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Author(s)	Chadha, Naresh M.; Madden, Niall
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A two-weight scheme for a time-dependent advection-diffusion problem

Naresh M. Chadha and Niall Madden

School of Mathematics, Statistics, and Applied Mathematics,
National University of Ireland, Galway, Ireland.
Naresh.Chadha@NUIGalway.ie, Niall.Madden@NUIGalway.ie
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Summary. We consider a family of two-weight finite difference schemes for a time-dependent advection-diffusion problem. For a given uniform grid-spacing in time and space, and for a fixed value of advection and diffusion parameters, we demonstrate how to optimally choose these weights by means of the notion of an equivalent differential equation. We also provide a geometric interpretation of the weights. We present numerical results that demonstrate that the approach is superior to other commonly used methods that also fit into the framework of a two-weight scheme.

1 Introduction

We consider the numerical solution of a one-dimensional advection-diffusion problem

$$\frac{\partial \Phi}{\partial t} + L\Phi = 0, \quad L := a\frac{\partial \Phi}{\partial x} - \varepsilon\frac{\partial^2 \Phi}{\partial x^2} \quad \text{for } (x,t) \in (0,l) \times (0,T], \tag{1a}$$

subject to the boundary and initial conditions

$$\Phi(0,t) = g_0(t), \quad \Phi(l,t) = g_l(t), \qquad t \in [0,T], \tag{1b}$$

$$\Phi(x,0) = f(x), \qquad x \in [0,l], \tag{1c}$$

were f, g_0 and g_l are known functions and are sufficiently smooth. It is assumed that ε and a, quantifying advection and diffusion processes respectively, are positive constants.

Models for the advection and diffusion of pollutants introduced into a fluid flow usually lead to problems of the form of (1) and its higher dimensional analogues. Many popular computer models for the two- and three-dimensional cases employ alternating direction implicit (ADI) techniques, where the problem is solved in only one coordinate direction over a fraction of a time-step. See, for example, the two-dimensional finite difference model DIVAST [3]. It solves a variant of the Navier-Stokes equations for calculating velocity fields, and then the time-dependent advection-diffusion equation for the solute transport problem, using a

space-staggered uniform grid. Consequently, one is restricted to solving the solute transport problem on a uniform mesh. This leads naturally to the following question: *how can one design a finite difference scheme which offers a sufficiently accurate solution to (1) on a uniform grid, and which can be easily extended to higher dimensional problems?*

We propose to answer this question in the framework of a two-weight scheme, the general form of which is two-weight scheme is presented in Section 2. This general form is analyzed in Section 3 to derive certain useful bounds which enable us to get an insight into the specific roles of the weights involved in the scheme, as well as determining conditions for stability. Furthermore, we demonstrate that there is a subtle interplay between these two weights which allows to devise a numerical method which offers better accuracy in comparison to other conventional methods.

In Section 4 we employ the notion of an *equivalent differential equation* [8], and obtain *optimal* values of the weights that eliminate first two leading terms in the truncation error. Furthermore, the optimal values of the weights are combined with results of Section 3 to determine a range of values of the discretization parameters, Δx and Δt, that produce a von Neumann stable solution, as well as satisfying necessary conditions to be non-oscillatory. In Section 5, we give numerical results that compare the proposed method with several well-known techniques that may be considered as special cases of the general two-weight scheme.

2 A general two-weight scheme

We construct a uniform finite difference, a tensor-product mesh $\{x_j, t^n\}$ on $[0,l] \times [0,T]$, where the grid points are defined as $(j\Delta x, n\Delta t), j = 1, \dots N, n = 0, \dots, M$; Δt and Δx are the time and space step lengths, respectively. We denote by u_j^n the value of a mesh function $\{u\}$ at a particular point.

Define the standard discrete difference operators:

$$D^0 u_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x}, \quad D^- u_j = \frac{u_j - u_{j-1}}{\Delta x},$$

$$\delta_{xx} u_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}, \quad \text{and} \quad \delta_t u_j^n = \frac{u_j^{n+1} - u_j^n}{\Delta t}.$$

We can now define a spatial finite difference operator, weighted with the parameter ϕ that balances between the standard second-order central difference operator, which may be unstable for small ε, and 2-point upwinding operator that is stable, but only first-order accurate:

$$L_\phi^N u_j := \big(-\varepsilon\delta_{xx} + a\delta_x \big) u_j, \quad \text{where } \delta_x := \phi D^- + (1-\phi) D^0.$$

We then introduce the parameter θ that weights the scheme between being implicit and explicit in nature, giving our general method for (1) as

$$\delta_t \Phi_j^n + L_\phi^N \left(\theta \Phi_j^{n+1} + (1-\theta)\Phi_j^n \right) = 0, \tag{2}$$

for $j = 1, \dots, N-1$ and $n = 1, \dots, M$.

