The von Neumann analysis and modified equation approach for finite difference schemes

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The von Neumann (discrete Fourier) analysis and modified equation technique have been proven to be two effective tools in the design and analysis of finite difference schemes for linear and nonlinear problems. The former has merits of simplicity and intuition in practical applications, but only restricted to problems of linear equations with constant coefficients and periodic boundary conditions. The later PDE approach has more extensive potential to nonlinear problems and error analysis despite its kind of relative complexity. The dissipation and dispersion properties can be observed directly from the PDE point of view: Even-order terms supply dissipation and odd-order terms reflect dispersion. In this paper we will show rigorously their full equivalence via the construction of modified equation of two-level finite difference schemes around *any wave number* only in terms of the amplification factor used in the von Neumann analysis. Such a conclusion fills in the gap between these two approaches in literatures.

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1. Introduction

The von Neumann (discrete Fourier) analysis and the modified equation technique have been proven to be two effective and fundamental tools in the design and analysis of finite difference schemes (even finite element or finite volume methods) for differential equations. The link between them is seemingly well-known and clear, but only in smooth regions of solutions or at low frequencies. The main purpose of this paper is to establish the *full connection* between them for *all wave number modes*, for which the modified equation is written in a very compact form just in terms of the amplification factor in the context of von Neumann analysis.

We consider time-dependent partial differential equations with constant coefficients,

$$\frac{\partial v}{\partial t} = \mathcal{L}_x v, \quad \mathcal{L}_x = \mathcal{L}(\partial_x) = \sum_{s=1}^{K} \alpha_s \partial_x^s, \tag{1.1}$$

where $\mathcal{L}_x$ represents linear differential operators with constant coefficients α_s. A conventionally used two-level difference scheme takes the form,

$$Bu^{n+1} = Au^n, \tag{1.2}$$

where the operator B is invertible; or explicitly (1.2) is expressed as

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$$\sum_{p=-N_1}^{N_2} B_p u_{j+p}^{n+1} = \sum_{p=-M_1}^{M_2} A_p u_{j+p}^n. \tag{1.3}$$

Here the discrete value u_j^n on the grid point (x_j, t_n) approximates the solution $v(x_j, t_n)$ of (1.1), $x_j = jh$, $t_n = n\tau$, $j \in \mathbb{Z}$, $n \in \mathbb{N}$, h represents the spatial mesh size and τ is the length of time step. This scheme has the stencil sizes of the implicit and explicit parts $N = N_1 + N_2 + 1$ and $M = M_1 + M_2 + 1$, respectively. The coefficients A_p and B_p are constant, satisfying a basic consistency condition,

$$\sum_{p=-N_1}^{N_2} B_p = \sum_{p=-M_1}^{M_2} A_p. \tag{1.4}$$

We are particularly concerned with explicit schemes, for which $N_1 = N_2 = 0$ and so $N = 1$. In fact, in our analysis, the implicit scheme (1.3) can be converted into an explicit one by a linear transformation.

To analyze and use the discrete algebraic equation (1.3) in the approximation of the solution of the continuous equation (1.1), four most basic and fundamental issues are the consistency, stability, convergence and wave propagation. The consistency describes whether (1.3) approximates (1.1). Once (1.3) is consistent with (1.1), the Lax-equivalence theorem states that the solution of (1.3) converges to the solution of (1.1) if and only if the scheme (1.3) is stable [10]. The wave propagation can be understood by using a so-called dispersion relation. All these issues can be addressed with the von Neumann analysis [2] and the modified equation technique [24]. The von Neumann analysis is relatively simple and intuitive, and the unique amplification factor implies the consistency, determines the stability of (1.3) and displays properties of wave propagations, despite the fact that it mostly applies to equations with constant coefficients and periodic boundary condition [16]. The modified equation can be interpreted as *the actual partial differential equation that the scheme (1.3) solves* [24]. This approach is originated in [4] and can be generalized for linear problems with variable coefficients or even nonlinear problems [8], the dissipation and dispersion effects of (1.3) can be understood from the partial differential equation point of view: Even order terms determines the dissipation and odd order terms represents the dispersion. This dissipative and dispersive information derived from the modified equation approach is very heuristic, unfortunately just valid for solutions in smooth regions or at low frequency modes [24]. Therefore the connection with the von Neumann analysis is only restricted there.

However, in many applications, for example, in the simulation of turbulent flows, aeroacoustic computations, or in the analysis of numerical boundary conditions, the understanding of numerical (e.g., oscillatory) phenomena and many others [3,18], one is more concerned with solution behaviors for a large range of wave numbers, particularly, middle- or large-wave-number, which arises a question how to derive modified equations for any wave number Fourier mode, or establish the full connection between these two approaches. This kind of missions has started earlier though just sporadic. For oscillatory (large-wave-number) parts, a formal analysis is presented in [16] for some specific schemes (e.g., the box scheme) and in [12] for the stable three-point generalized Lax-Friedrichs schemes. The oscillatory behavior of solutions can be illustrated rather clearly via the associated modified equation.

As such, the modified equation approach is worth reinspecting. It was pointed out in [7]: "Because of the lack of any theoretical foundation, this use has been accompanied by constant difficulties and results derived from modified equations have sometimes been regarded with apprehension. As a result a situation has arisen where authors either disregard entirely the technique or have an unjustified faith in its scope." Nevertheless, this approach is very heuristic in the design of numerical schemes and applicable to nonlinear problems [5,17,20,6,22], and therefore we hope to clarify the connection with the classical discrete Fourier analysis for the full range of wave number modes.

The full connection can be intuitively built as follows. Consider a Fourier mode $u_j^n = \lambda^n e^{ijkh}$, $i^2 = -1$, k is real. The frequency ω and the amplification factor λ are linked with $\lambda = e^{i\omega\tau}$, and thereby the dispersion relation $\omega = \omega(k; h, \tau)$ for (1.3). Then the (discrete) frequency ω is a function of k, but also of h and τ. We will simply write ω as $\omega = \omega(k)$, holding h, τ fixed later on. Then this Fourier mode can be expressed as

$$u_j^n = e^{-\omega_I n\tau} e^{ik[jh - v_p(k)n\tau]}, \tag{1.5}$$

where $v_p(k) = -\omega_R(k)/k$ is the phase speed, $\omega_R(k)$ and $\omega_I(k)$ are the real and imaginary parts of $\omega(k)$, respectively, i.e., $\omega(k) = \omega_R(k) + i\omega_I(k)$. Hence this mode propagates with the phase speed $v_p(k)$ and is dissipated with the rate $-\omega_I(k)$ at each step if $\omega_I > 0$, which is just the von Neumann criterion for stability[1]

$$|\lambda(k)| \leqslant 1. \tag{1.6}$$

To understand how the overall shape of the wave amplitudes around a fixed wave number k_0, let us think of k as the wave number around k_0, $k = k_0 + \tilde{k}$ and thereby $\omega = \omega_0 + \tilde{\omega}$, $\omega_0 = \omega(k_0)$, $\tilde{k}$ and $\tilde{\omega}$ are small. Then with the smoothness assumption of $\tilde{\omega}$ in terms of $\tilde{k}$, one obtains

$$\omega(k) = \omega(k_0) + \tilde{\omega}(k_0 + \tilde{k}) = \omega_0 + \sum_{s=1}^{\infty} \frac{\tilde{\omega}^{(s)}(k_0)}{s!} \tilde{k}^s, \quad \tilde{\omega}(k_0) = 0. \tag{1.7}$$

