Available online at http://scik.org
Eng. Math. Lett. 2022, 2022:2
https://doi.org/10.28919/eml/7444
ISSN: 2049-9337

INTUITIVE EXPLANATION OF NUMERICAL DIFFUSION WITH IMPLICIT SCHEME FOR ADVECTION EQUATION

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Abstract. We present a mathematical explanation about the false diffusion with an implicit scheme for advection equation using a Taylor approach. Typically for explain the numerical diffusion with an implicit scheme, it is explained using the Fourier approach as can be seen in the bibliographic review carried out in this paper.

Keywords: advection-diffusion; numerical diffusion; pure-advection; implicit-scheme.

2010 AMS Subject Classification: 35K57.

1. Introduction

Advection and advection-diffusion equations describe many physical processes. Pure advection is encountered, for example, in the case of inviscid fluid flow. The uni-dimensional linear case of pure advection, where some property ϕ is transported with a flow at a given velocity c, is represented by the following partial differential equation:

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

False diffusion, or numerical diffusion, is a common problem when numerically solving this equation with low order explicit time stepping schemes [1, 2], which is a consequence of the fact

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Received April 21, 2022

that the partial derivatives (in time and space) are replaced by a finite difference approximation,

$$\frac{\phi_i - \phi_{i-1}}{\Delta x} = \left(\frac{\partial \phi}{\partial x}\right)_i - \frac{\Delta x}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i + \mathcal{O}(\Delta x^2). \tag{2}$$

While the diffusive term vanishes as Δx goes to zero (thus maintaining consistency), in practice Δx is often significantly larger than zero, and false diffusion occurs. Only when the spatial and time discretisations are chosen in a manner such that $c\Delta t = \Delta x$, the diffusive terms cancel out, and a diffusion free solution can be obtained. For numerical stability it is necessary to always choose $c\Delta t \leq \Delta x$ when using an explicit time stepping scheme (this is known as the Courant-Friedrich-Lewy (CFL) condition [2]), so that avoiding false diffusion comes at a considerable computational cost, as a finer spatial discretisation requires a shorter time step. To evaluate the CFL condition, the Courant number is defined,

$$C \equiv \frac{c\Delta t}{\Delta x}. \tag{3}$$

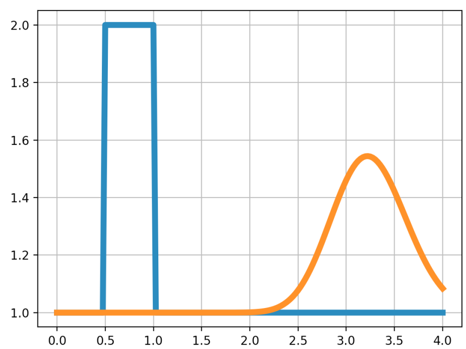
In order to avoid numerical instability, and thus to allow for larger time steps, an implicit time stepping scheme can be employed. Implicit time stepping schemes are stable even Numerical solutions of 1 with explicit and implicit time stepping are presented in fig. 1.

The graphs in figs. 1a, 1c and 1e show that while the implicit solution is numerically stable independently of the discretisation of time and space, it shows significant numerical diffusion in all cases, even when the CFL conditions is met. The explicit scheme, on the other hand, is unstable if $c\Delta t > \Delta x$ (fig. 1f), but yields a diffusion free solution if $c\Delta t = \Delta x$ (fig. 1b).

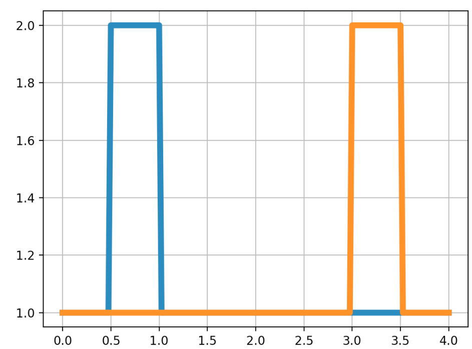
One possible approach to avoiding numerical diffusion in explicit schemes is to use higher order spatial discretisation [1, 3] but this increases the computational cost and can lead to instabilities [4].

