

NOTES AND CORRESPONDENCE

Accuracy of Multiply-Upstream, Semi-Lagrangian Advective Schemes II

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ABSTRACT

The degree of accuracy of various multiply-upstream semi-Lagrangian schemes is examined by analyzing the driven one-dimensional advection equation. The relationship between the order of accuracy of a given scheme and the order of the interpolations used, both to find the position of, and the value of the fields at, the departure point is established. In the process, it is shown how to construct a semi-Lagrangian scheme which is accurate to third-order.

1. Introduction

In practical integrations of the primitive meteorological equations using the multiply-upstream semi-Lagrangian approach, the departure point displacement (a , b) of a particle in a velocity field (u , v) over a time interval Δt has been estimated in a variety of ways. Robert (1981), and Robert et al. (1985) iterated twice the equations

$$\begin{aligned} a^{(m)} &= \Delta t u(x - a^{(m-1)}, y - b^{(m-1)}, t) \\ b^{(m)} &= \Delta t v(x - a^{(m-1)}, y - b^{(m-1)}, t), \end{aligned} \quad (1)$$

using a bicubic scheme to interpolate. Temperton and Staniforth (1986) iterated four times with a bilinear scheme, whereas McDonald and Bates (1987) found that iterating once with a bilinear scheme was sufficient to attain the accuracy they required. For smaller time steps, the latter authors found that using the grid point velocity to estimate the departure point displacement gave the level of accuracy needed; see Bates and McDonald (1982) and McDonald (1986). Another option used has been the 'non interpolating' approach of Ritchie (1986).

Although all of these integrations are not directly comparable, one can infer from them that for larger time steps the iterative procedure is necessary to estimate the departure point position. However, the question not clearly answered is the following. What is the lowest order interpolation scheme allied with the least number of iterations of (1) which gives solutions correct to a given degree of accuracy? Because iterating is potentially an expensive procedure, it is important to address this question, which is done in this note by analyzing semi-Lagrangian discrete approximations to the driven one-dimensional advection equation.

2. Accuracy

When performing an integration in a semi-Lagrangian and implicit manner using two time levels, the one-dimensional equation

$$\partial\psi(x, t)/\partial t + u(x, t)\partial\psi(x, t)/\partial x = \xi(x, t) \quad (2)$$

is assumed, when discretized in space and time, to have the solution

$$\begin{aligned} \Delta_L\psi/\Delta t - \bar{\xi}^L \\ = \{\psi[I\Delta x, (n+1)\Delta t] - \psi(I\Delta x - \hat{u}\Delta t, n\Delta t)\}/\Delta t \\ - \{\xi[I\Delta x, (n+1)\Delta t] + \xi(I\Delta x - \hat{u}\Delta t, n\Delta t)\}/2 = 0 \end{aligned} \quad (3)$$

where $x = I\Delta x$, and $t = n\Delta t$. In what follows, the advecting velocity \hat{u} will be defined either as the grid point velocity u_i^n or by means of the iterative procedure of Robert (1981) in which the m th guess of \hat{u} is expressed in terms of the $(m-1)$ 'st guess as follows:

$$\hat{u}^{(m)} = u\{I\Delta x - \hat{u}^{(m-1)}\Delta t/2, (n+1/2)\Delta t\}, \quad (4)$$

where $\hat{u}^{(0)} = u\{I\Delta x, (n+1/2)\Delta t\}$, and u is known only at the discrete points $(I\Delta x, n\Delta t)$.