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[1] The von Neumann criterion becomes $|\lambda(k)| \leqslant 1 + C\tau$ for some constant C if a zero term in the form $C_0 u$ is present in (1.1).

In this paper we always use the notation $\omega^{(s)}(k)$ to denote the s-th derivative of ω in terms of k and similarly for others. Then this Fourier mode propagates, see [21], in the form,

$$u_j^n \approx e^{-\omega_I(k_0)n\tau} \cdot e^{ik_0[jh - v_p(k_0)n\tau]} \cdot e^{i\tilde{k}[jh - G(k_0)n\tau]} \tag{1.8}$$

by ignoring higher order terms. Here $G(k_0) = -d\tilde{\omega}(k_0)/dk$ is the group velocity at k_0. Hence the principal part of this mode propagates with the phase speed $v_p(k_0)$ and is damped with the rate $-\omega_I(k_0)$ at each time step. The dispersion of (1.3) and other dissipation effects are reflected through $\tilde{\omega}(k_0 + \tilde{k})$.

We can depict the propagation of the overall shape of this wave amplitudes (wave packet) in terms of modified equations. Set

$$u_j^n = \alpha_j^n \tilde{u}_j^n, \quad \alpha_j^n = e^{i(n\omega_0\tau + jk_0h)}, \quad \tilde{u}_j^n = e^{i(n\tilde{\omega}\tau + j\tilde{k}h)}, \quad i^2 = -1. \tag{1.9}$$

With the change of $\tilde{k}$, $\tilde{u}_j^n$ is the wave packet around (k_0, ω_0). By comparing this with (1.7), and substituting $i\tilde{k}$ by ∂_x and $i\tilde{\omega}$ by ∂_t, the modified equation for $\tilde{u}_j^n$ is expressed in a compact form

$$\partial_t \tilde{u} = \frac{1}{\tau} \sum_{s=1}^{\infty} \frac{i^{-s}}{s!} [\ln \lambda]^{(s)}(k_0) \partial_x^s \tilde{u}, \quad [\ln \lambda]^{(s)}(k_0) = i\tilde{\omega}^{(s)}(k_0)\tau. \tag{1.10}$$

where $\lambda^{(s)}(k_0) = \frac{d^s \lambda(k_0)}{dk^s}$. In terms of the group velocity $G(k_0)$, (1.10) is rewritten as

$$\partial_t \tilde{u} + G(k_0)\partial_x \tilde{u} = -\sum_{s=2}^{\infty} \frac{i^{-(s-1)}}{s!} G^{(s-1)}(k_0) \partial_x^s \tilde{u}, \tag{1.11}$$

which implies that the wave packet of $\tilde{u}$ propagate with the group velocity $G(k_0)$, and the behavior is totally determined in terms of this unique quantity. This modified equation approach provides a PDE interpretation of the wave packet, through which we clarify its full connection with the von Neumann analysis: (i) *Take the von Neumann analysis for (1.3) to obtain the amplification factor $\lambda(k_0)$ for a fixed wave number k_0. Then we derive the modified equation (1.10) or (1.11) for the wave packet of $\tilde{u}$.* (ii) *On the other hand, as long as all coefficients of the modified equation at a fixed wave number k_0 are known, all derivatives of the amplification factor in the von Neumann analysis are obtained and thus the amplification factor $\lambda(k_0)$ is known.* Thus the von Neumann analysis and the modified equation technique are unified in a common framework and we can conveniently adopt either the von Neumann analysis or the modified equation to analyze the dissipation (stability) and dispersion (oscillations) of the scheme (1.3). We point out particularly that as $(k_0, w_0) = (0, 0)$, this modified equation (1.10) becomes that in [24] in a compact form,

$$\partial_t u = \frac{1}{\tau} \sum_{s=1}^{\infty} \frac{i^{-s}}{s!} [\ln \lambda]^{(s)}(0) \partial_x^s u. \tag{1.12}$$

This implies that the frequency defined by the dispersion relation for (1.3) be just the symbol of the modified equation (1.12).

We remark that although the above analysis is made only for (1.1) with constant coefficients, it works for the local stability or instability of the scheme (1.3) with variable coefficients or nonlinear problems. Indeed, we have developed a heuristic modified equation approach for nonlinear equations [13]. In a forthcoming contribution [14], we will investigate variable coefficient cases.

We organize this paper as follows. In Section 2 we will derive the modified equation rigorously. In Section 3 we present a throughout explanation about the full connection. In Section 4 we provide some simple discussions.

2. Modified equation for a wave packet around a fixed wave number

This section provides the derivation of a modified equation for a wave packet around a fixed wave number k_0 and the corresponding frequency $\omega_0 = \omega(k_0)$. Hence we make an ansatz,

$$u_j^n = \alpha_j^n \tilde{u}_j^n, \quad \alpha_j^n = e^{i(n\omega_0\tau + jk_0h)}, \quad \omega_0 = \omega(k_0). \tag{2.1}$$

This formulation somewhat corresponds to the setting in the Fourier analysis

$$u_j^n = e^{in\omega\tau} e^{ikjh}, \quad \tilde{u}_j^n = e^{in\tilde{\omega}\tau} e^{i\tilde{k}jh}, \quad \omega = \omega_0 + \tilde{\omega}, \quad k = k_0 + \tilde{k}, \tag{2.2}$$

and extends the analysis in [12,16] for highest frequency modes. As $(k_0, \omega(k_0)) = (0, 0)$, $\alpha_j^n \equiv 1$ and $u_j^n = \tilde{u}_j^n$.

