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Short note

On the spectral properties of shock-capturing schemes

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Abstract

In this short note we analyze the performance of nonlinear, shock-capturing schemes in wavenumber space. For this purpose we propose a new representation for the approximate dispersion relation which accounts to leading order for nonlinear effects. Several examples are presented, which confirm that the present theory yields an improved qualitative representation of the true solution behavior compared to conventional representations. The theory can provide useful guidance for the choice of the most cost-effective schemes for specific applications, and may constitute a basis for the development of optimized ones.
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1. Introduction

The numerical simulation of flow fields that include both shock waves and rich flow features (acoustic waves, turbulence) requires the use of high-fidelity numerical schemes that must be capable at the same time to handle flow discontinuities and accurately resolve a broad range of length scales, often orders of magnitude apart. It is well known [15] that the order of the truncation error of a numerical scheme only provides information on the asymptotic convergence rate to the exact solution, but it does not convey valuable informations on the actual error on a finite computational grid; rather, wave-propagation (spectral) properties of a difference scheme provide informations on the evolution of all Fourier modes supported on the grid. Linear, central difference approximations are ideal candidates to achieve quasi-spectral behavior in wavenumber space [4]. However, when the flow field includes shock waves whose location is not known in advance, such as for example supersonic jets in off-project conditions (see, e.g. Ref. [2]), the use of shock-capturing schemes becomes (almost) mandatory [4]. Shock-capturing schemes of formal order of accuracy higher than one are always nonlinear [6], i.e. they have a nonlinear behavior even when applied to linear equations, and most often incorporate some form of upwind-biasing. The nonlinear mechanisms in shock-capturing schemes may be represented either by a switch, such as for TVD schemes based on the use of flux (or slope) limiters [10], or on the adaptive

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or solution-biased choice of the stencil for the evaluation of the numerical flux, such as for ENO [5] and WENO [7] schemes. It is generally acknowledged that such nonlinear mechanisms have the main effect of activating (or enhancing) numerical dissipation (more or less) locally around discontinuities so as to prevent (or at least limit) the onset of Gibbs oscillations. Most often, modern shock capturing schemes have linear counterparts; for example, weighted essentially non-oscillatory (WENO) schemes may be turned into linear upwind schemes by disabling the nonlinear weights. The linear counterparts of shock-capturing schemes have occasionally been used in the literature (see, e.g. Ref. [16]) in order to gauge their performance in wavenumber space upon inspection of the approximate dispersion relation [8], i.e. the relation between the modified wavenumber and the reduced wavenumber, which can be consistently defined only for linear schemes. However, even though seldom stated explicitly , numerical tests show that the genuinely nonlinear mechanisms underlying shock-capturing schemes have a dramatic impact upon the computed solution, and their actual behavior may be very different from the one predicted on purely linear grounds.

In the present paper we analyze the wave propagation properties of shock-capturing schemes for smooth solutions, by attempting to define a suitable approximate dispersion relation (ADR). We point out that the issue of the behavior of shock-capturing schemes for shocked solutions is at least equally important, but is outside the scope of the present note; for a recent discussion on the topic the reader may consult Ref. [13] and reference therein.

The objective of the study is two-fold: (i) quantify the (leading order) effect of nonlinear mechanisms on the solution behavior in wavenumber space; and (ii) identify an error metric to be used as a basis of comparison for shock-capturing schemes designed for aeroacoustics applications. For this purpose, in Section 2 we define an ADR for nonlinear schemes; in Section 3 we illustrate the behavior of several low- and high-order shock-capturing schemes according to the new metric; and finally in Section 4 we compare the computational efficiency of those schemes.