The numerical diffusion caused by implicit schemes is often mentioned, but an explanation of its mathematical origin is difficult to find in the literature. Rood reviews and discusses the most commonly used advection solution schemes, taking into account numerical accuracy, diffusivity and computational cost [5]. The origin of the numerical diffusion in implicit schemes, however,

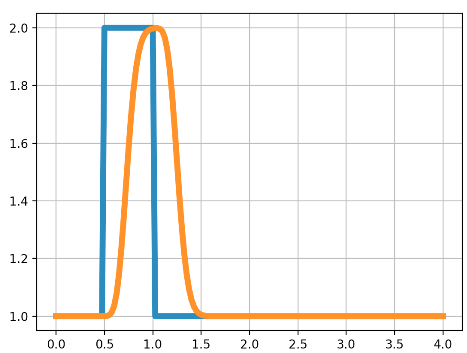
False diffusion also occurs in advection-diffusion equations (e.g. Navier-Stokes equations), where the simulated diffusivity is consequently over-predicted



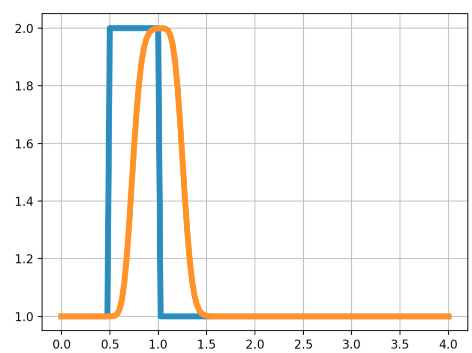
(A) Implicit time stepping with $c\Delta t = \Delta x$



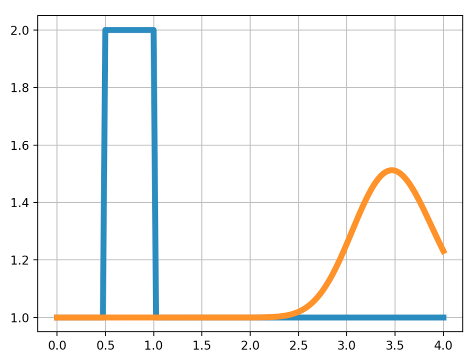
(B) Exlicit time stepping with $c\Delta t = \Delta x$



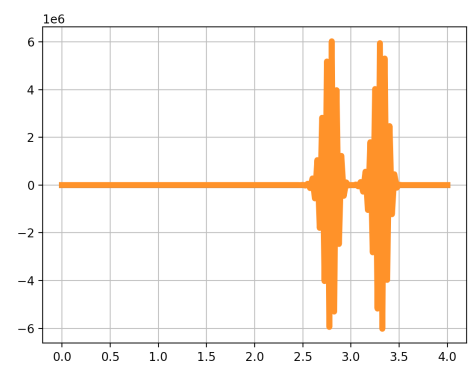
(C) Implicit time stepping with $c\Delta t = 0.1\Delta x$



(D) Explicit time stepping with $c\Delta t = 0.1\Delta x$



(E) Implicit time stepping with $c\Delta t = 1.1\Delta x$



(F) Explicit time stepping with $c\Delta t = 1.1\Delta x$

FIGURE 1. Numerical solution to eq. (1) with different parameters. On the left an implicit scheme is used, while on the right an explicit scheme is used.

is not discussed. Xue and Xie present an alternating direction implicit scheme for advection-diffusion equations that exhibits low numerical diffusion for low Peclet numbers, but as such is not suitable for pure advection [6]. They also indicate that numerical diffusion is mainly caused by interpolation between nodes, but do not offer a more detailed explanation. In a recent paper Wu et al. review existing time stepping schemes for advection-diffusion equations, and present a diffusion minimising numerical scheme [7]. But both, the reviewed and the newly presented scheme are explicit in nature, and implicit schemes are not discussed.

2. VON NEUMANN ANALYSIS

The von Neumann (or Fourier) stability analysis is a common approach to assess the numerical behaviour of different time stepping schemes for advection and advection-diffusion equations [8], and in pure advection, false diffusion can be explained by the reduction of the modulus of the amplification factor [9].

Long and Pepper introduce a "computational diffusion coefficient" based on the Courant number [10]. They indicate that the computational diffusion can be explained by the second spatial derivative from the Taylor expansion in the case of explicit schemes, and then generalise the diffusion coefficient based on Fourier analogy, but do not offer a more detailed explanation for the implicit case when $C > 1$.

3. TAYLOR BASED EXPLANATION

In this manuscript a more intuitive explanation for the occurrence of false diffusion in fully implicit schemes is offered, based on Taylor expansions of the terms of 1. The explanation is somewhat analogous to the case of the standard Euler scheme, but involves Taylor expansions in space and time. It shows that when using an implicit scheme to solve a pure advection equation, one is, in fact, solving an advection-diffusion equation.

