A new approach to design high-order schemes

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Abstract

In this paper a new approach, MPDE-aided method of undetermined coefficients, is proposed to design high-order finite difference schemes. This designing approach differs from other approaches in that it is constructed on the analysis theory of the modified partial differential equation. By this approach, not only the deduction of different schemes is unified, but also some multi-level highly accurate schemes are developed. Numerical tests for these high-order schemes are presented to verify their quality. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

There have been a great number of finite difference schemes developed for the solution of the unsteady advection equation. Most of these schemes are two-level explicit schemes (cf. [1,2,4,7–9,15]). Typical examples are presented as follows: the first-order upwind scheme is equivalent to two-node linear interpolation; the second-order Lax–Wendroff scheme is equivalent to three-node quadratic interpolation; the third-order QUICKEST scheme is equivalent to four-node cubic interpolation. In situations where the solution profile is sharp but smooth, or the wave frequency is high, the use of the above low-order schemes will cause over-smoothness to wave amplitude, or introduce spurious oscillation, or show significant phase error, thus cannot meet the needs of numerical simulation. Therefore, complicated Lagarangian or Hermitian interpolative polynomials are developed to design high-order accurate schemes (cf. [4,9,15]).

Although these methods are skillful and directional, they have some common defects. As two-level explicit schemes, they have to use at least \((N+1)\) nodes in one level to achieve \(N\)-th-order accuracy. When \(N\) is large, the schemes are surprisingly wide, thus neither compact nor efficient. Furthermore,
they usually need special procedures to deal with inflow or overflow boundaries, as well as handle locally refined meshes.

On the other hand, there are some multi-level schemes that can effectively overcome the above defects. Classical leapfrog scheme is the most familiar three-level scheme, which is simple and free of dissipation but introduces notable dispersive effect. Then, Iserles developed upwind leapfrog schemes, which combine the virtue of classical leapfrog scheme and upwinding method to achieve compact stencils and high accuracy, possessing the advantage of nondissipation and weak dispersion (cf. [5,6,10]). These examples inspire us to seek effective multi-level highly accurate schemes.

In the present paper, we propose a new approach to design high-order schemes. This approach possesses the great generality that it can be applied to the design of both two-level and multi-level schemes, both explicit and implicit ones. By this approach, we will unify the deduction of the above schemes introduced by different authors using different methods, as well as develop some highly accurate multi-level schemes. The theoretical tool of this approach is the Modified Partial Differential Equation (MPDE) analysis theory (cf. [3,11–14]).

2. MPDE aided method of undetermined coefficient

The one-dimensional unsteady advection of scalar \( u \) with constant positive velocity \( a \) is considered:

\[
    u_t + au_x = 0. \tag{1}
\]

Suppose that we apply a \( N \)-level, \( M \)-node finite difference scheme to approximate (1). The scheme generally takes the form

\[
    u_j^{n+1} + \sum_{l \neq 0} \alpha_l u_{j+1}^{n+1} = \sum_{m=0}^{N-2} \sum_k \beta_{mk} u_{j+k}^{n-m}, \tag{2}
\]

where \( \alpha_l (l = \pm 1, \pm 2, \ldots) \), \( \beta_{mk} (m = 0, 1, \ldots, N-2; k = 0, \pm 1, \pm 2, \ldots) \) are just the undetermined coefficients and there are totally \( M \) such unknowns. Consequently, \( M \) equations are needed to completely determine these coefficients.

Suppose that \( u \) is sufficiently smooth. Expanding (2) into Taylor series at grid point \((x_j, t_n)\) and collecting the terms, we get

\[
    P_{00} u + P_{10} u_t + P_{11} u_x + P_{20} u_{tt} + P_{21} u_{tx} + P_{22} u_{xx} + \cdots + P_{M0} \frac{\partial^M u}{\partial t^M} + \cdots + P_{MM} \frac{\partial^M u}{\partial x^M} + \cdots = 0, \tag{3}
\]

where the coefficients \( P_{ij} (i,j = 0,1,\ldots) \) are linear combinations of \( \alpha_l \), \( \beta_{mk} \) and, without loss of generality, we can let \( P_{10} = 1 \) after normalization. The basic consistency condition yields

\[
    P_{00}(\alpha_l, \beta_{mk}) = 0, \quad P_{11}(\alpha_l, \beta_{mk}) = a \tag{4}
\]

from which we can drop two unknowns.