2. General theory

For the sake of the analysis, let us consider the one-dimensional propagation of small disturbances in an unbounded domain, governed by the linear advection equation, with monochromatic sinusoidal initial conditions of wavelength λ (and wavenumber $w = 2\pi/\lambda$),

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \quad -\infty < x < +\infty, \quad u(x,0) = \hat{u}_0 e^{iwx}, \tag{1}$$

and assume $a > 0$. Let us consider a semi-discrete approximation of Eq. (1) on a grid with uniform spacing h and nodes $x_j = jh$,

$$\frac{dv_j}{dt} + av_j' = 0, \quad v_j(0) = \hat{u}_0 e^{ij\varphi}, \tag{2}$$

where $v_j(t) \approx u(x_j,t)$ and $\varphi = wh$ is the so-called reduced wavenumber [8]. If one assumes an explicit linear finite-difference approximation for the spatial derivative of v

$$v_j' = \frac{1}{h}\sum_{\ell=-q}^{r} a_\ell v_{j+\ell} \approx \left.\frac{\partial u}{\partial x}\right|_{x=x_j}, \tag{3}$$

Eq. (2) has the following exact solution [15]:

$$v_j(t) = \hat{v}(t)e^{ij\varphi}, \tag{4}$$

where the complex amplitude of the solution at time t is given by

$$\hat{v}(t) = e^{-i(at/h)\Phi(\varphi)}\hat{u}_0, \tag{5}$$

and $\Phi(\varphi)$ is the modified wavenumber [8] associated with the space discretization (3),

$$\Phi(\varphi) = \frac{1}{i}\sum_{\ell=-q}^{r} a_\ell e^{i\ell\varphi}. \tag{6}$$

Spectral schemes have $\Phi(\varphi) = \varphi$, and therefore the distance $|\Phi(\varphi) - \varphi|/\varphi$ can be usefully interpreted as a measure of the relative error associated with the finite-difference discretization.

Shock-capturing schemes typically use conservative approximations for the spatial derivative, so as to ensure convergence to weak solutions [9], based on the definition of a numerical flux $\hat{v}_{j+1/2}$ such that

$$v'_j = \frac{1}{h}(\hat{v}_{j+1/2} - \hat{v}_{j-1/2}), \tag{7}$$

where

$$\hat{v}_{j+1/2} = \hat{v}(v_{j-q+1}, \ldots, v_{j+r}); \tag{8}$$

note that $\hat{v}$ is, in general, a nonlinear function of its arguments, and therefore no analytical formula can be obtained for the ADR in this case.

However, even for nonlinear schemes one can (rather artificially) define an ADR by considering sinusoidal initial conditions with assigned reduced wavenumber $v_j(0) = \hat{v}_0 e^{ij\varphi}$, and time-advancing the solution up to a very small time (say τ), in order to rule out any error associated with time integration. The Fourier transform of the computed solution at time τ yields the complex amplitude of the mode associated with the reduced wavenumber φ, labeled here as $\hat{v}(\varphi;\tau)$, and therefore can exploit relation (5) to define a modified wavenumber

$$\Phi(\varphi) = -\frac{1}{i\sigma}\log\left(\frac{\hat{v}(\varphi;\tau)}{\hat{v}_0}\right), \tag{9}$$

where $\sigma = a\tau/h \ll 1$. On a finite grid of length L and nodes $j = 0, \ldots, N$, $h = L/N$, the supported Fourier modes have wavelenghts $\lambda_n = L/n$, $n = 0, \ldots, N/2$, and the corresponding reduced wavenumbers are $\varphi_n = 2\pi n/N$, and $0 \leqslant \varphi_n \leqslant \pi$. The above procedure is then repeated to define a modified wavenumber for all supported wavenumbers in practice, the DFT of the solution at φ_n is evaluated according to

$$\hat{v}(\varphi_n;\tau) = \frac{1}{N}\sum_{j=0}^{N-1} v_j(\tau) e^{-ij\varphi_n}, \tag{10}$$

and then relation (9) is exploited to define a modified wavenumber for all supported modes

$$\Phi(\varphi_n) = -\frac{1}{i\sigma}\log\left(\frac{\hat{v}(\varphi_n;\tau)}{\hat{v}_0(\varphi_n)}\right), \quad n = 0, \ldots, N/2. \tag{11}$$

