Supplementary Material

1 APPENDIX

1.1 Error Analysis

Theorem: Let $w_1 = w_1(y, y_1, y_2, y_3), w_2 = w_2(\theta, \theta_1, y, y_1, y_2)$ be differentiable functions, the maximum error attained by the Keller-Box shooting method with Jacobi iterative scheme for Eq. (40) is bounded.

Proof:

Discretize Eqs. (40) using Keller-Box method with Jacobi iterative scheme as follows

$$\begin{aligned}
\frac{y_i^{n+1} - y_{i-1}^n}{\delta h} + (y_1)_{i-1/2}^n &= 0, \\
\frac{(y_1)_i^{n+1} - (y_1)_{i-1}^n}{\delta h} + (y_2)_{i-1/2}^n &= 0, \\
\frac{(y_2)_i^{n+1} - (y_2)_{i-1}^n}{\delta h} + (y_3)_{i-1/2}^n &= 0, \\
\frac{(y_3)_i^{n+1} - (y_3)_{i-1}^n}{\delta h} + (W_1)_{i-1/2}^n &= 0
\end{aligned} \tag{S1}$$

Let the exact scheme be defined as:

$$\begin{aligned}
\frac{y_i^E - y_{i-1}^E}{\delta h} + (y_1)_{i-1/2}^E &= 0, \\
\frac{(y_1)_i^E - (y_1)_{i-1}^E}{\delta h} + (y_2)_{i-1/2}^E &= 0, \\
\frac{(y_2)_i^E - (y_2)_{i-1}^E}{\delta h} + (y_3)_{i-1/2}^E &= 0, \\
\frac{(y_3)_i^E - (y_3)_{i-1}^E}{\delta h} + (W_1)_{i-1/2}^n &= 0,
\end{aligned} \tag{S2}$$

such that at any grid point, errors of the solution follow:

$$\begin{aligned}
(e_1)_i^n &= y_1^n - y_1^E, \\
(e_2)_i^n &= (y_1)_i^n - (y_1)_i^E, \\
(e_3)_i^n &= (y_2)_i^n - (y_2)_i^E, \\
(e_4)_i^n &= (y_3)_i^n - (y_3)_i^E.
\end{aligned} \tag{S3}$$

Applying Mean Value Theorem, one can write

$$\begin{aligned} W_1(y_i^n,(y_1)_i^n,(y_2)_i^n,(y_3)_i^n) &- W_1(y_i^E,(y_1)_i^E,(y_2)_i^E,(y_3)_i^E) \\ &= (\bar{e}_1)_i^n.\nabla W_1(c_1,c_2,c_3), \end{aligned} \quad \text{(S4)}$$

in which

$$\begin{aligned} c_1 &= y_i^n+\varepsilon_1(y_2)_1^n, \\ c_2 &= (y_1)_i^n+\varepsilon_2(e_2)_i^n, \\ c_3 &= (y_2)_i^n+\varepsilon_3(e_3)_i^n, \end{aligned} \quad \text{(S5)}$$

$c_i\epsilon[0,1]$ for $i=1(1)3$, and $(\bar{e}_1)_i^n=[(e_1)_i^n,(e_2)_i^n,(e_3)_i^n]$.

Convergence error equations follow:

$$\begin{aligned} (e_1)^{n+1} &= (e_1)_{i-1}^n+\delta h(e_1)_{i-1/2}^n, \\ (e_2)_i^{n+1} &= (e_2)_{i-1}^n+\delta h(e_2)_{i-1/2}^n, \\ (e_3)_i^{n+1} &= (e_3)_{i-1}^n+\delta h(\hat{e}_1)_{i-1/2}^n\nabla W_1, \end{aligned} \quad \text{(S6)}$$

from Eq. (S6), one can infers the following inequalities

$$\begin{aligned} |(e_1)_i^{n+1}| &\leq |(e_1)_{i-1}^n|+\delta h|(e_2)_{i-1/2}^n|, \\ |(e_2)_i^{n+1}| &\leq |(e_2)_{i-1}^n|+\delta h|(e_3)_{i-1/2}^n|, \\ |(e_3)_i^{n+1}| &\leq |(e_3)_{i-1}^n|+\delta h|(\hat{e}_1)_{i-1/2}^n.\nabla W_1|. \end{aligned} \quad \text{(S7)}$$

