A LOW ORDER ADVECTION DISCRETIZATION SCHEME BASED ON AN ADDITIONAL GRADIENT EQUATION

Luiz Eduardo Bittencourt Sampaio, luizebs@vm.uff.br
Roney Leon Thompson, rthompson@mec.uff.br
Universidade Federal Fluminense (UFF – LMTA/PGMEC), Rua Passo da Pátria 156, bloco E, sala 216, Niterói, RJ, 24210-240, Brazil

Abstract. *Several numerical schemes have been proposed in the literature to deal with flows involving convection, but all of them present some spurious effects. It is generally agreed that a high order scheme is preferable, and that it must be complemented with some kind of limiting technique to avoid spurious oscillations, which necessarily leads to a low order approximation for small structures. In this paper we revisit some literature consensus regarding numerical schemes, like TVD enforcing, order of convergence, and the possible role in physical modeling of turbulence. We show that many literature recommendations in this respect come from a misleading error assessment used in the analysis and design of such schemes. A more physically-oriented error assessment tool is thus proposed, in which the initial reconstruction errors are separated from the errors due to the physical transport. Focusing on the latter and ignoring the former allowed the development of a preliminary scheme that, despite being based on first order stencils, provided improved results for all cases tested, when compared to several higher order traditional schemes in linear and non-linear convection. In the particular case of 1D linear convection in a uniform field, commonly used as benchmark for aero-acoustics, the total transport errors were of the order of machine precision, with virtually zero diffusion and dispersion.*

Keywords: Numerical schemes, convection, dispersion, diffusion, CFD.

1. INTRODUCTION

Traditional numerical discretization schemes are based on a pre-defined finite set of operations on the variable field that are performed for all time steps Lomax *et al.* (2001). In the design of a numerical scheme, the goal is to minimize an error according to some definition that is immutable from one time to the next. Generally, wavenumber analysis is employed to calculate this error for the continuous range of frequencies. During the discrete evolution of a waveform during a single time step, two types of errors are present: one due to the initial reconstruction of the field (which is the step that will allow to calculate the required derivatives for the Taylor series in Finite Difference Method, or a interpolated flux to be used in Finite Volume Method); and another one that arises from the discrete transport evolution, due to inaccuracies in spatial and temporal terms involved in the governing equations. While the first source of error cannot be avoided for a general initial waveform, the second can be overcome, at least for a limited set of initial fields.

During the choice of the coefficients in a computational stencil, no distinction is made between these two sources of errors, and the researcher generally loses the control over what he is aiming for in the search for the optimum scheme. For instance, if one tries to minimize the total L^2 error for the whole spectrum, frequencies that may never be represented by the mesh anyway will be accounted and will contribute to penalize the total "cost function". Worst than that, since each time step is treated equally, the error will be cumulative, and future waveforms will be contaminated by an error committed because of an optimization towards a mode that was not even present in the first place.

In this paper we propose to elect a set of initial waveforms for which we will be able to accurately predict the transport. The space spanned by this set is that of piecewise linear functions, and any error due to the initial reconstruction will be summarily ignored, under the reasoning that if a better representation is sought later, one can always apply some high order polynomial fitting or some filtering to smooth the field. Notice that in this case, the initial reconstruction errors makes no harm in this late high order reconstruction, as long as the transport evolution is accurately captured and the highest frequency present is inferior to the mesh spacing frequency, according to Nyquist criteria.

2. MOTIVATION

For the sake of clarity in the presentation, in this paper we will focus on the one dimensional pure convection transport equation. Let $\phi(t,x)$ be a function representing the quantity to be convected, subject to the following one dimension, linear, transport equation:

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0\,, \tag{1}$$

where u is the flow velocity convecting ϕ in the periodic domain Ω of length L_Ω.

We shall initially assume u as a uniform and constant field in the following discussion. In this case, the analytical solution is simply $\phi(t,x) = \phi^0(x - ut)$, where $\phi^0(x) = \phi(0,x)$ is the initial wave form.

Some remarks that inspired the developments presented in this paper are now drawn, regarding the evolution of a simple cosine wave of wavelength equal to twice the mesh spacing under linear convection in a uniform flow.

Remark 2.1 *For an odd number of quarter-wavelength convection distances, the mesh should be sampling the waveform at exactly the null points of the cosine and $\phi_i = 0$ for all grid points "i's".*

This means that the energy of the sampled analytical solution is null, and therefore is not to be conserved in a discrete environment. This does not correspond to the continuous domain (complete space of functions, without discretization) behavior, for which energy is known to be conserved, but this is the effect of the sampling operation.

Remark 2.2 *For a further quarter-wavelength advance, the sampled wave should yield the negative of the original field (π radians out of phase).*

This means that the exact solution, when mesh-sampled, is expected to periodically reappear, after a momentary disappearance at fractional times, as commented above. Therefore, there is a long-term, periodic conservation of energy.