In (3) and (4), the values of the fields at the departure point, $I\Delta x - \hat{u}\Delta t$, are not known and must be estimated by a suitable interpolation procedure. The question to be addressed is as follows. How closely does the finite difference equation (3) approximate the differential equation (2), if a given number of iterations of Eq. (4) are used to estimate \hat{u} ? This is done by expanding all of the quantities in Eq. (3) about the point $(I\Delta x, n\Delta t)$ using a Taylor series.

a. Scheme (a)

Consider first the accuracy of a model which uses a linear interpolation to approximate ψ and ξ at the departure point, that is,

$$\psi(I\Delta x - \hat{u}\Delta t, n\Delta t) = (1 - \hat{\alpha})\psi_{I-p}^n + \hat{\alpha}\psi_{I-p-1}^n \quad (5)$$

where

$$\hat{\alpha} = -p + \hat{u}\Delta t/\Delta x, \quad (6)$$

and $\psi_i^n = \psi(I\Delta x, n\Delta t)$. The integer p is such that the departure point lies between $(I-p)\Delta x$ and $(I-p-1)\Delta x$, and consequently, $0 \leq \hat{\alpha} < 1$.

Expanding all quantities except \hat{u} about $(I\Delta x, n\Delta t)$, and using (A1), it can be shown that

$$\frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = \left(\frac{\partial \psi}{\partial t}\right)_I^n + \hat{u} \left(\frac{\partial \psi}{\partial x}\right)_I^n - \xi_I^n + O(\Delta), \quad (7)$$

which is accurate to $O(\Delta)$, where Δ may equal Δt or Δx , depending on how the ratio $\Delta t/\Delta x$ behaves in the limit as Δx and Δt approach zero (see McDonald, 1984). This is true whether the velocity \hat{u} is estimated by using the grid point velocity u_I^n , or by iterating.

b. Schemes (b1) and (b2)

Next, consider the accuracy of models which use a quadratic interpolation to approximate ψ and ξ at the departure point, that is,

$$\psi(I\Delta x - \hat{u}\Delta t, n\Delta t) = 0.5\hat{\alpha}(1 + \hat{\alpha})\psi_{I-p}^n + (1 - \hat{\alpha})(1 + \hat{\alpha})\psi_{I-p}^n - 0.5\hat{\alpha}(1 - \hat{\alpha})\psi_{I-p+1}^n, \quad (8)$$

where $\hat{\alpha}$ is as defined in (6), and p is an integer such that $-0.5 \leq \hat{\alpha} < 0.5$. Again, expanding all quantities except \hat{u} about $(I\Delta x, n\Delta t)$, and using (A2) it can be shown that

$$\begin{aligned} \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = & \left(\frac{\partial \psi}{\partial t}\right)_I^n + \hat{u} \left(\frac{\partial \psi}{\partial x}\right)_I^n - \xi_I^n + \frac{\Delta t}{2} \left\{ \left(\frac{\partial^2 \psi}{\partial t^2}\right)_I^n \right. \\ & \left. - \hat{u}^2 \left(\frac{\partial^2 \psi}{\partial x^2}\right)_I^n - \left(\frac{\partial \xi}{\partial t}\right)_I^n + \hat{u} \left(\frac{\partial \xi}{\partial x}\right)_I^n \right\} + O(\Delta^2). \quad (9) \end{aligned}$$

Scheme (b1). If \hat{u} is approximated by the grid point velocity, u_I^n , one sees that the scheme is accurate to $O(\Delta t)$ or $O(\Delta x^2)$, whichever is larger.

The semi-Lagrangian part of this scheme is analogous to that used by Bates and McDonald (1982) to integrate a multilevel primitive equation model using real data. They found it to be superior to a scheme analogous to (a) which gave excessively smooth forecasts, and as good as a split-explicit Eulerian model to which it was compared, for advective time steps of 30 min and a spatial grid of 160 km.

