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A NEW DIFFERENCE SCHEME WITH MULTI-TIME LEVELS*

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In view of making the best use of information coming from past observational data, a new difference scheme with multi-time levels ($p > 3$) is suggested. Some mathematical characteristics of the scheme, which is called the retrospective scheme, are discussed. The numerical results of some examples show that the calculation accuracy of linear and nonlinear advection equations computed with the retrospective scheme is higher than that obtained via the leapfrog scheme. The scheme can be applied to many fields, such as meteorology, engineering physics, astronautics, environment and economy etc, where systematic observations are made normally.

Keywords: numerical computing, multi-initial values, self-memorization, the retrospective difference scheme
PACC: 0530, 0540

I. INTRODUCTION

In both forecast and simulation issues, a differential equation is generally discretized by using a difference scheme, such as the leapfrog scheme, the Euler scheme, or the Lax–Wendroff scheme with two or three time levels,[1] and then the difference equation is solved numerically if the initial condition is given. However, multi-time values before the initial time are required in solving the ordinary differential equation with the linear multi-step method. The values at these time levels are still computed from the given initial value by one of the above-mentioned schemes. That is to say, the one initial value principle invariably abides in the numerical computation; namely, the numerical integration uses only one initial value, which is taken from past observational data. Therefore, in view of utilizing the best information distilled from the observational data, the traditional method of solving differential equations, of course, is not perfect.

In view of further information obtained from observational data, first of all, the number of time levels p in a difference scheme should be enlarged. Hence an initial value problem of the differential equation is extended to a multi-value problem such as $p \geq 3$, i.e. more than three time levels are involved. In recent years, based on this idea, some new difference schemes have been conducted, one of which is the so-called self-memorization approach.[2] The differential equation is transformed to a difference-integral equation if the memory function is introduced into the numerical calculation, thus the forecast issue becomes a multi-initial value problem of the difference-integral equation. In order to estimate the memory function in the difference-integral equation from past observational data, various methods, such as least-squares, robust relaxation algorithm,[3] genetic algorithm,[4] etc, are used. The multi-time levels difference scheme is quite different from the traditional numerical computational scheme.

In order to improve computational precision, some skills in designing the difference scheme were conducted. Zeng *et al.*[5] suggested a flexible coefficient method to improve the precision in the weather forecast. Rivest *et al.*[6] deduced a three-level difference scheme, where some coefficients have to be determined empirically. Liu *et al.*[7] put forward a lattice Boltzmann method for two-dimensional (2D) convection diffusion. Cao *et al.*[8] discussed the conditions

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of stability and convergence for the P-R scheme for generalized nonlinear Schrödinger equations.

The weather forecast is normally regarded as an initial problem, so the values before or after an initial time t_0 are estimated from an initial value such as half-step integration. The multi-time level difference scheme suggested in this paper differs from previous schemes conceptually.

The retrospective scheme has been briefed in Ref.[9]. Here, some mathematics of the scheme has been deduced. Given an idealized velocity field, the evolutions of the field governed by the linear and nonlinear advection equations with the scheme have been calculated, and the analysis of calculations has been carried out.

Ⅱ. MATHEMATICAL PRINCIPLE

A. The retrospective difference scheme

A differential equation can be written as

$$\frac{\partial x}{\partial t} = F(x, \lambda, t), \tag{1}$$

where x is the physical quantity, t is the time and λ is a physical parameter. We introduce a memory function, $\beta(r,t)$, in which r is the space coordinate. As pointed out in Ref.[2], Eq.(1) can be transformed into a difference-integral equation

$$\beta(t)x(t) - \beta(t_{-p})x(t_{-p}) - \sum_{i=-p}^{0}(\beta(t_{i+1}) - \beta(t_i))x^m(t_i) - \int_{t_{-p}}^{t}\beta(\tau)F(\tau)\mathrm{d}\tau = 0, \tag{2}$$

where m stands for the median $x^m(t_i) \equiv x(t_m), t_i < t_m < t_{i+1}$; for simplicity, in the following context only the time variable t in β, x and F is still kept, while r and λ are omitted as we fix on the spatial point r. Equation(2) is called the self-memorization equation.