With the assumption that $\tilde{k} \ll 1$, it is shown in [21, p. 76] that the solution with the phase velocity $C(k_0 + \tilde{k})$, in correspond to (2.1), has the form

$$u(x, t) = \gamma(x, t)e^{i\tilde{k}(x - G(k_0)t)} e^{ik_0(x - C(k_0)t)}, \tag{2.3}$$

for some function $|\gamma(x, t)| \leqslant 1$.

In the following we will derive the modified equation for $\tilde{u}_j^n$, from which we can see clearly that $\tilde{u}$ propagates with the group velocity $G(k_0)$ and it is dissipated with the so-called *numerical diffusion*. Note that the principal part of (2.1) is damped

with the rate $-\omega_I(k_0)$, which is named as *a numerical damping*. It is evident that this is consistent with the traditional modified equation at $(\omega_0, k_0) = (0, 0)$. See [24].

Proposition 2.1. *The modified equation for the finite difference scheme* (1.3), *in terms of* $\tilde{u}_j^n$, *is*

$$\partial_t \tilde{u} = \frac{1}{\tau} \sum_{N=1}^{\infty} \frac{i^{-N}}{N!} \cdot [\ln \lambda]^{(N)}(k_0) \cdot \partial_x^N \tilde{u}, \quad i^2 = -1, \tag{2.4}$$

where the amplification factor $\lambda(k_0)$ *is expressed as*

$$\lambda(k_0) = \left[\sum_{p=-N_1}^{N_2} B_p e^{ik_0 ph} \right]^{-1} \cdot \sum_{p=-M_1}^{M_2} A_p e^{ik_0 ph}. \tag{2.5}$$

Note that the group velocity is defined as $G(k) = -\frac{d\omega(k)}{dk} = \frac{i}{\tau} \frac{d \ln \lambda(k)}{dk}$. *Then the modified equation can also be expressed as* (1.11).

Proof. Here we only prove for the explicit form of (1.3). For the general case, the theory of pseudo-differential operator should be applied [9], and the details are omitted here.

We substitute the ansatz (2.1) into (1.3) to obtain

$$e^{i\omega_0 \tau} \tilde{u}_j^{n+1} = \sum_{p=-M_1}^{M_2} A_p \alpha_p^0 \tilde{u}_{j+p}^n, \quad \alpha_p^0 = e^{ipk_0 h}. \tag{2.6}$$

Recall the operators

$$\tilde{u}(\cdot, t + \tau) = e^{\tau \partial_t} \tilde{u}(\cdot, t), \quad \tilde{u}(x + ph, \cdot) = e^{ph \partial_x} \tilde{u}(x, \cdot). \tag{2.7}$$

Then by ignoring the index j, (2.6) can be written as

$$e^{i\omega_0 \tau} e^{\tau \partial_t} \tilde{u} = \left(\sum_{p=-M_1}^{M_2} A_p \alpha_p^0 e^{ph \partial_x} \right) \tilde{u}. \tag{2.8}$$

Using the standard operator manipulation $e^{ph \partial_x} = \sum_{s=0}^{\infty} \frac{(ph \partial_x)^s}{s!}$ and taking into account the value of $\lambda^{(s)}(k)$ at $k = k_0, s = 0, 1, \ldots$

$$i^{-s} \lambda^{(s)}(k_0) = \sum_{p=-M_1}^{M_2} A_p (ph)^s e^{ipk_0 h} = \sum_{p=-M_1}^{M_2} A_p \alpha_p^0 (ph)^s, \tag{2.9}$$

we find that (2.8) can be written as

$$(e^{\tau \partial_t} - 1) \tilde{u} = e^{-i\omega_0 \tau} \left(\sum_{s=1}^{\infty} \frac{i^{-s}}{s!} \lambda^{(s)}(k_0) \partial_x^s \right) \tilde{u}, \tag{2.10}$$

where we have used $e^{i\omega_0 \tau} = \lambda(k_0)$. We proceed to use the operator manipulation again

$$\tau \partial_t = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} (e^{\tau \partial_t} - 1)^m, \tag{2.11}$$

and obtain

$$\tau \partial_t = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} \left[e^{-i\omega_0 \tau} \left(\sum_{s=1}^{\infty} \frac{i^{-s}}{s!} \lambda^{(s)}(k_0) \partial_x^s \right) \right]^m. \tag{2.12}$$

Now we denote

$$\Delta(k) := \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m} \left[\sum_{s=0}^{\infty} \frac{i^{-s}}{s!} [e^{-i\omega_0 \tau} \lambda(k) - 1]^{(s)} \partial_x^s \right]^m. \tag{2.13}$$

Here if we use the relation between λ and ω, $\lambda(k_0) = e^{i\omega_0 \tau}$ such that $e^{-i\omega_0 \tau} \lambda(k_0) - 1 = 0$, then $\Delta(k_0) = \tau \partial_t$. Thus we want to prove

$$\Delta(k) = \sum_{N=0}^{\infty} \frac{i^{(-N)}}{N!} [\ln \lambda(k)]^{(N)} \partial_x^N, \tag{2.14}$$

and then we obtain (2.4) by setting $k = k_0$.

For the simplicity of presentation below, we introduce notations of index sets and indexed functions:

Index set $M_{m,N}$. *For a fixed pair* (m, N), *an* (m, N) *non-negative index set* $M_{m,N} = \{(\sigma_0^N, \ldots, \sigma_N^N)\}$ *is so defined to satisfy:*

(i) $\sigma_s^N \geqslant 0$, for $0 \leqslant s \leqslant N$; and $\sigma_s^N = 0$ for $s > N$.
(ii) $\sum_{s=0}^{N} \sigma_s^N = m$.
(iii) $\sum_{s=0}^{N} s\sigma_s^N = N$.