Scheme (b2). What happens if \hat{u} is estimated using "centering in space and time"? Consider the simplest possible case, a single iteration of (4) using a linear interpolation,

$$\begin{aligned} \hat{u}^{(1)} = & u\{I\Delta x - u_I^{n+1/2}\Delta t/2, (n+1/2)\Delta t\}, \\ = & (1 - \hat{\gamma})u_{I-m}^{n+1/2} + \hat{\gamma}u_{I-m+1}^{n+1/2}, \quad (10) \end{aligned}$$

where

$$\hat{\gamma} = -m + \Delta t u_I^{n+1/2}/(2\Delta x), \quad (11)$$

and m is an integer such that $0 \leq \hat{\gamma} < 1$. Using Eq. (A1) yields

$$\hat{u}^{(1)} = \{u - (u\partial u/\partial x)\Delta t/2\}_I^{n+1/2} + O(\Delta t\Delta). \quad (12)$$

Using the following to approximate $u_I^{n+1/2}$,

$$u_I^{n+1/2} = (3u_I^n - u_I^{n-1})/2, \quad (13)$$

gives, after expanding u_I^{n-1} about $(I\Delta x, n\Delta t)$,

$$\hat{u}^{(1)} = \{u + (\partial u/\partial t - u\partial u/\partial x)\Delta t/2\}_I^n + O(\Delta t\Delta). \quad (14)$$

Substituting $\hat{u}^{(1)}$ into (9) one obtains

$$\begin{aligned} \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = & \left\{ \frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} - \xi \right\}_I^n \\ & + \frac{\Delta t}{2} \left\{ \left(\frac{\partial}{\partial t} - u \frac{\partial}{\partial x} \right) \left(\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} - \xi \right) \right\}_I^n + O(\Delta^2) \\ = & \left\{ \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L \right\}_1 + O(\Delta^2). \quad (15) \end{aligned}$$

Thus, a quadratic interpolation to estimate the departure point values of ψ and ξ , one iteration using a linear interpolation to "center in space", and Eq. (13) to "center in time" all combine to give accuracy to $O(\Delta^2)$.

It becomes clearer why the iterated estimate of the departure point position should yield superior forecasts for large Δt ; it raises the overall accuracy of the scheme from $O(\Delta t)$ to $O(\Delta t^2)$.

c. Schemes (c1), (c2), and (c3)

Consider now the accuracy of schemes which use a cubic interpolation to approximate ψ and ξ at the departure point, that is,

$$\begin{aligned} \psi(I\Delta x - \hat{u}\Delta t, n\Delta t) = & -\frac{1}{6}\hat{\alpha}(1 - \hat{\alpha})(1 + \hat{\alpha})\psi_{I-p-2}^n \\ & + \frac{1}{2}\hat{\alpha}(1 + \hat{\alpha})(2 - \hat{\alpha})\psi_{I-p-1}^n \\ & + \frac{1}{2}(1 - \hat{\alpha})(1 + \hat{\alpha})(2 - \hat{\alpha})\psi_{I-p}^n - \frac{1}{6}\hat{\alpha}(1 - \hat{\alpha})(2 - \hat{\alpha})\psi_{I-p+1}^n. \quad (16) \end{aligned}$$

As in (a), $0 \leq \hat{\alpha} < 1$. Expanding all quantities except \hat{u} about $(I\Delta x, n\Delta t)$, it can be shown by using (A3) that

$$\begin{aligned} \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = & \left(\frac{\partial \psi}{\partial t}\right)_I^n + \hat{u} \left(\frac{\partial \psi}{\partial x}\right)_I^n - \xi_I^n \\ & + \frac{\Delta t}{2} \left\{ \left(\frac{\partial^2 \psi}{\partial t^2}\right)_I^n - \hat{u}^2 \left(\frac{\partial^2 \psi}{\partial x^2}\right)_I^n - \left(\frac{\partial \xi}{\partial t}\right)_I^n + \hat{u} \left(\frac{\partial \xi}{\partial x}\right)_I^n \right\} \\ & + \frac{\Delta t^2}{6} \left\{ \left(\frac{\partial^3 \psi}{\partial t^3}\right)_I^n + \hat{u}^3 \left(\frac{\partial^3 \psi}{\partial x^3}\right)_I^n - \frac{3}{2} \left(\frac{\partial^2 \xi}{\partial t^2}\right)_I^n - \frac{3\hat{u}^2}{2} \left(\frac{\partial^2 \xi}{\partial x^2}\right)_I^n \right\} \\ & + O(\Delta^3). \quad (17) \end{aligned}$$

Scheme (c1). If the grid point velocity, u_I^n , is used to approximate \hat{u} the scheme is accurate to $O(\Delta t) + O(\Delta x^3)$. The model of McDonald (1986) is analogous to this. He reported acceptable 24 h forecasts using a primitive equation model with $\Delta t = 1$ h and a space discretization of 160 km. This analysis indicates that the time truncation error was not yet dominating the space truncation error for these forecasts.