Following this procedure one is able to construct an ADR that accounts to leading order for the nonlinear effects embodied in shock-capturing schemes. Several caveats are in order here. In first place, one should recognize that the solution spectra at time τ obtained by means of shock-capturing schemes contain a whole range of wavenumbers rather than the primary one only, as would be the case for linear schemes; at later times those secondary (spurious) modes interact with each other and with the primary one, thus affecting its evolution. In second place, in general several Fourier modes of $O(1)$ amplitude are present at the same time, and, unlike the linear case, their evolution cannot be analyzed separately. These aspects place a stringent bound on the range of applicability of the present (quasi-linear) theory, and will be discussed in greater detail in the next section. Finally, one might observe that the computed ADR in principle depends upon the choice of the initial complex amplitude of the Fourier modes ($\hat{v}_0(\varphi_n)$); we have found that this is not the case, and for all schemes considered here there is no significant influence of the choice of $\hat{v}_0(\varphi_n)$ on the reported ADR.

3. ADR of common shock-capturing schemes

For illustrative purposes in the present study we have considered a limited number of shock-capturing schemes, including: (i) second-order TVD schemes of the type developed by Osher and Chakravarthy [10], with the minmod (MM), superbee (SB) and Van Leer (VL) flux limiters (see, e.g. Ref. [6] for a comprehensive discussion on limiters); (ii) the third-order TVDM (total variation diminishing in the means) compact scheme of Cockburn and Shu [3] with minmod limiter (CS3); and (iii) schemes of the WENO class [7], with formal order of accuracy of three (WENO3), five (WENO5) and seven (WENO7). For an extensive review of the properties of WENO schemes, as well as for a compilation of weights and smoothness indicators, the reader is referred to the work of Balsara and Shu [1]. We point out that, even though results are shown only for a limited number of schemes, the analysis can be applied in principle to any scheme.

The main results are reported in Fig. 1, in terms of the real and the imaginary part of the modified wavenumber; we recall that (see Eq. (5)), the real part of Φ is associated with the approximate phase speed, i.e. with the dispersion properties of the discretization scheme, while the imaginary part of Φ is related to its 'numerical dissipation'. For comparison purposes, in Fig. 2 we also report the ADR of the linear counterparts of the schemes listed above. For this purpose we recall that second-order TVD schemes may be thought of as a blend of first-order upwind (UW1) and second-order central (C2) differencing, and that disabling the nonlinear weights of WENO schemes one is left with the linear upwind schemes of the cor-