Indexed function H_N. *For a smooth function* $f(k) = e^{-i\omega_0\tau}\lambda(k) - 1$ *with the index* $(\sigma_0^N, \ldots, \sigma_N^N) \in M_{m,N}$, *we denote indexed functions*

$$H_N(s, \sigma_s^N)(k) = C_{m-\sigma_N^N - \cdots - \sigma_{s+1}^N}^{\sigma_s^N} \left(\frac{f^{(s)}}{s!}\right)^{\sigma_s^N}(k), \quad s = 1, \ldots, N, \tag{2.15}$$

where $C_m^\sigma = \frac{m!}{\sigma!(m-\sigma)!}$ *are the standard binomial coefficients.*

With the above notations, we have $H_N(s, 0) = 1$ and write (2.13) as

$$\Delta(k) = \sum_{N=1}^{\infty}\sum_{m=1}^{\infty}\frac{(-1)^{m+1}}{m} \sum_{(\sigma_0^N,\ldots,\sigma_N^N)\in M_{m,N}} i^{-N}\prod_{s=0}^{N}H_N(s,\sigma_s^N)\partial_x^N. \tag{2.16}$$

Note that for $N > 1$ and $k \sim k_0$,

$$\left[\frac{\lambda'(k)}{\lambda(k)}\right]^{(N-1)} = \left[\ln(1 + e^{-i\omega_0\tau}\lambda(k) - 1)\right]^{(N)} = \sum_{m=1}^{\infty}\left[\frac{(-1)^{m+1}}{m}\left((e^{-i\omega_0\tau}\lambda(k) - 1)^m\right)^{(N)}\right], \tag{2.17}$$

where we have used the fact that there exists $0 < \delta \ll 1$ such that $|e^{-i\omega_0\tau}\lambda(k) - 1| \leqslant \delta$ for $k \sim k_0$. Therefore in order to prove (2.4), it suffices to show for each pair (m, N),

$$\sum_{(\sigma_0^N,\ldots,\sigma_N^N)\in M_{m,N}}\prod_{s=0}^{N}H_N(s,\sigma_s^N) = \frac{1}{N!}\left[(e^{-i\omega_0\tau}\lambda(k) - 1)^m\right]^{(N)}. \tag{2.18}$$

Then we complete the proof immediately.

We verify (2.18) by induction. In the proof process of (2.18), we denote $f = e^{-i\omega_0\tau}\lambda(k) - 1$. It is easy to see that (2.18) holds for $N = 1$. This is because $m = 1$ if $N = 1$.

Now we assume that (2.18) holds for N. Then we want to prove that it holds also for $N + 1$, i.e.,

$$\frac{1}{(N+1)!}[f^m]^{(N+1)} = \frac{1}{(N+1)!}\frac{d}{dk}[f^m]^{(N)} = \sum_{(\sigma_0^{N+1},\ldots,\sigma_{N+1}^{N+1})\in M_{m,N+1}}\prod_{s=0}^{N+1}H_{N+1}(s,\sigma_s^{N+1}). \tag{2.19}$$

For this purpose, we denote by D_ℓ^N the differential operation for $\sigma_\ell^N \geqslant 1, \ell = 0, \ldots, N$,

$$D_\ell^N\left[\prod_{s=0}^{N}H_N(s,\sigma_s^N)\right] := \prod_{s\neq\ell}H_N(s,\sigma_s^N) \cdot \frac{d}{dk}H_N(\ell, \sigma_\ell^N). \tag{2.20}$$

Observe that for $0 \leqslant \ell \leqslant N$,

$$D_\ell^N\left[\prod_{s=0}^{N}H_N(s,\sigma_s^N)\right] = \prod_{s\neq\ell,\ell+1}H_N(s,\sigma_s^N) \cdot (\sigma_{\ell+1}^N + 1)(\ell + 1)$$

$$\cdot C_{m-\sigma_N^N-\cdots-(\sigma_{\ell+1}^N+1)}^{\sigma_\ell^N-1}\left(\frac{f^{(\ell)}}{\ell!}\right)^{\sigma_\ell^N-1} \tag{2.21}$$

$$\cdot C_{m-\sigma_N^N-\cdots-\sigma_{\ell+2}^N}^{\sigma_{\ell+1}^N+1}\left(\frac{f^{(\ell+1)}}{(\ell+1)!}\right)^{\sigma_{\ell+1}^N+1}.$$

Denote

$$\bar{\sigma}_s^{N+1} = \begin{cases} \sigma_{\ell+1}^N + 1, & \text{for } s = \ell + 1, \\ \sigma_\ell^N - 1, & \text{for } s = \ell, \\ \sigma_s^N, & \text{otherwise.} \end{cases} \tag{2.22}$$

Then so defined index $(\bar{\sigma}_0^{N+1}, \ldots, \bar{\sigma}_{N+1}^{N+1}) \in M_{m,N+1}$. In fact we calculate:

$$\begin{aligned}
\sum_{s=0}^{N+1} s \cdot \bar{\sigma}_s^{N+1} &= \sum_{s\neq\ell,\ell+1} s \cdot \bar{\sigma}_s^{N+1} + \ell \cdot \bar{\sigma}_\ell^{N+1} + (\ell + 1) \cdot \bar{\sigma}_{\ell+1}^{N+1} \\
&= \sum_{s\neq\ell,\ell+1} s \cdot \sigma_s^N + \ell \cdot (\sigma_\ell^N - 1) + (\ell + 1) \cdot (\sigma_{\ell+1}^N + 1) \\
&= \sum_{s=0}^{N} s \cdot \sigma_s^N + 1 \\
&= N + 1,
\end{aligned} \tag{2.23}$$

and

$$\sum_{s=0}^{N+1} \bar{\sigma}_s^{N+1} = \sum_{s=0}^{N} \sigma_s^N = m. \tag{2.24}$$

Thus (2.21) is rewritten as

$$D_\ell^N \left[\prod_{s=0}^{N} H_N(s, \sigma_s^N) \right] = (\sigma_{\ell+1}^N + 1)(\ell + 1) \prod_{s=0}^{N+1} H_{N+1}(s, \bar{\sigma}_s^{N+1}). \tag{2.25}$$

With careful check of the above process, we find that if $(\sigma_{0,\kappa}^N, \ldots, \sigma_{N,\kappa}^N) \in M_{m,N}$ satisfies,

$$\sigma_{s,\kappa}^N = \begin{cases} \bar{\sigma}_\kappa^{N+1} - 1, & \text{for } s = \kappa + 1, \\ \bar{\sigma}_\kappa^{N+1} + 1, & \text{for } s = \kappa, \\ \bar{\sigma}_s^{N+1}, & \text{otherwise}, \end{cases} \tag{2.26}$$

there holds

$$D_\kappa^N \left[\prod_{s=0}^{N} H_N(s, \sigma_{s,\kappa}^N) \right] = (\bar{\sigma}_{\kappa+1}^{N+1})(\kappa + 1) \prod_{s=0}^{N+1} H_{N+1}(s, \bar{\sigma}_s^{N+1}). \tag{2.27}$$

We collect all terms with the indices $(\sigma_{0,\kappa}^N, \ldots, \sigma_{N,\kappa}^N) \in M_{m,N}$ satisfying (2.26) and sum up to obtain

$$\begin{aligned} m_{\kappa=0}^N D_\kappa^N \left[\prod_{s=0}^{N} H_N(s, \sigma_{s,\kappa}^N) \right] &= \sum_{\kappa=0}^{N} (\kappa + 1) \cdot \bar{\sigma}_{\kappa+1}^{N+1} \cdot \prod_{s=0}^{N+1} H_{N+1}(s, \bar{\sigma}_s^{N+1}) \\ &= \sum_{\kappa=0}^{N+1} \kappa \cdot \bar{\sigma}_\kappa^{N+1} \cdot \prod_{s=0}^{N+1} H_{N+1}(s, \bar{\sigma}_s^{N+1}) \\ &= (N+1) \prod_{s=0}^{N+1} H_{N+1}(s, \bar{\sigma}_s^{N+1}). \end{aligned} \tag{2.28}$$

This means that the differentiation operation on $[f^m]^{(N)}$ generates *partial* terms in $[f^m]^{(N+1)}$.