Scheme (c2). If \hat{u} is computed using one iteration of a linear interpolation to “center in space” and Eq. (13) to “center in time”, the overall accuracy of the scheme is raised to $O(\Delta t^2)$ as can be seen by substituting Eq. (14) into Eq. (17):

$$\frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = \left\{ \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L \right\}_1 + O(\Delta t^2) + O(\Delta^3). \quad (18)$$

This is analogous to the scheme described in McDonald and Bates (1987) where $\Delta t = 1.5$ h was used with a spatial grid of 160 km to obtain accurate forecasts, and also to Method 2 of Temperton and Staniforth (1986) who reported satisfactory integrations of a shallow water model with $\Delta t = 2$ h for a spatial discretization of 100 km.

Looking at Eq. (17) it is clear that using a cubic interpolation to estimate ψ and ξ at the departure point gives rise to the possibility of constructing an $O(\Delta^3)$ accurate scheme provided, among other things, that \hat{u} is calculated to $O(\Delta^3)$. This latter can be done as follows.

Scheme (c3). First, when centering in time, use three levels,

$$u_I^{n+1/2} = (15u_I^n - 10u_I^{n-1} + 3u_I^{n-2})/8, \quad (19)$$

and secondly, when centering in space use a quadratic interpolation and iterate twice. The first iteration yields, using (A2),

$$\begin{aligned} \hat{u}^{(1)} &= u \{ I\Delta x - u_I^{n+1/2} \Delta t/2, (n+1/2)\Delta t \}, \\ &= \{ u - (u\partial u/\partial x)\Delta t/2 + (u^2\partial^2 u/\partial x^2)\Delta t^2/8 \}_I^{n+1/2} \\ &\quad + O(\Delta t\Delta^2). \end{aligned} \quad (20)$$

Iterating again gives, using Eq. (A2),

$$\begin{aligned} \hat{u}^{(2)} &= u \{ I\Delta x - \hat{u}^{(1)}\Delta t/2, (n+1/2)\Delta t \}, \\ &= u_I^{n+1/2} - \frac{\Delta t}{2} \hat{u}^{(1)} \left(\frac{\partial u}{\partial x} \right)_I^{n+1/2} \\ &\quad + \frac{\Delta t^2}{8} \{ \hat{u}^{(1)} \}^2 \left(\frac{\partial^2 u}{\partial x^2} \right)_I^{n+1/2} + O(\Delta t\Delta^2), \end{aligned} \quad (21)$$

$$\begin{aligned} &= \{ u - (u\partial u/\partial x)\Delta t/2 + [u^2\partial^2 u/\partial x^2 \\ &\quad + 2u(\partial u/\partial x)^2]\Delta t^2/8 \}_I^{n+1/2} + O(\Delta t\Delta^2). \end{aligned} \quad (22)$$

A third iteration will not improve the order of accuracy unless it is accompanied by a cubic interpolation. Also, looking at (21), it becomes clear that it would have been sufficient to use a linear interpolation when computing $\hat{u}^{(1)}$ to attain $O(\Delta t\Delta^2)$ accuracy for $\hat{u}^{(2)}$. Temperton and Staniforth (1986) iterate four times using a bilinear interpolation in their Scheme 3. The above indicates that a bilinear followed by a biquadratic interpolation might have yielded an improved result.