For simplicity, we take equal intervals Δt, for multi-time $t_i = t_0 + i\Delta t$, (i=1,0,–1,–2,$\cdots$, $-p$), where t_0 is the initial time, and p is called the retrospective order. Taking the median $x^m(t_i)$ as the mean of two values at adjacent times, i.e.

$$x^m(t_i) = \frac{1}{2}[x(t_0 + (i+1)\Delta t) + x(t_0 + i\Delta t)],$$

we can write Eq.(2) as

$$x(t_1) = \sum_{i=-p}^{0}\alpha_i x(t_0 + i\Delta t) + \frac{1}{\beta(t_1)}\int_{t_{-p}}^{t_1}\beta(\tau)F(\tau)\mathrm{d}\tau, \tag{3}$$

where

$$\alpha_{-p} = \frac{1}{2\beta(t_1)}[\beta(t_0 - p\Delta t) + \beta(t_0 - (p-1)\Delta t)],$$
$$\alpha_i = \frac{1}{2\beta(t_1)}[\beta(t_0 + (i+1)\Delta t) - \beta(t_0 + (i-1)\Delta t)],$$
$$\alpha_0 = \frac{1}{2\beta(t_1)}[\beta(t_0) - \beta(t_0 - \Delta t)],$$
$$i = -p+1, -p+2, \cdots, -1.$$

Furthermore, replacing the integration by summation, Eq.(3) can be discretized as

$$x(t_1) = \sum_{i=-p}^{0}\alpha_i x(t_0 + i\Delta t) + \sum_{i=-p}^{0}\theta_i F(t_0 + i\Delta t)\Delta t, \tag{4}$$

in which $\theta_i = \beta(t_i)/\beta(t_1)$.

Consider a one-dimensional advection equation

$$\frac{\partial u}{\partial t} + C\frac{\partial u}{\partial s} = 0, \tag{5}$$

i.e.
$$\frac{\partial u}{\partial t} = F(u,t) = -C\frac{\partial u}{\partial s}, \tag{6}$$

where s is the spatial coordinate, u is the velocity, and C is a constant velocity of advection. For the spatial point r_j, the self-memorization equation (6) can be deduced as

$$\beta(j,t)u(j,t) = \beta(j,t_{-p})u(j,t) + \sum_{i=-p}^{0}[\beta(j,t_{i+1}) - \beta(j,t_i)]u^m(j,t_i) - C\int_{t_{-p}}^{t}\beta(j,\tau)\frac{\partial u(j,\tau)}{\partial s}\mathrm{d}\tau. \tag{7}$$

While making a prediction with Eq.(4), we use p values of $x(t_i)$ and p fields of $F(t_i)$ before the initial time t_0, therefore $\beta(t_i)$ in Eq.(4) plays an important role in memorizing $p+1$ values of x and $p+1$ fields of F. This is the reason why we call $\beta(t_i)$ the memory function, and is the mathematical basis for proposing the memory function. Observational data in time $t_0, t_{-1}, \cdots, t_{-p}$ are used in the weather forecast and the computation, hence the difference scheme is called the retrospective difference scheme.

Using the same notations in the difference schemes in the numerical mathematics, i.e. denoting

$$\beta_j^{n+1} \equiv \beta(j,t), \beta_j^{n-1} \equiv \beta(j,t_{-1}), \cdots$$
$$u_j^{n+1} \equiv u(j,t), u_{j+1}^{n+1} \equiv u(j+1,t), \cdots$$
$$\mu = -C\Delta t/\Delta s,$$

replacing the integration by summation from $n-p$ to $n+1$, using a central difference for space, and taking

retrospective order p, then the retrospective scheme of Eq.(7) can be written as

$$u_j^{n+1} = \alpha_{-p} u_j^{n-p} + \sum_{i=-p}^{0} \alpha_i (u_j^{n+1})^m + \sum_{i=-p}^{1} (\theta_i u_{j+1}^{n+i} - \tilde{\theta}_i u_{j-1}^{n+i}), \tag{8}$$

where

$$\alpha_{-p} = \beta_j^{n-p}/\beta_j^{n+1},$$
$$\alpha_i = (\beta_j^{n+i+1} - \beta_j^{n+i})/\beta_j^{n+1},$$
$$\theta_i = \beta_{j+1}^{n+i}/2\beta_j^{n+1},$$
$$\tilde{\theta}_i = \beta_{j-1}^{n+i}/2\beta_j^{n+1}.$$