On the other hand, for each term in $[f^m]^{(N+1)}$, in each index $(\sigma_0^{N+1}, \ldots, \sigma_{N+1}^{N+1}) \in M_{m,N+1}$, we can find all indices $(\sigma_0^N, \ldots, \sigma_N^N) \in M_{m,N}$ satisfying (2.26) such that (2.28) holds. That is, every term of $[f^m]^{(N+1)}$ can be obtained via the differentiation operation on the corresponding terms of $[f^m]^{(N)}$.

Thus we complete the proof of (2.19). Hence (2.18) holds. □

3. The Full connection between two approaches

In Section 2 we derived the modified equation (2.4) for the scheme (1.3). In this section we present a throughout explanation about its full connection with the von Neumann analysis in terms of consistency, stability and wave propagation, although it is quite clear from the previous discussions. We assume again that (1.1) takes an explicit form

$$\mathcal{L}_x v = \sum_{s=1}^{K} \alpha_s \partial_x^s v, \tag{3.1}$$

where α_s are constant, $s = 1, 2, \ldots, K$. The symbol of the operator $\mathcal{L}_x$ is a polynomial, denoted by

$$S_L(k) = \mathcal{L}(ik). \tag{3.2}$$

Then the elementary solution $u(x, t)$ of (1.1), with the initial data $v_0(x) = e^{ikx}$, is

$$v(x, t) = e^{ikx} \cdot e^{S_L(k)t}. \tag{3.3}$$

We still discuss the explicit case of (1.3) only, and the implicit case can be explained in parallel but more tedious.

3.1. Consistency and accuracy

The concepts of consistency and accuracy in the present context illustrate how well the scheme (1.3) approximates Eq. (1.1), usually in smooth regions of the solutions. Using the von Neumann analysis, we just need to compare the solution $u_j^n = \lambda^n e^{ikjh}$ of the scheme (1.3) with the solution (3.3) at (x_j, t_n). Write $u_j^n = e^{i\omega n\tau} e^{ikjh}$. Then we compare $S_L(k)$ with $\omega(k)$ at $k = 0$,

$$\omega(k) = \sum_{s=1}^{\infty} \frac{\omega^{(s)}(0)}{s!} k^s, \tag{3.4}$$

where we use the fact that $\omega(0) = 0$. Thus we say the scheme (1.3) is consistent with Eq. (1.1) if there holds

$$i\sum_{s=1}^{K}\frac{\omega^{(s)}(0)}{s!}k^s = S_L(k). \tag{3.5}$$

If the scheme has accuracy of order $q, q \geqslant 1$, in addition that the consistency condition (3.5) is satisfied, there holds,

$$\omega^{(s)}(0) = 0, \quad s = K+1, \ldots, K+q-1. \tag{3.6}$$

It is exactly the same using the modified equation (2.4) at small-wave-number $k_0 = 0$,

$$\partial_t u = \frac{1}{\tau}\sum_{s=1}^{\infty}\frac{i^{-s}}{s!} \cdot [\ln\lambda]^{(s)}(0) \cdot \partial_x^s u, \tag{3.7}$$

where we use the consistency condition (1.4) such that $\lambda(0) = 1$. Noting that

$$\lambda^{(s)}(0) = i^s h^s \sum_p p^s A_p, \tag{3.8}$$

we obtain

$$[\ln\lambda]^{(s)}(0) = C_s i^s h^s, \tag{3.9}$$

where $C_s(A_p)$ are real constants, depending on A_p, and they are easily calculated without using the tedious Taylor series expansion in [24]. Then the modified equation (1.12) is written as

$$\partial_t u = \frac{1}{\tau}\sum_{s=1}^{\infty}\frac{C_s}{s!}h^s\partial_x^s u. \tag{3.10}$$

In comparison of (1.1) and (3.10), we have the following interpretation for consistency and accuracy.

Consistency. *The scheme (1.3) is consistent with (1.1) if*

$$\frac{C_s}{\tau}\cdot\frac{h^s}{s!} = \alpha_s, \quad s = 1, \ldots, K, \tag{3.11}$$

are satisfied.

Accuracy. *The scheme (1.3) approximates (1.1) with the accuracy of order $q, q \geqslant 1$ in space if*

$$C_s h^s = \begin{cases} s! \cdot \alpha_s \tau, & 1 \leqslant s \leqslant K, \\ 0 & K < s \leqslant K+q-1 \end{cases} \tag{3.12}$$

and $C_{q+K} h^K/\tau$ is bounded.

We are particularly interested in the advection (hyperbolic) equation of the form

$$v_t + cv_x = 0, \quad c > 0, \tag{3.13}$$

since most effective algorithms for hyperbolic systems or convective-dominated problems are related to this simple equation. Assume that the explicit scheme (1.3) for (3.13) is symmetric, $M_1 = M_2 = M$. The maximal accuracy is of order $2M$. And it is of order $q, q \leqslant 2M$ if the consistency conditions

$$\sum_{p=-M}^{M} p^m A_p = (-v)^m, \quad m = 0, 1, \ldots, q, \tag{3.14}$$

are satisfied, where the Courant number is $v = c\tau/h$. In fact, (3.14) is equivalent to

$$[\ln\lambda]^{(s)}(0) = \begin{cases} -ihv, & s = 1, \\ 0, & 1 < s \leqslant q. \end{cases} \tag{3.15}$$

For upwind-biased schemes, we just need to set $A_p = 0$ for some p to derive the scheme with the restriction (3.15).

3.2. Stability

Eq. (1.1) is (strictly) dissipative if the real part of $S_L(k)$ is (negative) non-positive for all non-zero wave number k. Similar arguments apply to the finite difference scheme (1.3) and the von Neumann criterion (1.6) put a constraint in order to make the scheme (1.3) stable. We note that many schemes are not strictly dissipative for some wave number modes. In other words, $|\lambda(k_0)| = 1$ for some $k_0 \in [-\pi/h, \pi/h]$. For instance, the Lax-Friedrichs has the property that $\lambda(0) = \lambda(\pi/h) = 1$. See Fig. 1. To make clearer the dissipative property of a difference scheme, the von Neumann analysis uses the Taylor series expansion for $\lambda(k)$ at such wave numbers.