Substituting Eq. (19) into Eq. (22) and expanding u_I^{n-1} and u_I^{n-2} about $n\Delta t$ yields

$$\begin{aligned} \hat{u}^{(2)} &= \left\{ u + \frac{\Delta t}{2} \left(\frac{\partial u}{\partial t} - u \frac{\partial u}{\partial x} \right) + \frac{\Delta t^2}{8} \left[\frac{\partial^2 u}{\partial t^2} - 2 \frac{\partial u}{\partial t} \frac{\partial u}{\partial x} \right. \right. \\ &\quad \left. \left. - 2u \frac{\partial^2 u}{\partial x \partial t} + 2u \left(\frac{\partial u}{\partial x} \right)^2 + u^2 \frac{\partial^2 u}{\partial x^2} \right] \right\}_I^n + O(\Delta t\Delta^2). \end{aligned} \quad (23)$$

Substituting Eq. (23) into Eq. (17) gives

$$\frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L = \left\{ \frac{\Delta_L \psi}{\Delta t} - \bar{\xi}^L \right\}_1 + \Delta t^2 (T_2)_I^n + O(\Delta^3) \quad (24)$$

where T_2 is given by Eq. (A4).

This is the analogue of the Temperton and Staniforth (1986) Scheme 3, with the reservation expressed above. They found it gave good results for a shallow water model with $\Delta t = 3$ h on a 100 km grid.

The above suggests a general procedure. To attain $O(\Delta t\Delta^r)$ accuracy in calculating \hat{u} , estimate it using r iterations, the first of which uses a linear, the second a quadratic, the third a cubic, and so on until the last, which uses an r th order interpolation. Simultaneously, use $(r+1)$ levels to center in time.

3. Construction of higher order schemes

All of the ingredients which make up scheme (c3) are potentially accurate to $O(\Delta^3)$. This gives rise to the question as to whether (2) can be solved in a semi-Lagrangian manner to this level of accuracy, not with only two time levels. Thus, to answer the question, the three-time level approach must be examined. This involves using

$$\begin{aligned} \Delta_{2L}\psi/2\Delta t - \bar{\xi}^{2L} &= \{ \psi [I\Delta x, (n+1)\Delta t] \\ &\quad - \psi [I\Delta x - 2\tilde{u}\Delta t, (n-1)\Delta t] \} / 2\Delta t \\ &\quad - \{ \xi [I\Delta x, (n+1)\Delta t] + \xi [I\Delta x - 2\tilde{u}\Delta t, (n-1)\Delta t] \} / 2 \\ &= 0 \end{aligned} \quad (3a)$$

as a finite difference approximation to (2), and

$$\tilde{u}^{(m)} = u \{ I\Delta x - \tilde{u}^{(m-1)}\Delta t, n\Delta t \}, \quad (4a)$$

where $\tilde{u}^{(0)} = u(I\Delta x, n\Delta t)$, to center in space. Of course, the question of centering in time does not arise.

If ψ and ξ are estimated at the departure point by means of a cubic interpolation and \tilde{u} is evaluated by iterating twice, using a linear followed by a quadratic interpolation, as in (c3), one obtains

$$\begin{aligned} \frac{\Delta_{2L}\psi}{2\Delta t} - \bar{\xi}^{2L} &= \left\{ \left(1 - \Delta t u \frac{\partial}{\partial x} \right) \left(\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} - \xi \right) + \Delta t^2 T_3 \right\}_I^n \\ &\quad + O(\Delta^3) \end{aligned} \quad (25)$$

where T_3 is given by Eq. (A5). So this scheme is also accurate to $O(\Delta t^2)$, but the errors are four times as large as in Eq. (24), as can be seen by comparing T_2 and T_3 . This was pointed out by Temperton and Staniforth (1986) as a possible advantage of the two-time level approach.

This scheme is the one-dimensional analogue of the model of Robert et al. (1985) who, however, iterate twice with a bicubic interpolation to ‘center in space’. This analysis indicates that they might retain the same accuracy while improving their efficiency by using a bilinear followed by a biquadratic interpolation. They reported accurate integrations of a multilevel primitive equation model with $\Delta t = 1.5$ h for a spatial grid of 190 km.