In this regard, this paper shows it is possible to develop a numerical scheme that is able to conserve energy in a long term, periodic manner, without the dispersive errors which would result from conservation enforcement from one time-step to the next. In order to achieve this, a fundamental feature that must be contemplated is the ability to capture the disappearance/reappearance of structures, as commented above. This is clearly against the traditional idea of enforcing TVD at every time step, as this would eliminate any possibility of resurgence of the original shape.It is also against the use of conservative schemes, as commonly done in LES along with a physical model to dissipate energy.

Remark 2.3 *At an odd number of quarter-wavelength traveling distances, the analytical solution for the original problem becomes a sine wave, since the travelled distance corresponds to a one-fourth wavelength.*

To capture this sine wave, one could think about using a staggered mesh, which would allow a sampling that coincides with the sine peaks. Or alternatively, one could use the same original collocated mesh, where a new independent equation for the derivative of ϕ (or gradient in more dimensions) is solved – the rationale being that the sine can be expressed as a derivative of the cosine wave of the same frequency. This latter approach is chosen in this paper and a possible implementation is outline in the next section.

3. A NEW PROPOSAL USING AN INDEPENDENT GRADIENT EQUATION

We will now show a general framework for developing consistent numerical schemes that can present minimum or zero errors, at least for the 1-D linear convection in uniform field. The new proposal algorithm can be split into three parts, for the sake of clarity: the general transport equations, which includes an additional independent equation for the gradient transport; the reconstruction functions; and the time advancing step, in which discrete solution for the transport equations is found.

The spatial derivative of Eq. 1 is:

$$\frac{\partial G}{\partial t} + u\frac{\partial G}{\partial x} + \frac{\partial u}{\partial x}G = 0\,. \tag{2}$$

In the complete space of functions, Eq. 2 is redundant as it is derived from Eq. 1 – satisfying the latter automatically implies satisfying the former. However, in a truncated discrete environment, this is not the case, and Eq. 2 provides complementary information to the convective transport of ϕ. This (solving for an independent equation for the derivative) was the key missing link, absent in all previous numerical schemes of the literature. To isolate the influences of the second and third terms in the left hand side of Eq. 2, we note that the third term becomes zero in a uniform flow field, while the second term becomes zero when ϕ is linear (G is constant). The second term on the left hand side of Eq. 2 is the convection of G and accounts for the change in the spatial derivative (G) due to the shape of the reconstructed function, upon convection. This term alone has the ability to bring upwind information even if unbiased schemes are used in all spatial derivatives.

The reconstruction step aims at rebuilding a continuous function with the limited information available – the fields ϕ and G. We will require that the reconstructed function be continuous, but we will not enforce continuity in its derivatives, to keep the computational costs low. With the values of ϕ and G at two adjacent mesh nodes, x_j and x_{j+1}, one can find the intersection point $(x_{Int}, \phi(x_{Int}))$ and then reconstruct the function at any location in between these two nodes. The reconstructed field ϕ consists of piecewise linear segments, each of them extending from one intersection point (found between x_j and x_{j+1}) to the next (located between x_{j+1} and x_{j+2}), while the reconstructed G is assumed constant in the same piecewise intervals. This process can be repeated for every pair of adjacent nodes at a generic time $t = t_m = m\Delta t$ (m is an integer number) so that the reconstructed fields ϕ and G are analytically known everywhere for $t = t_m$.

Equations 1 and 2 can then be advanced from t_m to t_{m+1}, using the last know reconstructed fields as the "initial condition" ($t = t_m$). Generally, for the proposed reconstruction, the second term on the LHS of Eq. 2 is null because of the piecewise linear reconstruction. Only exception is when an intersection point crosses a mesh node location. In this case, by solving the jump condition we find that a simple gradient update is sufficient to represent this crossing. For the particular reconstruction chosen in this work, it can be mathematically proven that this gradient update reduces to a traditional first order upwind calculation for the nodes where the crossing occurs.