Here, $\alpha_{-p}, \alpha_i, \theta_i, \tilde{\theta}_i$ are called memory coefficients, Eqs.(4)and (8) are multi-time level difference schemes derived from a difference-integration equation. Generally, the median is given by

$$(u_j^{n+1})^m = \frac{1}{2}(u_j^{n+i+1} + u_j^{n+i}). \tag{9}$$

B. The multi-level average scheme

Forward difference schemes with different times $x(t-\Delta t), x(t-2\Delta t), \cdots, x(t-p'\Delta t)$ are written as

$$x(t) - x(t-\Delta t) = \Delta t F(t-\Delta t), \tag{10}$$
$$x(t) - x(t-2\Delta t) = 2\Delta t F(t-2\Delta t), \tag{11}$$
$$\cdots\cdots$$
$$x(t) - x(t-p'\Delta t) = p'\Delta t F(t-p'\Delta t), \tag{12}$$

where $t = t_0 + \Delta t$, $p' = p+1$. Adding up from Eq.(10) to Eq.(12), we obtain

$$x(t) = \sum_{i=1}^{p'} \alpha_i x(t-i\Delta t) + \sum_{i=1}^{p'} \theta_i F(t-i\Delta t), \tag{13}$$

where $\alpha_i \equiv 1/p', \theta_i = i\Delta t/p'$.

Obviously, Eqs.(13) and (4) are the same in form. However, the coefficients of the former are defined from numerical calculation viewpoint, and the latter is given by means of a special algorithm based on observational data. Both schemes contain $p+1$-time levels. Equation (13) is called the average scheme with the multi-time levels.

In view of the process yielding Eq.(13), the multi-level scheme can be deduced directly and simply from a traditional scheme. This proves that the retrospective difference scheme derived from the difference-integral equation is rational.

C. The multi-level binomial scheme

Differentiating Eq.(1) yields

$$\frac{\partial^2 x}{\partial t^2} = \frac{\partial F}{\partial t}. \tag{14}$$

Then performing the same procedure up to p order, we obtain

$$\frac{\partial^p x}{\partial t^p} = \frac{\partial^{p-1} F}{\partial t^{p-1}}. \tag{15}$$

The correspondent forward difference schemes of Eqs.(1), (14) and (15) are written as

$$\begin{aligned}
\Delta x(t) =& x(t+\Delta t) - x(t) = F(t), \\
\Delta^2 x(t) =& \Delta x(t+\Delta t) - \Delta x(t) \\
=& x(t+2\Delta t) - 2x(t+\Delta t) + x(t) \\
=& (F(t+\Delta t) - F(t))\Delta t, \\
& \cdots\cdots \\
\Delta^p x(t) =& \Delta^{p-1} x(t+\Delta t) - \Delta^{p-1} x(t) \\
=& \sum_{i=0}^{p} (-1)^i C_p^{p-i} x(t+(p-i)\Delta t) + x(t) \\
=& \sum_{i=0}^{p} (-1)^i C_{p-1}^{p-i} F(t+(p-i)\Delta t)\Delta t \\
& p = 2, 3, \cdots.
\end{aligned} \tag{16}$$

Equation (16) can be turned into the following form

$$x(t) = \sum_{i=0}^{p} \alpha_i x(t+(p-i)\Delta t) + \sum_{i=1}^{p} \theta_i F(t+(p-i)\Delta t), \tag{17}$$

where

$$\alpha_i = (-1)^{i+1} C_p^{p-i}, \qquad \theta_i = (-1)^i C_{p-1}^{p-i} \Delta t.$$

Equation (17), similar to the above multi-level average scheme, is called the multi-level binomial scheme, for its coefficients are taken as a binomial structure. The multi-level scheme Eq.(17) is derived from the differential and difference principles. Obviously, both Eqs.(13) and (17) are regarded as special cases of the self-memorization equation if particular values are put into the memory function.