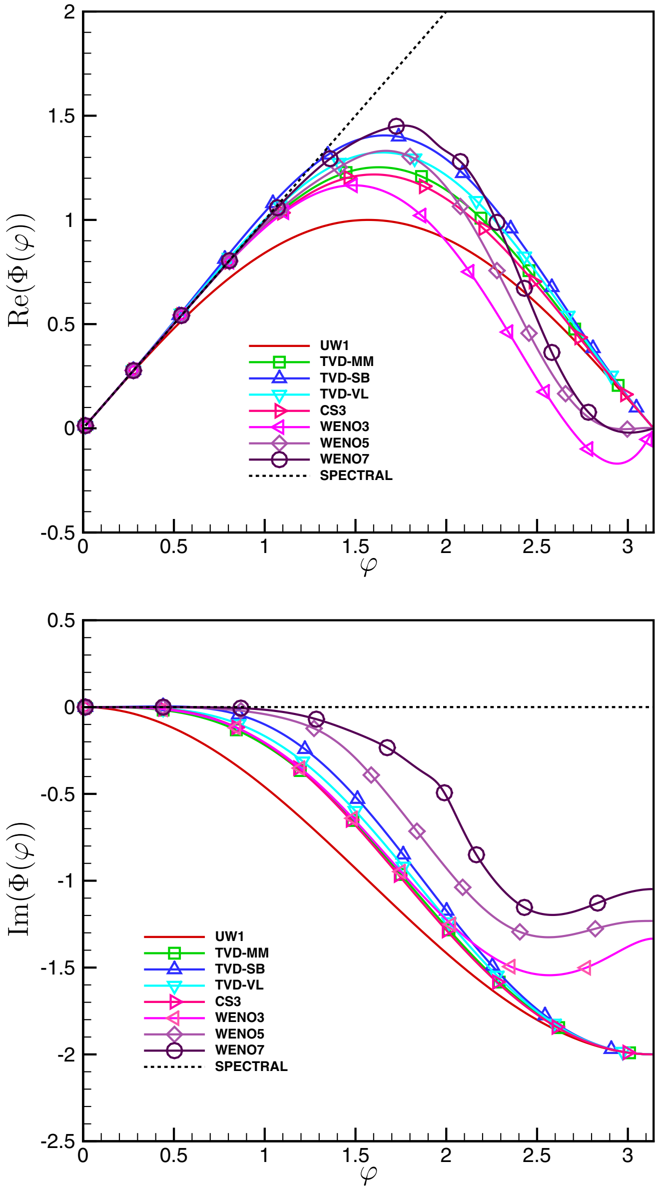

Fig. 1. Approximate dispersion relation for various shock-capturing schemes.

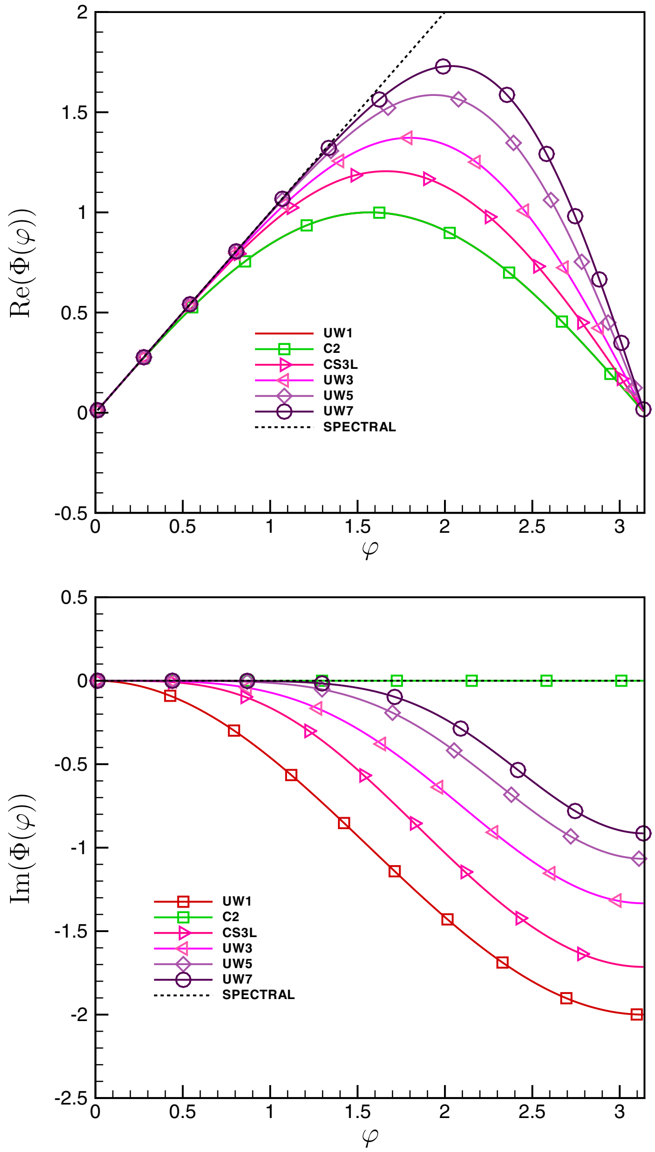

Fig. 2. Approximate dispersion relation for various linear finite-difference schemes.

responding order (UW3, UW5, UW7). The linear version of Cockburn and Shu's scheme is a third-order compact upwind scheme that we have labeled here as CS3L; for a discussion on the ADR of compact upwind schemes see, e.g. Ref. [11].