In terms of the modified equation (2.4), the dissipative property of the difference scheme (1.3) becomes obvious, and the stability requirement can be clarified as follows.

(i) Small-wave-number. At small-wave-number $k_0 = 0$, $\tilde{u}_j^n$ coincides with u_j^n and thus the modified equation is (1.12). The dissipation effect of the scheme (1.3) is reflected in terms of even-order derivative of (1.12) or (3.10),

$$-[\ln \lambda]^{(2s)}(0) > 0, \quad \text{or} \quad (-1)^{s-1}C_{2s} > 0, \tag{3.16}$$

which is just the explicit expression of $\mu(2s)$ at the small-wave-number in [24, Page 167]. Indeed, the lowest even-order term is determinant. As $s = 1$, it is the usual von Neumann numerical viscosity, which plays a decisive role in dissipating small-wave-number modes.

(ii) Large-wave-number. In many applications, large-wave-number modes are much more concerned. In view of (2.1), the mode is divided into two parts α_j^n and $\tilde{u}_j^n$, and thereby the dissipation effects are correspondingly distinguished into two categories:

1. **Strong dissipation.** This type of dissipation comes from the fixed mode $\alpha_j^n = e^{-\omega_I(k_0)n\tau} \cdot e^{i[jh - v_p(k_0)n\tau]}$, which is a traveling wave solution of the PDE,

$$v_t + v_p(k_0)v_x = -\omega_I(k_0)v, \tag{3.17}$$

where $-\omega_I(k_0)v$ plays a damping effect if $\omega_I(k_0) > 0$. Such an effect is thus termed as *a numerical damping*. For a dissipative scheme $|\lambda(k_0)| \leqslant 1$, this dissipation forces most Fourier modes to decay exponentially in time. However, it does not take any effect at small-wave-number $k_0 = 0$, or for neutrally stable schemes such as the box scheme with $|\lambda(k)| \equiv 1$. Even for some strongly stable schemes such as the Lax-Friedrichs scheme, in which this dissipation effect vanishes at the largest-wave-number since $\lambda(\pi/h) = 1$, as shown in Fig. 1. Then the weak dissipation described below will play a crucial role.

2. **Weak dissipation.** This type of dissipation can be seen from the modified equation (1.10) for $\tilde{u}$. As usual, consider an elementary solution of (1.10) in the form, just similar to the small wave number case (1.12),

$$\tilde{u}(x, t) = e^{\gamma t}e^{i\tilde{k}x}. \tag{3.18}$$

Then γ must satisfy

$$\gamma = \frac{1}{\tau}\sum_{s=1}^{\infty} \frac{[\ln \lambda]^{(s)}(k_0)}{s!}\tilde{k}^s = i\sum_{s=1}^{\infty}\frac{\tilde{\omega}^{(s)}(k_0)}{s!}\tilde{k}^s. \tag{3.19}$$

Thus the weak dissipation effect is reflected with the real part of γ,

$$Re\gamma = -\sum_{s=1}^{\infty}\frac{\tilde{\omega}_I^{(s)}(k_0)}{s!}\tilde{k}^s. \tag{3.20}$$

This is just the imaginary part of $\omega(k)$ at $k = k_0$, consistent with that by the Taylor series expansion in the von Neumann analysis.
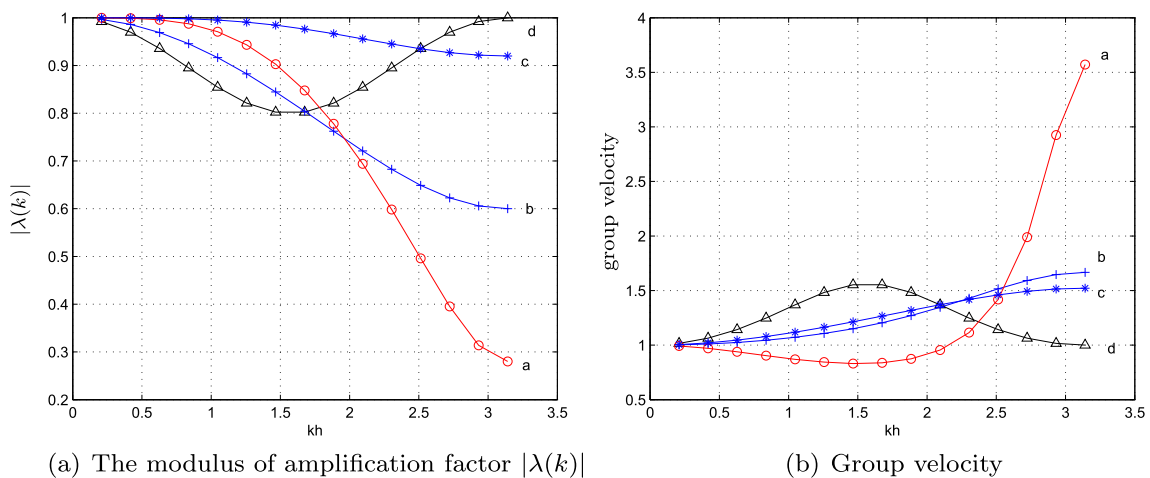

Fig. 1. Comparison of several 3-point first and second order upwind scheme: The Lax–Wendroff scheme labeled "a"; the first order upwind scheme labeled "b"; the Warming-Beam scheme labeled "c" and the Lax–Friedrichs scheme labeled "d". The Courant number $v = c\tau/h = 0.8$, $c = 1$.

(a) The modulus of amplification factor $|\lambda(k)|$ (b) Group velocity

In Fig. 1 (a), we display the modulus of the amplification factors for several popular schemes: (a) The Lax-Wendroff scheme; (b) the upwind scheme; (c) the second order Warming-Beam scheme and (d) the Lax-Friedrichs scheme. As is well-known, the Lax-Friedrichs and the upwind schemes are of first order and have strong numerical viscosities at small wave numbers; while the Lax-Wendroff [11] and the Warming-Beam schemes [23] are of second order and the dissipation effect at small wave numbers are reflected through four-order terms in their respective modified equations. However, at large wave numbers, the situations change: The Lax-Wendroff scheme has the strongest numerical damping, while the Lax-Friedrichs does not have any amplitude error there. Once the data is polluted by the highest frequency mode of the form $(-1)^{j+n}$, the Lax-Friedrichs solution will exhibit oscillatory phenomena, see [12]. These examples highlight the fact that it is necessary to analyze the amplitude error for all wave number modes when investigating the dissipative property of a finite difference scheme.