To seek the other \( M-2 \) equations, we carry out the procedure of self-elimination on (3) (note: do not use the original Eq. (1) itself) and obtain the MPDE perfectly equivalent to (2) (cf. [3,11–14]):

\[
    u_t + au_x = Q_2 u_{xx} + Q_3 u_{xxx} + Q_4 u_{xxxx} + \cdots, \tag{5}
\]
where the coefficients $Q_i$ ($i = 1, 2, 3, \ldots$) are polynomials of $\alpha_i, \beta_{mk}$. To make scheme (2) reach the highest accuracy, we force

$$Q_2(\alpha_i, \beta_{mk}) = 0, \quad Q_3(\alpha_i, \beta_{mk}) = 0, \ldots, \quad Q_{M-1}(\alpha_i, \beta_{mk}) = 0$$

from which we solve out the left $M - 2$ unknowns and definitely determine scheme (2), which achieves $(M - 1)$th-order accuracy.

One problem remains in the application of the above idea. That is, when $M$ is large ($M \geq 5$), the coefficients $Q_i$ in (5) may be high-degree polynomials of the unknowns $\alpha_i, \beta_{mk}$, which makes the system of nonlinear equations (6) seemingly unsolvable. However, the following theorem ensures that, in fact, (6) can be reduced to linear simultaneous equations.

**Theorem 1.** Suppose $L$ is an integer satisfying $2 \leq L \leq M - 1$, if we have in (5)

$$Q_2 = Q_3 = \cdots = Q_{L-1} = 0$$

then

$$Q_L = P_{LL} - aP_{L,L-1} + a^2 P_{L,L-2} - \cdots + (-a)^L P_{L,0},$$

where $P_{Li}$ ($i = 0, 1, \ldots, L$) are the coefficients in (3) and are linear combinations of the unknowns $\alpha_i, \beta_{mk}$.

**Proof.** This is rather a work of algebraic substitution. The only thing we need to take notice of is the equivalence of the substitution, which means that we should not use (1) in the procedure. From (5) and (7) we get

$$u_t + au_x = Q_1 \frac{\partial^L u}{\partial x^L} + \text{HOD}(L),$$

where HOD$(L)$ denote those derivative terms with order higher than $L$. Note that (9) and (3) are equivalents provided (7) holds true. By repeated self-differentiation and substitution, (9) yields

$$\frac{\partial^{p+q} u}{\partial t^p \partial x^q} = \frac{\partial^{p+q-1}}{\partial t^{p-1} \partial x^q} \left(-au_x + Q_1 \frac{\partial^L u}{\partial x^L} + \text{HOD}(L)\right)$$

$$\equiv (-a) \frac{\partial^{p+q} u}{\partial t^{p-1} \partial x^{q+1}} + \text{HOD}(L + p + q - 2)$$

$$\equiv (-a)^2 \frac{\partial^{p+q} u}{\partial t^{p-2} \partial x^{q+2}} + \frac{\partial^{p+q-1}}{\partial t^{p-2} \partial x^{q+1}} \left(Q_1 \frac{\partial^L u}{\partial x^L} + \text{HOD}(L)\right) + \text{HOD}(L + p + q - 2)$$

$$\equiv (-a)^2 \frac{\partial^{p+q} u}{\partial t^{p-2} \partial x^{q+2}} + \text{HOD}(L + p + q - 2)$$

$$= \cdots$$

$$\equiv (-a)^p \frac{\partial^{p+q} u}{\partial x^{p+q}} + \text{HOD}(L + p + q - 2)$$

$$p + q = 2, 3, \ldots, L, \quad p, q = 0, 1, 2, \ldots.$$  \hspace{1cm} (10)

Substitute (10) into (3) and we easily find $Q_L$ expressed as the very form in (8). \qed
Now we permit $L$ to take the values of 0, 1. From (8) it is obvious that $Q_0 = P_{00}$, $Q_1 = P_{11} - a$.