The results quantitatively unveil some interesting facts, most of which are already (loosely though) acknowledged. The effect of limiters on second-order TVD schemes is beneficial for performance in wavenumber space in that they have better dispersion properties than C2 scheme, and less numerical dissipation than UW1, whereas limiting has a minor effect on the performance of the CS3 scheme. The analysis also indicates that the TVD-SB scheme has a slightly unstable behavior at low wavenumbers, where $\mathrm{Im}(\Phi) > 0$ (though not clearly visible in the figure); this is associated with the well known 'squaring' effect caused by the superbee limiter, and is compensated by its nonlinear stability properties. With regard to the behavior of WENO schemes, they exhibit similar dispersion performances but less numerical dissipation with respect to low-order ones, and propagate marginally resolved waves (i.e. for $\varphi \approx \pi$) at negative phase speed. The spectral properties (both dispersion and dissipation) of WENO schemes are dramatically deteriorated upon activation of the nonlinear weigths, and linear analysis brings little (if any) information on the actual solution behavior. In order to investigate this point more clearly, we have analyzed the evolution of the amplitude of (initially) isolated Fourier modes corresponding to $\varphi = \pi/8$, $\pi/4$ and $\pi/2$. The results of simulations of the linear advection equation performed with the WENO5 scheme are reported in Fig. 3; in the same figure we also report the theoretically predicted time evolution (as from Eq. (5))

$$|\hat{v}(\varphi, t)| = |\hat{v}_0(\varphi)| e^{(at/h)\mathrm{Im}[\Phi(\varphi)]}, \tag{12}$$

where the modified wavenumber Φ is either extracted from the simulation according to Eq. (11) or predicted on linear grounds according to Eq. (6) for UW5, which is the linear version of WENO5. The figure clearly indicates that linear analysis predicts a much slower decay of the Fourier modes, while the quasi-linear analysis described in Section 2 provides quantitatively correct prediction for the amplitude of the modes up to a time, which is shorter for marginally resolved waves, when higher order effects related to the onset of spurious modes become important. For the same scheme we have also computed the solution starting from initial conditions containing a broad range of wavenumbers,

$$v_j(0) = \sum_{m=1}^{N/2} A_m^0(\varphi_m) e^{i\theta_m} e^{ij\varphi_m}, \tag{13}$$

where the initial amplitude of the modes are distributed according to

$$A_m^0(\varphi_m) = e^{-(\varphi_m/(\pi/8))^2} \tag{14}$$

and θ_m are random phases. The computed amplitude spectra at time $t = 8$ are shown in Fig. 4 together with the predictions obtained from the quasi-linear ADR for WENO5 and the linear ADR for UW5. Even though in this case nonlinear interaction between $O(1)$ modes are certainly not negligible, the figure shows rather good agreement at low wavenumbers with the quasi-linear ADR. At higher wavenumbers a spectrum 'wake' consisting of spurious modes arises, which is not accounted for in the present theory.

The same qualitative behavior shown here for WENO5 has been observed for all the schemes we have considered. The overall indication is that the quasi-linear ADR here proposed can be used to get a more precise (even though incomplete) idea on the qualitative behavior of the solution of wave propagation problems provided by shock-capturing schemes compared to the commonly used linear ADR.