4. NUMERICAL EXPERIMENTS

Several 1D tests were performed in order to compare the new proposal with traditional high order schemes. Linear convection in uniform flow were captured within machine accuracy with the present proposal, while 4th order and higher schemes, with and without limiting techniques (like TVD) needed several mesh nodes to provide similar accuracy. The error convergence rates for the test case involving the linear convection transport of a gaussian pulse with an increasing number of mesh nodes are presented in Fig. 1, for the optimized DRP-7 (Tam and Webb, 1993), WENO Levy *et al.* (2001), and the present algorithm. A theoretical 4^{th} order line is also shown. It is worth commenting that high order discretization must not be the guiding principle for designing or choosing numerical schemes. In fact, the algorithm here presented, despite being based only on first order upwind, provided truncation error accurate results. It is not even possible to infer the order of the present proposal by looking at Fig. 1. At least in the cases presented in this work, it seems that correctly representing the physics is more important than the order of convergence. Notice that all limited schemes in the literature revert to low order near the mesh cut-off, as the case with WENO in Fig. 1. It takes a lot of mesh refinement before one can take full advantage of the 4th order accuracy (i.e., getting a sixteen-fold smaller error when doubling the mesh). There are a number of practical situations (like in turbulence) in which one knows the expected size of the smaller structure that must be well captured by the scheme, and the full benefit of a 4th order scheme will only be appreciated with a mesh that fits many nodes inside this smallest mode. This would not be necessary with a low order schemes that privilege the transport physics errors instead of the initial reconstruction errors.

The results are also machine precision accurate for linear convection in multi-dimensional cases, as shown in Fig. 2

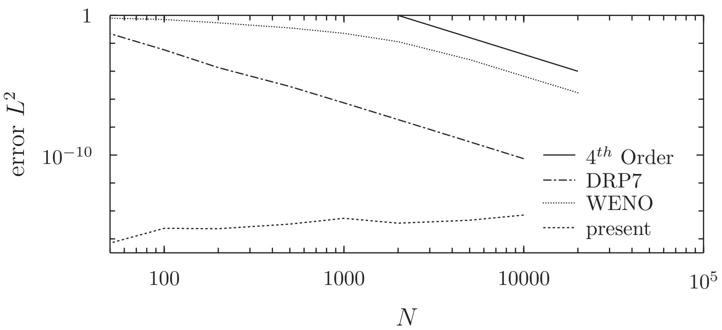
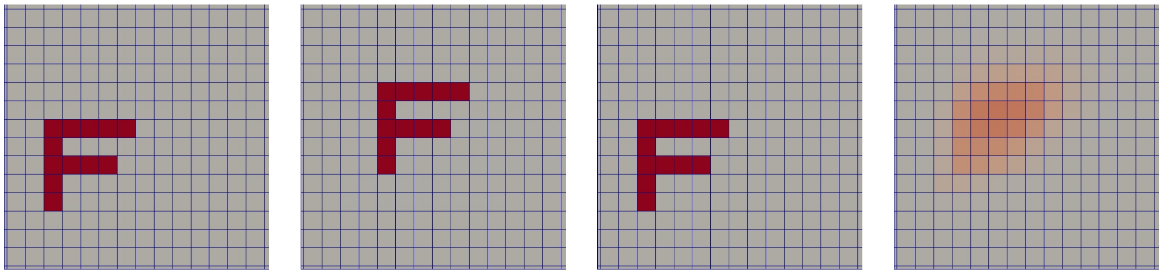


Figure 1. Convergence rates for the error measured at $t = 5$.

for the pure linear convection of a passive scalar that initially assumes the letter "F" shape. The shape is perfectly recovered after a multiple of mesh space convection distance for the new scheme, while all limited traditional schemes tested (MUSCL is the one shown in the figure) presented some blurring effect, as expected.



(a) new scheme $t = 0$ (b) new scheme $t = 2$ (c) traditional $t = 0$ (d) traditional $t = 2$

Figure 2. Pure linear convection in 2D.

For non-linear convection, the new scheme also shown superior accuracy, along with an ability to change the size of the structures without incurring in spurious dispersion or dissipation, suggesting it could be able to capture the turbulence energy cascade towards the subgrid modes without any subgrid model.

5. FINAL REMARKS

The author hopes this work has helped elucidate some controversial topics in the CFD and turbulence simulations community. The separation of the initial waveform reconstruction error from the transport error allows the development of better schemes. It made possible the design of a numerical scheme based on first order *upwinding* that are exact at least for the simpler linear convection in uniform flow field, despite being only first order in space and second in time, and it showed that preference for high order scheme with TVD should be revisited.

6. ACKNOWLEDGEMENTS

The authors acknowledges the support from CNPq.

7. REFERENCES

Levy, D., Puppo, G. and Russo, G., 2001. "Central weno schemes for hyperbolic systems of conservation laws". *MATH. MODEL. NUMER. ANAL*, Vol. 33, pp. 547–571.

Lomax, H., Pulliam, T.H. and Zingg, D.W., 2001. *Fundamentals of computational fluid dynamics*. Scientific Computation. Springer-Verlag, Berlin. ISBN 3-540-41607-2.

Tam, C.K.W. and Webb, J.C., 1993. "Dispersion-relation-preserving finite difference schemes for computational acoustics". *J. Comput. Phys.*, Vol. 107, No. 2, pp. 262–281. ISSN 0021-9991.

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