As an example, the neutrally stable box scheme has no amplitude error at all. That is to say, both the strong and weak dissipation vanish. This scheme takes the compact form for the linear advection equation (3.13), see [16, Page 117],

$$(\mu_x \delta_t + v \mu_t \delta_x) u_{j+1/2}^{n+1/2} = 0, \tag{3.21}$$

where $\mu_x u_{j+1/2}^n = \frac{1}{2}(u_j^n + u_{j+1}^n)$, $\delta_x u_{j+1/2}^n = u_{j+1}^n - u_j^n$, and similarly for μ_t and δ_t. It can be written in a purely transport form

$$[\mathcal{D}_t + c\mathcal{D}_x] u_{j+1/2}^{n+1/2} = 0, \tag{3.22}$$

where $\mathcal{D}_t = \mu_t^{-1}\delta_t/\tau$ and $\mathcal{D}_x = \mu_x^{-1}\delta_x/h$. The amplification factor is

$$\lambda(k) = \frac{\cos\frac{1}{2}kh - iv\sin\frac{1}{2}kh}{\cos\frac{1}{2}kh + iv\sin\frac{1}{2}kh}, \tag{3.23}$$

and $|\lambda(k)| \equiv 1$. In order to stabilize the scheme, the time-average technique is used, see [16, Page 176],

$$[\mathcal{D}_t + c\mathcal{M}_t\mathcal{D}_x] u_{j+1/2}^{n+1/2} = 0, \tag{3.24}$$

with $\mathcal{M}_t = 1 + (\theta - \frac{1}{2})\tau\mathcal{D}_t$. Now the amplification factor of (3.24) is

$$\lambda(k) = \frac{(1 - 2v + 2v\theta)e^{ikh} + (1 + 2v - 2v\theta)}{(1 + 2v\theta)e^{ikh} + (1 - 2v\theta)}. \tag{3.25}$$

Such a manipulation actually adds some artificial viscosity at small wave numbers and numerical damping at large wave numbers, see Fig. 2. The modified equation for (3.24) can be obtained through calculating the amplification factor $\lambda(k)$ in (3.25). At $k = 0$, we have $\lambda(0) = 1$, $[\ln\lambda]'(0) = -c\tau i$ and $[\ln\lambda]''(0) = (ih)^2 v^2 (2\theta - 1), \ldots$, and thus the modified equation is

$$\partial_t u + c\partial_x u = c^2 \tau(\theta - 1/2)\partial_x^2 u + \cdots. \tag{3.26}$$

Hence as $\theta > 1/2$, we introduce artificial viscosity which suppresses oscillations caused by low frequency modes. For $k \neq 0$, we also have $|\lambda(k)| < 1$ uniformly if $\theta > 1/2$, as shown in Fig. 2, which provides the numerical damping (strong dissipation). We do not write out the explicit expression of $|\lambda(k)|$, which is tedious but does not help too much.
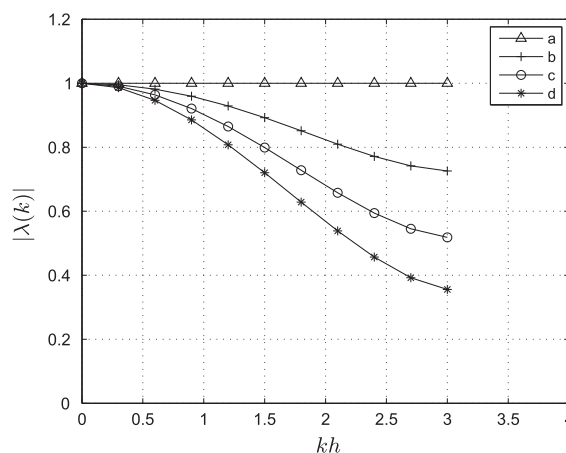

Fig. 2. Amplitude errors of the modified box scheme. The Courant number is taken to be $v = 0.8$ and the parameter θ is taken to be 0.5, 0.58, 0.66 and 0.74, respectively, for *a, b, c* and *d*.

3.3. Dispersion and wave propagation

To understand the behavior of the solution by (1.3), it is necessary to look at the dispersion relation between the wave number k and the frequency $\omega, \omega = \omega(k)$. For this, there are two main elements: Phase speed and group velocity [19]. The phase speed is the rate at which the phase of the wave propagates in space while the group velocity is the velocity with which the wave packet propagates through space. The von Neumann analysis works on this well, as we pointed out in the introduction section that the finite difference solution can be expressed in terms of the phase speed and group velocity (cf. (1.8)),

$$u_j^n = e^{-\omega_I(k_0)n\tau} \cdot e^{ik_0[jh - v_p(k_0)n\tau]} \cdot e^{i[\tilde{k}jh + \tilde{\omega}(k_0 + \tilde{k})n\tau]}, \tag{3.27}$$

where we set $k = k_0 + \tilde{k}$, $\omega(k) = \omega(k_0) + \tilde{\omega}(k_0 + \tilde{k})$ and $v_p(k_0) = -\omega_R(k_0)/k_0$. Note again that

$$\tilde{\omega}(k_0 + \tilde{k}) = \sum_{s=1}^{\infty} \frac{\tilde{\omega}^{(s)}(k_0)}{s!} \tilde{k}^s, \text{ and } -\tilde{\omega}'(k_0) = G(k_0). \tag{3.28}$$

Thus (1.8) is just (3.27) by ignoring higher order terms of $\tilde{\omega}$ in (3.28). This provides the interpretation of phase speed and group velocity through the von Neumann analysis (cf. [21]).

The modified equation (2.4) is obviously obtained via transforming $i\tilde{\omega}$ into ∂_t and $i\tilde{k}$ into ∂_x formally, or it is written as

$$\partial_t \tilde{u} + G(k_0)\partial_x \tilde{u} = \sum_{s=2}^{\infty} \frac{i^{-s}}{s!} [\ln \lambda]^{(s)} \partial_x \tilde{u}, \tag{3.29}$$

i.e., (1.11). Thus it provides a PDE interpretation of group velocity and $\tilde{u}$ can be understood as the wave packet around the wave number k_0.

Thus we unify the two approaches to depict the wave propagation, particularly the propagation of wave packets.