It is important to discuss the accuracy and consistency of the difference scheme with multi-time levels, but it is difficult to do so. As an example, we will make a deduction only for a special case. The accuracy and the consistency of multi-level binomial scheme with p=4 are studied as follows, for the accuracy in forecasting the summer monsoon is quite high

by using a self-memorization regional climatic model when p=4.[10]

On the basis of the Fourier analysis and the exponential expression,[11] supposing

$$x(t) = g\exp(-\mathrm{i}kt), \tag{18}$$

then $\dfrac{\mathrm{d}^4x}{\mathrm{d}t^4} = (-\mathrm{i}k)^4 g\exp(-\mathrm{i}kt) = (-\mathrm{i}k)^4 x$ with p=4. Its difference is

$$\begin{aligned}\Delta_t^4 x(t) =& \frac{1}{\Delta t^4}[x(t+4\Delta t) - x(t+3\Delta t) \\ &+ 6x(t+2\Delta t) - 4x(t+\Delta t) + x(t)] \\ =& \frac{1}{\Delta t^4} g\exp(-\mathrm{i}kt)[\exp(-4\mathrm{i}k\Delta t) - 4\exp(-3\mathrm{i}k\Delta t) \\ &+ 6\exp(-2\mathrm{i}k\Delta t) - 4\exp(-\mathrm{i}k\Delta t) + 1] \\ =& (-\mathrm{i}k)^4 x[1 + 2(-\mathrm{i}k\Delta t) + O((-\mathrm{i}k\Delta t)^2)] \\ =& [1 + 2(-\mathrm{i}k\Delta t) + O((-\mathrm{i}k\Delta t)^2)]\frac{\mathrm{d}^4x}{\mathrm{d}t^4}, \end{aligned} \tag{19}$$

i.e. $\Delta_t^4 \equiv [1 + 2(-\mathrm{i}k\Delta t) + O((-\mathrm{i}k\Delta t)^2)]\dfrac{\mathrm{d}^4}{\mathrm{d}t^4}$. Its accuracy is $O(\Delta t)$.

The difference scheme of Eq.(17) is written as

$$\begin{aligned}&\frac{x^{n+4} - 4x^{n+3} + 6x^{n+2} - 4x^{n+1} + x^n}{\Delta t^4} \\ =& \frac{F^{n+3} - 3F^{n+2} + 3F^{n+1} - F^n}{\Delta t^3}. \end{aligned} \tag{20}$$

Here x^{n+4}, x^{n+3}, x^{n+2}, x^{n+1}, F^{n+3}, F^{n+2}, F^{n+1} are approximately expressed via the Taylor expansion at x^n, F^n respectively. Then the consistency of differential equation (20) is

$$\begin{aligned}\frac{\partial^4 x}{\partial t^4} - \frac{\partial^3 F}{\partial t^3} =& \Delta t\left(-\frac{2}{3}\frac{\partial^4 F}{\partial t^4} + 2\frac{\partial^5 x}{\partial t^5}\right) \\ &+ (\Delta t)^2\left(\frac{5}{4}\frac{\partial^5 F}{\partial t^5} - \frac{13}{6}\frac{\partial^6 x}{\partial t^6}\right) + \cdots \\ =& l_4\left(\frac{\partial^4 F}{\partial t^4}\right) + l_5\left(\frac{\partial^5 F}{\partial t^5}\right), \end{aligned} \tag{21}$$

where $l_4 = \dfrac{3}{4}\Delta t$, $l_5 = -\dfrac{11}{12}(\Delta t)^2$.

Equation (21) is equivalent to Eq.(15) at $p = 4$. When $l_4 > 0$, and the ratio of l_4 to l_5 is about Δt, the dissipation terms on the right-hand side of Eq.(21) are very important for the stability of the difference scheme.

Up to now, three new difference schemes with multi-time levels—the retrospective difference scheme, the multi-level average scheme and the multi-level binomial scheme—have been derived and discussed.

Ⅲ. NUMERICAL CALCULATION

As an example, we still take the three time levels, but utilize all the information of observations at t and $t - \Delta t$. The retrospective scheme of the advection equation (8) is adopted, and an idealized field is computed using

$$u(x,t) = a\sin(mx - \sigma t), \tag{22}$$

where

$$\begin{aligned}&m = 2\pi/L_x, L_x = 3600\mathrm{km}, \sigma = 2\pi/T, \\ &T = 5\mathrm{d} = 5\mathrm{d}\times 24\mathrm{h/d}, x_i = \mathrm{i}\Delta x, \Delta x = 300\mathrm{km}, \\ &t_\tau = \tau\Delta t, \Delta t = 1\mathrm{h}, \sigma = mc, a = 10\mathrm{m/s}, c = 8.3\mathrm{m/s}. \end{aligned}$$