It now becomes obvious how to construct an $O(\Delta^3)$ accurate scheme: the $O(\Delta t^2)$ errors in T_2 and T_3 cancel if one takes $\frac{2}{3} \times$ Eq. (24) $- \frac{1}{3} \times$ Eq. (25). Thus, the finite difference equation

$$\frac{4}{3} \left\{ \frac{\Delta_L \psi}{\Delta t} - \bar{\xi} L \right\} - \frac{1}{3} \left\{ \frac{\Delta_{2L} \psi}{2\Delta t} - \bar{\xi} 2L \right\} = 0 \quad (26)$$

will yield an $O(\Delta^3)$ accurate scheme. This can be written as

$$\begin{aligned} & \{ 7\psi[I\Delta x, (n+1)\Delta t] - 8\psi[I\Delta x - \hat{u}\Delta t, n\Delta t] \\ & + \psi[I\Delta x - 2\hat{u}\Delta t, (n-1)\Delta t] \} / 6\Delta t \\ & + \{ -3\xi[I\Delta x, (n+1)\Delta t] - 4\xi[I\Delta x - \hat{u}\Delta t, n\Delta t] \\ & + \xi[I\Delta x - 2\hat{u}\Delta t, (n-1)\Delta t] \} / 6 = 0. \quad (27) \end{aligned}$$

If one uses a cubic interpolation to approximate ψ and ξ at the departure point, a linear interpolation to evaluate $\hat{u}^{(1)}$ and $\hat{u}^{(2)}$, a quadratic interpolation to evaluate $\hat{u}^{(2)}$ and $\hat{u}^{(2)}$, and Eq. (19) to ‘center in time’ when evaluating \hat{u} , then Eq. (27) yields an $O(\Delta^3)$ accurate scheme. Expanding about $(I\Delta x, n\Delta t)$ and substituting gives

$$\begin{aligned} & \left[\left[1 + \frac{\Delta t}{3} \left(2 \frac{\partial}{\partial t} - u \frac{\partial}{\partial x} \right) + \frac{\Delta t^2}{6} \frac{\partial}{\partial t} \left(\frac{\partial}{\partial t} - 2u \frac{\partial}{\partial x} \right) \right] \right. \\ & \left. \times \left[\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} - \xi \right] \right]^n + O(\Delta^3) = 0. \quad (28) \end{aligned}$$

It would be interesting to test this scheme in a realistic setting to see if the promise of high accuracy in both Δt and Δx held up in practice.

4. Concluding remarks

The order of accuracy of the various approaches to integrating the advection equation with forcing term in a semi-Lagrangian and implicit manner has been examined. In the process, it has been shown how to construct a scheme which is accurate to $O(\Delta^3)$. The procedure generalizes to higher order in Δ . As a result, it should be possible to construct semi-Lagrangian schemes which are accurate to any desired order.

The foregoing analysis also helps to explain the results obtained by Pudykiewicz and Staniforth (1984) and McDonald (1984), who tested the semi-Lagrangian procedure by advecting a cone at constant angular velocity about a point in the (x, y) plane. They found that for large Δt using \hat{u} as estimated by (4) gave superior results to using $\hat{u} = u_I^n$. It is now clear that the

former choice of \hat{u} yields a scheme accurate to $O(\Delta t^2)$ whereas the latter yields one accurate only to $O(\Delta t)$, as Staniforth and Pudykiewicz (1985) had speculated.

APPENDIX

It is easy to show the following by expanding ϕ in a Taylor series about $I\Delta x$. (It is not necessary to assume any relationship between p and $\hat{\alpha}$ to obtain these results.)