Combining conditions (4), (6) and Theorem 1, we immediately obtain the following:

**Theorem 2.** To completely determine the unknowns $\alpha_i$, $\beta_{mk}$ and make scheme (2) achieve the highest $(M - 1)$th-order accuracy, we only need to solve the linear simultaneous equations

$$
P_{LL}(\alpha_i, \beta_{mk}) - aP_{L,L-1}(\alpha_i, \beta_{mk}) + a^2P_{L,L-2}(\alpha_i, \beta_{mk}) - \cdots + (-a)^L P_{L0}(\alpha_i, \beta_{mk}) = 0,
$$

for $L = 0, 1, \ldots, M - 1$. (11)

In most cases, linear system (11) has a unique solution which is just what we want. However, there are situations where (9) is irregular. Then, one needs to reduce the accuracy condition, say, $(M - 2)$th-order instead of $(M - 1)$th-order. Or else, only simply tries another $M$-node stencil and rebuilds (11).

3. Application of the approach

Now we apply the new approach, stated above, in the design of finite difference schemes. Here, for demonstration, we take the 3-level, 10-node explicit stencil shown in Fig. 1(a), by which the unknown $u_j^{n+1}$ can be approximated as

$$
u_j^{n+1} = \sum_{i=-2}^{2} a_i u_{j+i}^n + \sum_{j=-2}^{2} b_i u_{j+1}^{n-1},
$$

where $a_i$ and $b_i$ are the coefficients to be determined. By the different choice of these coefficients, we can get many meaningful schemes, both familiar and unfamiliar. If $b_i = 0$, $i = -2, -1, \ldots, 2$, (12) is reduced to a 2-level scheme and we can easily obtain, from (3), (11), the first-order upwind, the second-order Lax–Wendroff, the third-order QUICKEST, the fourth-order Lagrangian interpolative schemes (cf. [9,15]) by involving 2, 3, 4, 5 points, respectively. If we adopt the particular 3-level stencils as in Figs. 1(b)–(d), we will solve out by (11) the leapfrog, upwind leapfrog,
space-extending upwind leapfrog schemes (cf. [6,10]), which are the typical examples of multi-level schemes.

Now, we select some other particular stencils as in Figs. 1(c)–(h), we will work out from (11) four high-order accurate schemes, which have not been investigated yet. They achieve fifth-, seventh-, seventh-, ninth-order, respectively, and we will denote them separately as 6P5O, 8P7O-1, 8P7O-2 and 10P9O. Their concrete expressions are as follows:

6P5O:

\[
\begin{align*}
    u_j^{n+1} &= \frac{c(2c + 1)(2c - 1)}{c + 2} u_j^{n-1} + 2(1 + 2c)(1 - 2c)u_j^n + \frac{c(1 + 2c)(1 - 2c)}{2 - c} u_j^{n+1} \\
    &+ \frac{c(c + 1)(2c + 1)}{2 - c} u_j^{n-1} + (2c - 1)(2c + 1)u_j^{n-1} + \frac{c(c - 1)(1 - 2c)}{2 + c} u_j^{n+1},
\end{align*}
\]

8P7O-1:

\[
\begin{align*}
    u_j^{n+1} &= \frac{4c(2c - 1)(2c + 1)(c + 1)}{(2 + c)(3 + c)} u_j^{n-1} + \frac{8(1 - c)(1 - 2c)(1 + 2c)(1 + c)}{(2 - c)(2 + c)} u_j^n \\
    &+ \frac{4c(1 + 2c)(1 - 2c)(1 - c)}{(2 - c)(3 - c)} u_j^{n-1} + \frac{c^2(c + 1)^2(1 - 2c)(1 + 2c)}{6(c - 2)(c - 3)} u_j^{n-2} \\
    &+ \frac{4c(c + 1)^2(1 + 2c)(1 - c)}{3(c - 2)} u_j^{n-1} + (c - 1)(1 - 2c)(1 + 2c)(1 + c)u_j^{n-1} \\
    &+ \frac{4c(1 - c)^2(1 + c)(2c - 1)}{3(c + 2)} u_j^{n-1} + \frac{c^2(1 - c)^2(1 - 2c)(1 + 2c)}{6(c + 2)(c + 3)} u_j^{n+1},
\end{align*}
\]