The time-step Δt is 1 h in the integration with the retrospective scheme. Firstly, the 48h time series is calculated with Eq.(22), which is called a real-time series hereafter. Secondly, the memory coefficients α_{-p}, α_i, θ_i, $\tilde{\theta}_i$ in Eq.(8) are estimated by means of the least-squares method with the 48h time series. Finally the prediction is made by both the leapfrog scheme and the retrospective scheme to 600d (600d×24h/d=14400h), taking p=2,3,4,5,6 respectively. It is shown that the root-mean-square errors (RMSEs) of the retrospective scheme are much smaller than those of the leapfrog scheme (Fig.1).

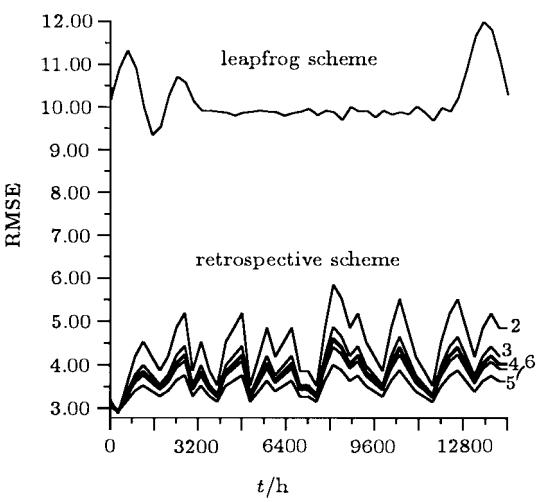


Fig.1. Variation of RMSEs between the linear advection equation integration and the idealized field: RMSEs, the root-mean-square errors; h, hour; 2, 4 and 6 represent retrospective orders p=2, 4 and 6 respectively; the curves of p=4 and 6 are nearly overlapped. The RMSEs are smallest at p=5.

Figure 2 shows the time series computed with both difference schemes and an idealized field at L=3600km, and p=5. In Fig.2 a sawtooth curve, which is caused by computational solution, appears when using the leapfrog scheme. Before integrating 40 time steps (88h), i.e. before the idealized field reaches a peak, the values computed with the retrospective

scheme and the leapfrog scheme are all close to that of the idealized field. But over the peak, the values computed with the leapfrog scheme depart more and more from the true solution. While the idealized field reaches the second peak, the phase of the leapfrog scheme is hardly in accord with that of the idealized field. However, the curve of the retrospective scheme is still in agreement with that of the idealized field, though there is a phase lag between them.

Figure 3 shows the variation of velocity $\boldsymbol{u}$ among the idealized field, the retrospective scheme and the leapfrog scheme as given different space scales L_x. The image integrated with the retrospective scheme is in good accordance with that of idealized field except for some details. But the image calculated via the leapfrog scheme differs considerably from the idealized field.

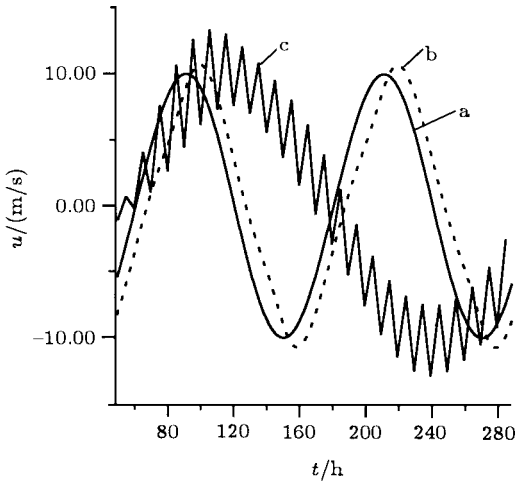


Fig.2. Variation of velocity u computed by the idealized field (a), the retrospective difference scheme (b) and the leapfrog scheme (c), for L_x=3600km and p=5.