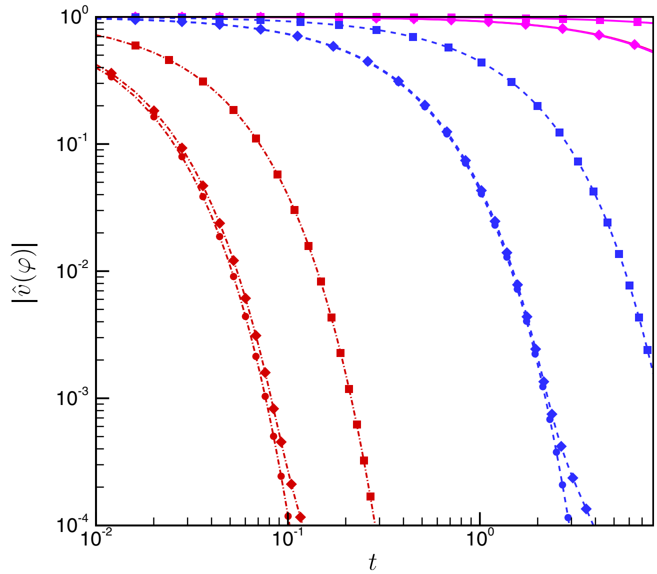

Fig. 3. Time evolution of isolated Fourier modes amplitude. ◆, computed (WENO5); ●, quasi-linear ADR (WENO5); ■, linear ADR (UW5). —, $\varphi = \pi/8$; - - - -, $\varphi = \pi/4$; –·–·–, $\varphi = \pi/2$.

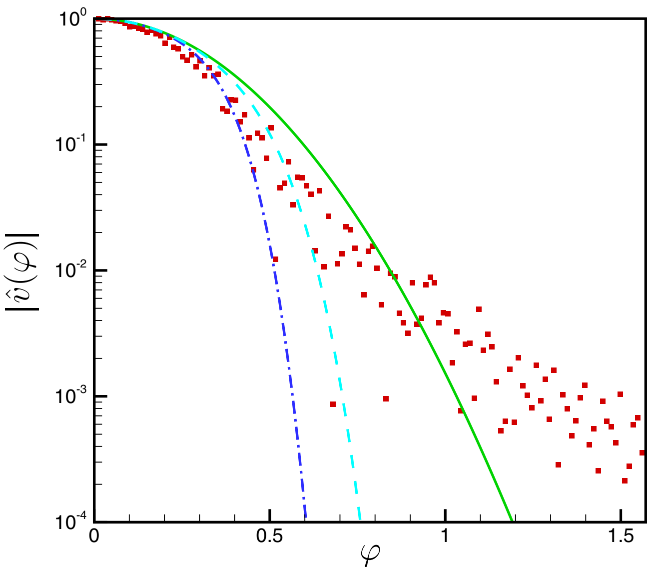

Fig. 4. Computed amplitude spectra at $t = 8$ (square symbols). —, initial conditions; –·–·–, quasi-linear ADR (WENO5); - - - -, linear ADR (UW5).

4. Performance analysis

The next step is exploiting the new ADR representation to obtain an improved numerical error metric to compare the performance of different schemes, and potentially to design optimized ones. The analysis of the error of linear finite-difference schemes for spatial discretization has been the subject of previous studies by Colonius and Lele [4] and by the present author [12]. The main result of those studies is that, for wave propagation problems involving a range of wavenumbers $0 \leqslant w \leqslant \bar{w}$, the maximum relative error (defined as the distance in the L_2 norm from the exact solution) is given by

$$e_0(\bar{\varphi}) = \frac{1}{\bar{\varphi}} \max_{0 \leqslant \varphi \leqslant \bar{\varphi}} |\Phi(\varphi) - \varphi|, \tag{15}$$

where $\bar{\varphi} = \bar{w}h$, and is therefore entirely dependent upon the ADR of the scheme under consideration. In addition, assuming that time integration is performed by means of an explicit Runge–Kutta scheme at fixed value of the Courant number, the incurred computational cost is

$$C \sim \frac{v}{\bar{\sigma}\bar{\varphi}^{n_{\mathrm{D}}+1}}, \tag{16}$$

where n_{D} is the number of spatial dimensions and v is a measure of the CPU time per grid point per time step required by the scheme. The specific values of v used in the present analysis (reported in Table 1) have been obtained by measuring the CPU time required by the various schemes for the solution of Burgers equation, and include the time for performing Lax–Friedrichs flux splitting. Such values are meant only for indicative purposes, as the actual figures sensitively depend upon the specific implementation and computer architecture. The idea is then to exploit the results of linear analysis to evaluate the performance of shock-capturing schemes for wave propagation problems assuming that they can be characterized in terms of their quasi-linear