If eq. (1) holds for all $x \in [0,L]$ and for all $t>0$, then it must hold for any particular x_i, at any point in time t_n:

$$\left(\frac{\partial \phi}{\partial t}\right)_i^n + c\left(\frac{\partial \phi}{\partial x}\right)_i^n = 0 \tag{4}$$

If an implicit scheme chosen, the spatial derivative is evaluated in t_{n+1},

$$\left(\frac{\phi_i^{n+1}-\phi^n}{\Delta t}\right)_i + c\left(\frac{\partial\phi}{\partial x}\right)_i^{n+1} = 0 \tag{5}$$

Approximating the spatial derivative at time t_{n+1} using a Taylor expansion, the following expression is obtained,

$$\left(\frac{\partial\phi}{\partial x}\right)_i^{n+1} = \left(\frac{\partial\phi}{\partial x}\right)_i^n + \frac{\partial}{\partial t}\left(\frac{\partial\phi}{\partial x}\right)_i^n \Delta t + O(\Delta t^2) \tag{6}$$

According to Schwartz's theorem, mixed second derivatives can be interchanged, so that

$$\left(\frac{\partial\phi}{\partial x}\right)_i^{n+1} = \left(\frac{\partial\phi}{\partial x}\right)_i^n + \frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial t}\right)_i^n \Delta t + O(\Delta t^2) \tag{7}$$

But, according to eq. (2),

$$\left(\frac{\partial\phi}{\partial t}\right)_i^n = -c\left(\frac{\partial\phi}{\partial x}\right)_i^n, \tag{8}$$

So that the Taylor series now contains a second derivative in x,

$$\left(\frac{\partial\phi}{\partial x}\right)_i^{n+1} = \left(\frac{\partial\phi}{\partial x}\right)_i^n - c\left(\frac{\partial^2\phi}{\partial x^2}\right)_i^n \Delta t + O(\Delta t^2) \tag{9}$$

Replacing the first two terms in eq. (3) one obtains

$$\left(\frac{\phi_i^{n+1}-\phi^n}{\Delta t}\right)_i + c\left[\left(\frac{\partial\phi}{\partial x}\right)_i^n - c\left(\frac{\partial^2\phi}{\partial x^2}\right)_i^n \Delta t\right] = 0 \tag{10}$$

which, after re-arranging terms, yields the following advection-diffusion equation,

$$\left(\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)_i + c\left(\frac{\partial\phi}{\partial x}\right)_i^n = c^2\left(\frac{\partial^2\phi}{\partial x^2}\right)_i^n \Delta t. \tag{11}$$

11 indicates that when using a fully implicit scheme to solve 1, a non-zero term appears on the right hand side, which is proportional to the second spatial derivative, thus resulting in (false) diffusion. The diffusive term is multiplied by the times step, which indicates that false diffusion cannot be prevented completely, but its magnitude can be manipulated by adjusting the time step. This is consistent with [10].

4. Conclusion

In this manuscript an intuitive mathematical explanation for the occurrence of numerical diffusion when solving the pure advection equation is presented. As opposed to the von Neumann analysis, which focuses on the numerical error, this approach makes use of the Taylor expansion of the equation, and shows that solving the pure advection equation using an implicit time stepping scheme, effectively results in the solution of an advection-diffusion equation

Conflict of Interests

The author(s) declare that there is no conflict of interests.

References

[1] C. Hirsch, Numerical computation of internal and external flows, Butterworth-Heinemann, Oxford, (2007)

[2] J. H. Ferziger, M. Perić, Computational methods for fluid dynamics, Springer. (1980)

[3] S. Palankar, Numerical heat transfer and fluid flow, Taylor & Francis Group. (1980)

[4] P. Smolarkiewicz, A simple positive definite advection scheme with small implicit diffusion, Mon. Weather Rev. 11 (1983), 479-486.

[5] R. B. Rood, Numerical advection algorithms and their their role in atmospheric transport and chemistry models, Rev. Geophys. 25 (1987), 71-100

[6] X. Yuqun, C. Xie, A characteristic alternating direction implicit scheme for the advection-dispersion equation, Develop. Water Sci. 36 (1988), 63-688

[7] H. Wu, P. Fu, J. P. Morris, et al. ICAT: A numerical scheme to minimize numerical diffusion in advection-dispersion modeling and its application in identifying flow channeling, Adv. Water Resources. 134 (2019).

[8] P. Wesseling, von Neumann stability conditions for the convection-diffusion equation, IMA J. Numer. Anal. 16 (1996), 583-598.

[9] M. T. Odman, A quantitive analysis of numerical diffusion introduced by advection algorithms in air wuality models, Atmospheric Enviro. 31 (1997), 1933-1940.

[10] P. Long, D. Pepper, An examination of some simple numerical schemes for calcultaing scalar advection, J. Appl. Meteorol. 20 (1981), 146-156.