Setting $\nabla W_1=[\bar{W}_1^1,\bar{W}_1^2,\bar{W}_1^3]$, Eq. (S7) can be expressed as

$$\begin{aligned} |(e_3)_i^{n+1}| &\leq |(e_3)_{i-1}^n|+\delta h|\Sigma_{j=1}^3(e_j)_{i-1/2}^n\hat{W}_1^j|, \\ &\leq |(e_3)_{i-1}^n|+\delta h\Sigma_{j=1}^3|(e_j)_{i-1/2}^n\bar{W}_1^j|, \end{aligned} \quad \text{(S8)}$$

such that

$$\begin{aligned} |(e_3)_i^{n+1}| &\leq |(e_3)_{i-1}^n|+\delta h|\Sigma_{j=1}^3(e_j)_{i-1/2}^n\hat{W}_1^j|, \\ &\leq |(e_3)_{i-1}^n|+\delta h\Sigma_{j=1}^3|(e_j)_{i-1/2}^n\bar{W}_1^j|. \end{aligned} \quad \text{(S9)}$$

Then

$$\begin{aligned} (e_1)_i^n &= max_{i=1(1)N}|(e_1)_i^n|, \\ (e_2)_i^n &= max_{i=1(1)N}|(e_2)_i^n|, \\ (e_3)_i^n &= max_{i=1(1)N}|(e_3)_i^n|, and \\ (\bar{e})^n &= max[max_{i=1(1)N}(e_1=1(1)N)_i^n]. \end{aligned} \quad \text{(S10)}$$

where N represents the number of nodes. Equations. (S8) and (S9) can be written in the form

$$\begin{aligned} e_1^{n+1} &\leq e_1^n + \delta h e_2^n + \bar{M}_1 O(\delta h)^2, \\ e_2^{n+1} &\leq e_2^n + \delta h e_3^n + \bar{M}_2 O(\delta h)^2, \\ \bar{e}^{n+1} &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)\bar{e}^n + \bar{M}_3 O(\delta h)^2. \end{aligned} \tag{S11}$$

Evaluating $n = 0, 1$,and n in the above expression, one can write

$$\begin{aligned} \bar{e}^1 &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)\bar{e}^0 + \bar{M}_3 O(\delta h)^2, \\ \bar{e}^2 &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^2 \bar{e}^0 + [1 + (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)]\bar{M}_3 O(\delta h)^2, \\ \bar{e}^n &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^n \bar{e}^0 + [1 + (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|) + ..., \\ &+ (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^{n-1}]\bar{M}_3 O(\delta h)^2. \end{aligned} \tag{S12}$$

Taking the sum of the nth term yields

$$\begin{aligned} \bar{e}^n &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^n \bar{e}^0 + \left(\frac{[1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|]^n}{4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|} \right) \bar{M}_3 O(\delta h)^2, \\ &\leq (1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^n \bar{e}^0 + EXP(4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)\bar{M}_3 O(\delta h)^2. \end{aligned} \tag{S13}$$

By virtue of Eq. (S13), Eq. (S11) becomes

$$\begin{aligned} e_1^n &\leq (1 + \delta h)[(1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^n \bar{e}^0 + EXP(4(n-1)\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)\bar{M}_3 O(\delta h)^2], \\ &+ \bar{M}_1 O(\delta h)^2, \end{aligned} \tag{S14}$$

$$\begin{aligned} e_2^n &\leq (1 + \delta h)[(1 + 4\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)^n \bar{e}^0 + EXP(4(n-1)\delta h \Sigma_{j=1}^4 |\bar{W}_1^j|)\bar{M}_3 O(\delta h)^2], \\ &+ \bar{M}_2 O(\delta h)^2. \end{aligned} \tag{S15}$$

Equations (S14) and (S15) give the maximum error bounds for Eqs. (44)-(51). Thus, error for Eqs. (33) with the condition expressed in Eqs. (34) and (35) can be shown in the similar way (see [18]).