For the linear interpolation,

$$\begin{aligned} & (1 - \hat{\alpha})\phi_{I-p} + \hat{\alpha}\phi_{I-p-1} \\ & = \phi_I - (p + \hat{\alpha})\Delta x \left(\frac{\partial \phi}{\partial x} \right)_I + \sum_{l=2}^{\infty} \frac{\Delta x^l}{l!} \left(\frac{\partial^l \phi}{\partial x^l} \right)_I W_1^l(\hat{\alpha}, p). \quad (A1) \end{aligned}$$

For the quadratic interpolation,

$$\begin{aligned} & 0.5\hat{\alpha}(1 + \hat{\alpha})\phi_{I-p-1} + (1 - \hat{\alpha})(1 + \hat{\alpha})\phi_{I-p} \\ & - 0.5\hat{\alpha}(1 - \hat{\alpha})\phi_{I-p+1} = \phi_I - (p + \hat{\alpha})\Delta x \left(\frac{\partial \phi}{\partial x} \right)_I \\ & + (p + \hat{\alpha})^2 \frac{\Delta x^2}{2} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_I + \sum_{l=3}^{\infty} \frac{\Delta x^l}{l!} \left(\frac{\partial^l \phi}{\partial x^l} \right)_I W_2^l(\hat{\alpha}, p). \quad (A2) \end{aligned}$$

For the cubic interpolation,

$$\begin{aligned} & -\frac{1}{6}\hat{\alpha}(1 - \hat{\alpha})(2 - \hat{\alpha})\phi_{I-p+1} + \frac{1}{2}(1 - \hat{\alpha})(1 + \hat{\alpha})(2 - \hat{\alpha})\phi_{I-p} \\ & + \frac{1}{2}\hat{\alpha}(1 + \hat{\alpha})(2 - \hat{\alpha})\phi_{I-p-1} - \frac{1}{6}\hat{\alpha}(1 - \hat{\alpha})(1 + \hat{\alpha})\phi_{I-p-2} \\ & = \phi_I - (p + \hat{\alpha})\Delta x \left(\frac{\partial \phi}{\partial x} \right)_I + (p + \hat{\alpha})^2 \frac{\Delta x^2}{2} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_I \\ & - (p + \hat{\alpha})^3 \frac{\Delta x^3}{6} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_I + \sum_{l=4}^{\infty} \frac{\Delta x^l}{l!} \left(\frac{\partial^l \phi}{\partial x^l} \right)_I W_3^l(\hat{\alpha}, p). \quad (A3) \end{aligned}$$

The $W_r^l(\hat{\alpha}, p)$ are polynomials in $\hat{\alpha}$ and p , and are defined in McDonald (1984). If p and $\hat{\alpha}$ are related as in (6) then, $\Delta x^l W_r^l(\hat{\alpha}, p) / \Delta t$ is of order Δ^{l-1} , where Δ may be Δt or Δx depending on how the ratio $\Delta t / \Delta x$ behaves in the limit as Δt and Δx approach zero. {See (15)–(17) in Section 2b of McDonald (1984), in which there is an error in (17), the last term of which should read $O[(\Delta x / \Delta t)^l]$.

The $O(\Delta t^2)$ terms in Eqs. (24) and (25) are constructed as follows:

$$\begin{aligned} t_1 & = \partial / \partial t (\partial / \partial t - 2u\partial / \partial x) (\partial \psi / \partial t + u\partial \psi / \partial x - \xi) / 6 \\ t_2 & = u\partial / \partial x (\partial / \partial t + u\partial / \partial x) (\partial \psi / \partial t + u\partial \psi / \partial x - \xi) / 6 \\ & - (\partial / \partial t + u\partial / \partial x) (\partial \xi / \partial t + u\partial \xi / \partial x) / 12 - (\partial \psi / \partial x) \\ & \times (\partial / \partial t + u\partial / \partial x - 3\partial u / \partial x) (\partial u / \partial t + u\partial u / \partial x) / 24 \\ T_2 & = t_1 + t_2 \quad (A4) \end{aligned}$$

$$T_3 = t_1 + 4t_2. \quad (A5)$$

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