psi_{-5} = \psi_{0^-} - 5h_1\psi'_{0^-} + ... + \frac{(5h_1)^6}{6!}\psi''''''_{0^-} + ... \tag{A.38}$$

$$\psi_{+1} = \psi_{0^+} + h_2\psi'_{0^+} + ... + \frac{(h_2)^6}{6!}\psi''''''_{0^+} + ... \tag{A.39}$$

Replacing all $\psi_{0^+}^{(n)}$ derivatives with $\psi_{0^-}^{(n)}$ derivatives in above equations:

$$\begin{aligned}\psi_{+1} = \quad & \psi_{0^-}\left(1+\frac{\zeta_{12}h_2^2}{2!}+\frac{\zeta_{12}^2h_2^4}{4!}+\frac{\zeta_{12}^3h_2^6}{6!}\right)+\rho_{21}\psi'_{0^-}\left(h_2+\frac{\zeta_{12}h_2^3}{3!}+\frac{\zeta_{12}^2h_2^5}{5!}\right)\\ & +\psi''_{0^-}\left(\frac{h_2^2}{2!}+\frac{2\zeta_{12}h_2^4}{4!}+\frac{3\zeta_{12}^2h_2^6}{6!}\right)+\rho_{21}\psi'''_{0^-}\left(\frac{h_2^3}{3!}+\frac{2\zeta_{12}h_2^5}{5!}\right)\end{aligned}$$

$$+\psi_{0^-}^{''''}\left(\frac{h_2^4}{4!}+\frac{3\zeta_{12}h_2^6}{6!}\right)+\rho_{21}\psi_{0^-}^{'''''}\left(\frac{h_2^5}{5!}\right)+\psi_{0^-}^{''''''}\left(\frac{h_2^6}{6!}\right) \tag{A.40}$$

Differentiating equation A.35 twice with respect to x:

$$\psi_{-2}^{''}=\psi_{0^-}^{''}-2h_1\psi_{0^-}^{'''}+\frac{(2h_1)^2}{2!}\psi_{0^-}^{''''}-\frac{(2h_1)^3}{3!}\psi_{0^-}^{'''''}+\frac{(2h_1)^4}{4!}\psi_{0^-}^{''''''}-\ldots \tag{A.41}$$

Following the intermediate steps, we get the final relationship:

$$\begin{aligned}\psi_{-2}^{''}= \quad & \psi_{-5}\left(b_{26}-2h_1b_{36}+\frac{(2h_1)^2}{2!}b_{46}-\frac{(2h_1)^3}{3!}b_{56}+\frac{(2h_1)^4}{4!}b_{66}\right)+\\ & \psi_{-4}\left(b_{25}-2h_1b_{35}+\frac{(2h_1)^2}{2!}b_{45}-\frac{(2h_1)^3}{3!}b_{55}+\frac{(2h_1)^4}{4!}b_{65}\right)+\\ & \psi_{-3}\left(b_{24}-2h_1b_{34}+\frac{(2h_1)^2}{2!}b_{44}-\frac{(2h_1)^3}{3!}b_{54}+\frac{(2h_1)^4}{4!}b_{64}\right)+\\ & \psi_{-2}\left(b_{23}-2h_1b_{33}+\frac{(2h_1)^2}{2!}b_{43}-\frac{(2h_1)^3}{3!}b_{53}+\frac{(2h_1)^4}{4!}b_{63}\right)+\\ & \psi_{-1}\left(p_1-2h_1p_2+\frac{(2h_1)^2}{2!}p_3-\frac{(2h_1)^3}{3!}p_4+\frac{(2h_1)^4}{4!}p_5\right)+\\ & \psi_{0}\left(b_{21}-2h_1b_{31}+\frac{(2h_1)^2}{2!}b_{41}-\frac{(2h_1)^3}{3!}b_{51}+\frac{(2h_1)^4}{4!}b_{61}\right)+\\ & \psi_{+1}\left(b_{22}-2h_1b_{32}+\frac{(2h_1)^2}{2!}b_{42}-\frac{(2h_1)^3}{3!}b_{52}+\frac{(2h_1)^4}{4!}b_{62}\right)\end{aligned} \tag{A.42}$$

where $p_1 = a\cdot b_{21}+b_{22}+b_{23}+b_{24}+b_{25}+b_{26}$, $p_2 = a\cdot b_{31}+b_{32}+b_{33}+b_{34}+b_{35}+b_{36}$, $p_3 = a\cdot b_{41}+b_{42}+b_{43}+b_{44}+b_{45}+b_{46}$, $p_4 = a\cdot b_{51}+b_{52}+b_{53}+b_{54}+b_{55}+b_{56}$ and $p_5 = a\cdot b_{61}+b_{62}+b_{63}+b_{64}+b_{65}+b_{66}$. This relation gives the seven-point second derivative approximation at two sample points before the interface. The relation at two sample points ahead of the interface is obtained by interchanging $h_2 \rightleftharpoons -h_1$, $\psi_{-1} \rightleftharpoons \psi_{-3}$, $\psi_0 \rightleftharpoons \psi_{-4}$, $\psi_{+1} \rightleftharpoons \psi_{-5}$ and $n_1^2 \rightleftharpoons n_2^2$.