8P7O-2:

\[
\begin{align*}
    u_j^{n+1} &= \frac{2c(1 - c)^2(2c - 1)(2c + 1)}{3(2 + c)(3 + c)} u_j^{n-1} + \frac{2c(2c - 1)(2c + 1)(2 - c)}{c + 2} u_j^n \\
    &+ 2(1 - 2c)(1 + 2c)(1 - c)u_j^n + \frac{2c(1 - 2c)(2c + 1)(1 - c)}{3(3 - c)} u_j^{n+1} \\
    &+ \frac{c(c + 1)(1 - 2c)(1 + 2c)}{3(3 - c)} u_j^{n-1} + 2c(2c + 1)(1 - c)u_j^{n-1} \\
    &+ \frac{(1 + 2c)(2c - 1)(1 - c)(2 - c)}{2 + c} u_j^{n-1} + \frac{2c(1 - c)^2(2 - c)(2c - 1)}{3(c + 2)(c + 3)} u_j^{n+1},
\end{align*}
\]

10P9O:

\[
\begin{align*}
    u_j^{n+1} &= \frac{c(1 - c)^2(1 + c)(2c + 1)(2c - 1)}{3(c + 3)(c + 4)} u_j^{n-1} + \frac{4c(2c - 1)(2c + 1)(1 + c)(2 - c)}{3(c + 3)} u_j^n \\
    &+ 2(1 - c)(1 - 2c)(1 + 2c)(1 + c)u_j^n + \frac{4c(1 - c)(1 - 2c)(1 + 2c)(c + 2)}{3(3 - c)} u_j^{n+1}.
\end{align*}
\]
where \( c \) is the Courant number in the above expressions. All the four linear schemes are stable for \( 0 \leq c \leq \frac{1}{2} \). The main reason for introducing such schemes is that they achieve high accuracy in the numerical simulation of some severe problems of the linear advection equation (1). Here we present two test examples.

The first example is the pure advection of a combination of a half-ellipse profile and a triangular profile. Exactly, the initial value condition to (1) is

\[
\begin{cases}
4 \sqrt{1 - (x - 1)^2} & \text{if } 0 \leq x \leq 2, \\
4 - 8|x - 3.5| & \text{if } 3 \leq x \leq 4, \\
0 & \text{otherwise}
\end{cases}
\]

and the velocity is \( a = 1 \). We choose grid size \( \Delta x = 0.01 \) and time step \( \Delta t = 0.004 \), so the Courant number \( c = 0.4 \). The test results after 500-step \( (t = 2.0) \) and 2500-step \( (t = 10.0) \) computation by applying the four schemes are shown in Fig. 2.

We can see that all the four schemes cause little smoothness to the wave and show little phase error. However, the 6P5O scheme introduces some spurious oscillation near the left endpoint (an inflection point) of the half-ellipse and this becomes apparent when \( t \geq 10.0 \). This effect is much like that of the Lax–Wendroff scheme. Nevertheless, the other three schemes are almost free of this and give satisfactory results, maintaining sharp profile.

The second example is the pure advection of a high-frequency oscillation wave. The velocity is still \( a = 1 \) and the initial value to (1) is

\[
\begin{cases}
e^{-16(x-0.5)^2}\sin 40\pi x & \text{if } 0 \leq x \leq 1, \\
0 & \text{otherwise}
\end{cases}
\]

The grid size and time step are the same as those in the first example. The test results after 500-step and 2500-step computation are shown in Fig. 3. Note that the 6P5O scheme shows remarkable increase of the wave amplitude when \( t = 10.0 \). This is due to accumulation of the spurious wave introduced by the scheme itself. Therefore, the 6P5O scheme should not be used in this situation. On the other hand, the performance of the other three schemes are quite good. They all maintain most of the wave amplitude and show little phase error.

4. Conclusions

We have proposed a new practical scheme-designing approach whose application is based on the results of Theorems 1 and 2. The approach can unify the deduction of arbitrary schemes for the
Fig. 2. Numerical simulation for the first initial condition at Courant number of 0.4. Solutions after 500 time steps ($t=2.0$) and 2500 time steps ($t=10.0$).
Fig. 3. Numerical simulation for the second initial condition at Courant number of 0.4. Solutions after 500 time steps ($t = 2.0$) and 2500 time steps ($t = 10.0$).
pure advection model and is especially efficient in the design of multi-level, high-order schemes, although the selection of effective stencils may need some trials. By this approach, some extremely accurate schemes are developed and their merits are verified by numerical tests. It is evident that this approach can be naturally generalized to the design of finite difference schemes for any linear governing equations.

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