4. Some extensions and discussion

The von Neumann analysis has the advantage of simplicity, intuition and easy implementation and it can supply at least local information about properties of dissipation and dispersion, even though there are the severe restriction over constant coefficients of PDE and periodic boundary conditions, and even counterexamples about the frozen coefficient method which leads to the instability of variable coefficients problems [15]. In contrast, the application of the modified equation approach may be much more extensive. For example, the modified equation can be derived for the monotone scheme for nonlinear hyperbolic conservation laws [8].

In the sequel, we discuss several aspects concerning the von Neumann analysis and the modified equation approach.

4.1. Multidimensional extension

It is straightforward to extend the one-dimensional case to the following multidimensional case

$$v_t = \mathcal{L}_{\mathbf{x}}(v) = \sum_{s=1}^{K} \alpha_s \cdot \nabla_{\mathbf{x}}^s v \tag{4.1}$$

with periodic boundary conditions, where $\mathbf{x} = (x_1, \ldots, x_d) \in [-\pi, \pi]^d$, $\nabla_{\mathbf{x}} = (\partial_{x_1}, \ldots, \partial_{x_d})$, α_s are constant vectors and $\nabla_{\mathbf{x}}^s$ is defined as convention. With a uniform partition of the domain so that $\mathbf{x_j} = (j_1, \ldots, j_d)h$, $j_\ell \in \{0, 1, \ldots, J\}$, and $h = 2\pi/J$ is the mesh size, a linear scheme is

$$\sum_{\mathbf{q} \in \mathcal{N}_1} B_{\mathbf{q}} u_{\mathbf{j}}^{n+1} = \sum_{\mathbf{p} \in \mathcal{N}_2} A_{\mathbf{p}} u_{\mathbf{j+p}}^n, \tag{4.2}$$

where $B_{\mathbf{q}}, A_{\mathbf{p}}$ are constants depending on τ/h, and $\mathcal{N}_1$ and $\mathcal{N}_2$ are the finite sets to index the neighbors of the point $\mathbf{x_j}$ (we use bold letters to denote vectors). Then just as one-dimensional case, we use the von Neumann analysis to obtain accuracy, stability and dispersion results by setting the Fourier mode $u_{\mathbf{j}}^n = \lambda^n(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{j}h}$ to study the amplification factor,

$$\lambda(\mathbf{k}) = \left[\sum_{\mathbf{q} \in \mathcal{N}_1} B_{\mathbf{q}} e^{i\mathbf{k}\cdot\mathbf{p}h} \right]^{-1} \sum_{\mathbf{p} \in \mathcal{N}_2} A_{\mathbf{p}} e^{i\mathbf{k}\cdot\mathbf{p}h}. \tag{4.3}$$

The only difference is that we use multiple indices here.

The modified equation for (4.2) is also the same with multiple indices by setting

$$u_{\mathbf{j}}^n = \alpha_{\mathbf{j}}^n \tilde{u}_{\mathbf{j}}^n, \quad \alpha_{\mathbf{j}}^n = e^{i(\omega(\mathbf{k_0})n\tau + \mathbf{k_0}\cdot\mathbf{j}h)}, \quad \tilde{u}_{\mathbf{j}}^n = e^{i(\tilde{\omega}n\tau + \tilde{\mathbf{k}}\cdot\mathbf{j}h)}. \tag{4.4}$$

Then we derive a modified equation for $\tilde{u}_{\mathbf{j}}^n$, which is similar to (2.4) via replacing ∂_x by $\nabla_{\mathbf{x}}$.

4.2. System cases

Consider system cases,

$$\mathbf{v}_t = \mathcal{L}_\mathbf{x}(\mathbf{v}) = \sum_{s=1}^{K} \alpha_s \cdot \nabla_\mathbf{x}^s \mathbf{v} =: P(\nabla_\mathbf{x})\mathbf{v}, \tag{4.5}$$

where $\mathbf{v}$ is a vector-valued function, and α_s are constant matrices in addition to the aforementioned $\nabla_\mathbf{x}$. The von Neumann analysis can proceed, almost the same as before, by setting

$$\mathbf{u}_\mathbf{j}^n = \hat{\mathbf{u}}^n(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{j}h}, \tag{4.6}$$

as we consider the following finite difference scheme for (4.5),

$$\sum_{\mathbf{q}\in\mathcal{N}_1} B_\mathbf{q}\mathbf{u}_{\mathbf{j}+\mathbf{q}}^{n+1} = \sum_{\mathbf{p}\in\mathcal{N}_2} A_\mathbf{p}\mathbf{u}_{\mathbf{j}+\mathbf{p}}^n, \tag{4.7}$$

where $\mathbf{u}_\mathbf{j}^n$ is the numerical solution approximating $\mathbf{v}(\mathbf{x}_\mathbf{j}, t_n)$, $\hat{\mathbf{u}}^n(\mathbf{k})$ is a vector-valued function of $\mathbf{k}$. Then the amplification matrix is

$$G(\mathbf{k}, \tau) = \left[\sum_{\mathbf{q}\in\mathcal{N}_1} B_\mathbf{q}e^{i\mathbf{k}\cdot\mathbf{q}h}\right]^{-1} \sum_{\mathbf{p}\in\mathcal{N}_2} A_\mathbf{q}e^{i\mathbf{k}\cdot\mathbf{p}h}. \tag{4.8}$$

Thus the von Neumann analysis of consistency, stability and dispersion property of (4.7) is just how to compare the amplification matrix (4.8) with the Fourier symbol $P(i\mathbf{k})$ of (4.5), or more precisely, we need to compare $G(\mathbf{k}, \tau)$ with $e^{\tau P(i\mathbf{k})}$. We refer to [15] for details.

However, the derivation of the modified equation for (4.7) becomes much more involved. This is left for the future.

4.3. Multi-level methods

Multi-level methods, such as the leap-frog scheme, can be considered similarly. The difference is, as pointed out in [1], that in the von Neumann analysis, the amplification factor associated with a wave number generally has $(L-1)$ roots for an L-level scheme, while the coefficients of the modified equation provide information for only the principal root.

4.4. Variable coefficients and nonlinear cases

For problems with variable coefficients or even nonlinear cases, the von Neumann analysis does not seem straightforward to apply. A usual strategy is to adopt the frozen coefficient method at a point, even though there are some counterexamples to display the invalidity of this approach [15]. On the other hand, the modified equation approach seems much flexible to apply for such cases and even for discontinuous solutions (shocks) [5,8]. In this sense, the modified equation has more potential in practical applications. In [13] we have developed a heuristic modified approach for nonlinear problems, but just restricted to conservation laws. For a general problem, we still work in progress [14].

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