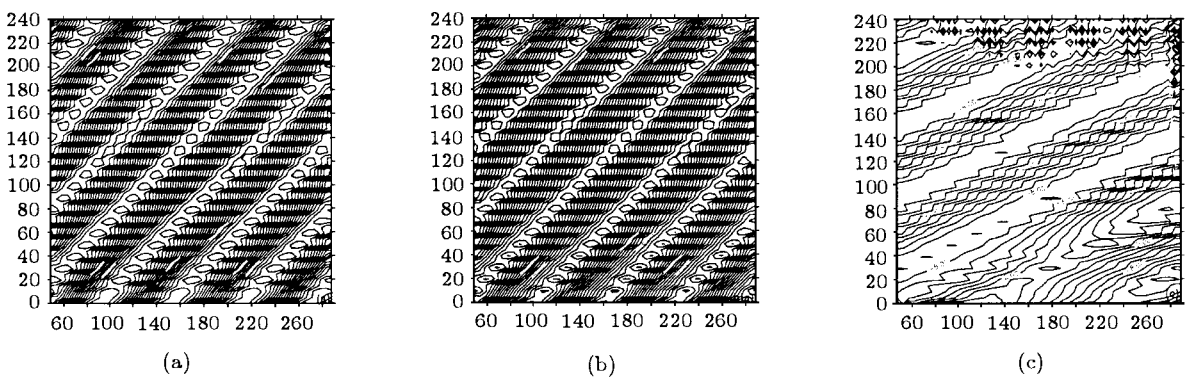


Fig.3. Variation of velocity $\vec{u}$ as L_x given different spatial scales for the idealized field (a), the retrospective difference scheme (b) and the leapfrog scheme (c). Unit: coordinate, L_x, 30km; abscissa, t, h.

Similarly, a nonlinear one-dimensional advection equation is

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial s} = 0, \tag{23}$$

namely, $\dfrac{\partial u}{\partial t} = -\dfrac{1}{2}\dfrac{\partial u^2}{\partial s} = F(u,t).$

Its retrospective scheme is written as

$$u_j^{n+1} = \alpha_{-p}u_j^{n-p} + \sum_{i=-p}^{0}\alpha_i(u_j^{n+1})^m + \sum_{i=-p}^{1}[\theta_i(u_{j+1}^{n+i})^2 - \tilde{\theta}_i(u_{j-1}^{n+i})^2], \tag{24}$$

where

$$\begin{aligned}\alpha_{-p} &= \beta_j^{n-p}/\beta_j^{n+1},\\ \alpha_i &= (\beta_j^{n+i+1} - \beta_j^{n+i})/\beta_j^{n+1},\\ \theta_i &= \beta_{j+1}^{n+i}/4\beta_j^{n+1},\\ \tilde{\theta}_i &= \beta_{j-1}^{n+i}/4\beta_j^{n+1}.\end{aligned} \tag{25}$$

The median given is the same as Eq.(9).

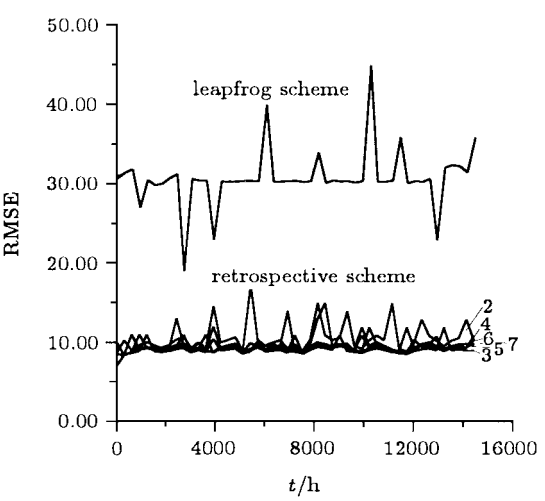


Fig.4. Variation of RMSEs between the nonlinear advection equation integration and the idealized field: RMSEs, the root-mean-square errors; 2, 4 and 6 represent retrospective orders p=2, 4 and 6 respectively; both curves of p=4 and 6 are nearly overlapped.