Table 1
Estimate of CPU time per grid point per time step for several shock-capturing schemes (cost is normalized by the CPU time needed for UW1)

UW1	TVD-MM	TVD-SB	TVD-VL	CS3	WENO3	WENO5	WENO7
1	1.786	1.942	1.775	3.220	2.682	5.607	7.613

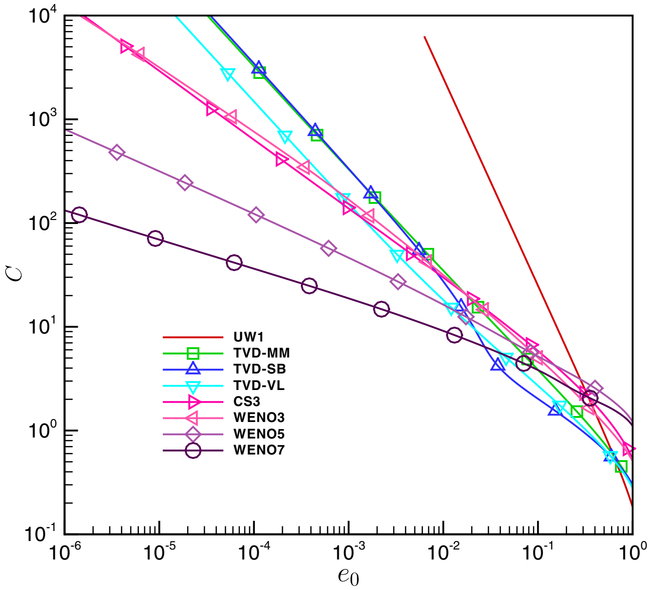

Fig. 5. Cost vs. error level plots (in one space dimension) for several shock-capturing schemes.

ADR. In Fig. 5 we report the cost vs. error plot thus obtained for the shock-capturing schemes considered in the present paper for one-dimensional problems (i.e. $n_D = 1$). The figure seems to indicate that high-order shock-capturing schemes of the WENO class become more cost-effective when relatively strict error tolerances are placed (i.e. for error levels $e_0 \leqslant 10^{-2}$); when coarser representations are sought for, classical second-order TVD scheme seem to be best candidates. Taking this analysis literally, one might think of constructing shock-capturing schemes optimized for specific error levels (as done in Ref. [12] for linear schemes), trying to modify their quasi-linear ADR. This could be done, for example, acting on the WENO weights or smoothness evaluators.

We again remark that the overall solution error is affected by the generation of spurious modes and by non-linear mode interactions; these features are not accounted for in the present analysis, and actual error levels can be even one order of magnitude larger than those predicted from Eq. (15). The simplified analysis, however, has at least two merits: (i) it provides a lower bound for the overall error; (ii) it provides a basis for the comparison of performance of nonlinear schemes other than case-by-case, as usually done in the literature (see, e.g. Ref. [14]).

5. Concluding remarks

In this note we have defined an approximate dispersion relation for nonlinear, shock-capturing schemes. Despite its limitations, the theory is proven to be more accurate in predicting the qualitative solution for wave propagation problems than conventional linear representations. Computed results indicate that nonlinear mechanisms generally degrade the solution behavior of shock-capturing schemes compared to their linear counterparts, to an extent that is not predictable on purely linear grounds. One of the applications of the present theory is the definition of a new error metric for shock-capturing schemes which (though only approximate) may provide some general guidance for the selection of the most cost-effective scheme under specific restrictions of the solution error, as well as for the development of optimized schemes.

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