The computation of Eq.(24) is the same as Eq.(8), and the computational results are drawn in Fig.4. The RMSEs of the retrospective difference scheme are from one third to one fourth of the RMSEs of the leapfrog scheme when the retrospective order p is set to be several integers. But the RMSEs of either the retrospective scheme or the leapfrog scheme of the nonlinear advection equation are greater than those of linear advection equation. However, as the RMSEs are statistic, sometimes the RMSEs computed for the nonlinear advection equation are likely to be smaller than those of linear advection equation for some given L_x. Given certain values to retrospective order p, sometimes the RMSEs curves interrelate given different values of L_x, which may be caused by nonlinear interaction. Figure 5 is similar to Fig.3. The variation of the velocity $\boldsymbol{u}$ with time step is presented in Fig.5, from which the advantage of the retrospective scheme is also demonstrated.

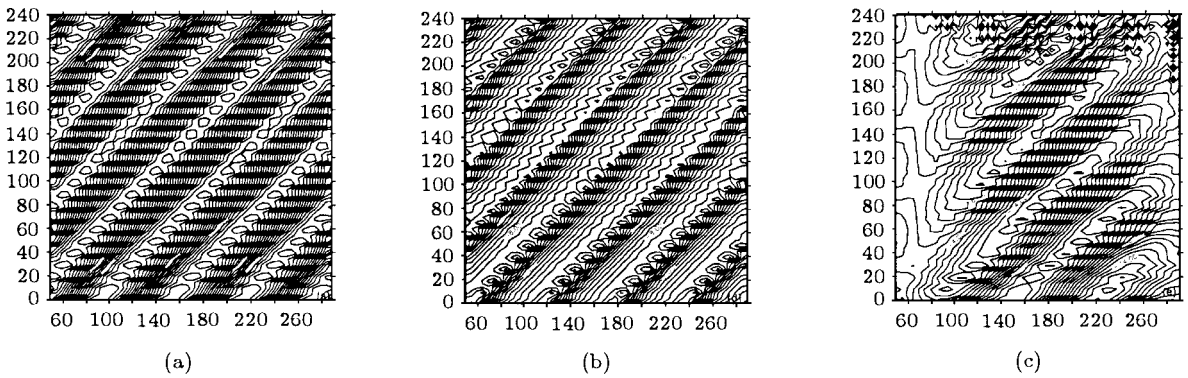


Fig.5. Variation of the velocity $\vec{u}$ with L_x given different spatial scales in the nonlinear advection equation for the idealized field (a), the retrospective difference scheme (b) and the leapfrog scheme (c). Unit: coordinate, L_x, 30km; abscissa, t, h.

IV. CONCLUSION

Forecasting with the retrospective scheme may be written as

$$\begin{aligned}\hat{x}(t_1) =& f(x(t_0), x(t_{-1}), \cdots, x(t_{-p});\\ & F(t_0), F(t_{-1}), \cdots, F(t_{-p})),\end{aligned} \tag{26}$$

at $t_2 = t_1 + \Delta t = t_0 + 2\Delta t$,

$$\begin{aligned}\hat{x}(t_2) =& f(x(t_1), x(t_0), \cdots, x(t_{-p+1});\\ & F(t_1), F(t_0), \cdots, F(t_{-p+1})),\\ & \cdots\cdots\cdots\cdots\end{aligned} \tag{27}$$

at $t_{q+1} = t_q + \Delta t = t_0 + (q+1)\Delta t$, we obtain

$$\begin{aligned}\hat{x}(t_{q+1}) =& f(x(t_{q-p}), x(t_{q-p+1}), \cdots, x(t_q);\\ & F(t_{q-p}), F(t_{q-p+1}), \cdots, F(t_q)),\end{aligned} \tag{28}$$

where q is the number of prediction time step. If $\hat{x}(t_1)$ and $\hat{x}(t_2)$ are obtained by Eqs.(26) and (27) respectively, involving p observational data of x and F, but only one value is different, namely, $x(t_{-p})$ replaced by $x(t_1)$, then when p is adequate to guarantee the computational stability, the prediction can be influenced only by randomness.

A new time integration of the differential equation, whose purpose is to make the difference scheme contain more information of both observed space points and fields, has been suggested. It is possible that in the process of time integration the time smoothing can be withdrawn, because the memorial coefficients in the scheme play a role of time smoothing. Hence, in terms of the idealized field data we demonstrate that the accuracy and efficiency of the retrospective scheme are higher than those of the leapfrog scheme. However, the difference scheme with the multi-time levels is prosperous; it can be applied to various fields.[12,13] But its mathematics and computations will be studied further.

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