Several studies, such as [2], consider schemes that involve a weighted spatial discretization. For example, fixing $\theta = 0$, certain values of ϕ lead to some of the

schemes considered in [2]. Moreover, for different combinations of θ and ϕ in (2), one obtains various standard difference-schemes used for linear advection-diffusion problems. For example,

- $\theta = 0$ and $\phi = 0$ correspond to forward Euler with central differencing.
- $\theta = 0$ and $\phi = a\Delta t/\Delta x$ give the standard Lax-Wendroff scheme.
- $\theta = 1$ and $\phi = 0$ give the backward Euler method with central differencing.
- $\theta = 1/2$ gives Crank-Nicolson type methods.

3 Analysis of the scheme

In this section, we shall analyze the general scheme and derive some useful bounds for the weights involved in the scheme using various standard concepts, e.g., method of lines, and stability analysis. These bounds shall be used in Section 4. Furthermore, the geometric interpretation of these bounds enables us to get an insight into their specific roles in the scheme.

First, note that the scheme (2) can be rewritten as

$$A_1\Phi_{j-1}^{n+1} + B_1\Phi_j^{n+1} + C_1\Phi_{j+1}^{n+1} = A_2\Phi_{j-1}^{n} + B_2\Phi_j^{n} + C_2\Phi_{j+1}^{n}, \tag{3}$$

$$\text{where,}\quad A_1 = -\frac{\theta}{2}(c+\psi), \qquad B_1 = 1+\theta\psi, \qquad C_1 = \frac{\theta}{2}(c-\psi),$$

$$A_2 = \frac{1-\theta}{2}(c+\psi), \quad B_2 = 1-(1-\theta)\psi, \quad C_2 = \frac{1-\theta}{2}(-c+\psi),$$

where $s := \varepsilon\Delta t/(\Delta x)^2$, $c := a\Delta t/\Delta x$, $\psi := 2s + \phi c$. The scheme is consistent as $A_1+B_1+C_1 = A_2+B_2+C_2$. Next, we derive bounds for the weights in Sections 3.1, 3.2, 3.3 using a notion of monotonicity, some standard concepts from method of lines, and stability analysis, respectively.

3.1 Using a notion of monotonicity

We rewrite the scheme (2) in a semi-discretized form as follows

$$\frac{d\Phi_j}{dt} = \sum_i \alpha_i(\Phi_{i+j} - \Phi_i),$$

$$\alpha_{-1} = \frac{a(1+\phi)}{2\Delta x} + \frac{\varepsilon}{\Delta x^2}; \quad \alpha_1 = -\frac{a(1-\phi)}{2\Delta x} + \frac{\varepsilon}{\Delta x^2}.$$

A necessary (but not itself sufficient) condition for the monotonicity of the scheme in this form is $\alpha_i \geq 0$, for all $i \neq 0$. This yields

$$\phi \geq 1 - 2s/c. \tag{4}$$

Remark 1. One may obtain the bound (4) using eigenvalue analysis. Consider the linear system that is solved at each time-step in the form (3). The eigenvalues of the matrix are given by $\lambda_j = B_1 + 2\sqrt{A_1C_1}\cos\left(j\pi/(M-1)\right)$, for $j = 1, 2, \ldots, M-1$. For solution to be spatially non-oscillatory, real eigenvalues are required (see [4]). This gives $A_1C_1 \geq 0 \implies (1/4)\theta^2(c^2-\psi^2) \leq 0$, which leads to (4).

3.2 Using the method of lines

As stated in Section 1, we assume that a and ε are constant. So, on an unbounded domain, one may apply Fourier analysis. We rewrite the difference scheme (2) as the following system of ordinary differential equations:

$$\frac{d\Phi_j}{dt} = -L_\phi^N \Phi_j, \qquad L_\phi^N \equiv -\varepsilon\delta_{xx} + a\delta_x. \tag{5}$$

We denote the Fourier transform of the operator L_ϕ^N by $\hat{L}_\phi^N(\beta) = e^{-\mathrm{i}j\beta} L_\phi^N e^{\mathrm{i}j\beta}$. A sufficient condition for von Neumann stability is

$$S_L \subseteq S, \quad S_L = \{-\Delta t \hat{L}_\phi^N(\beta) \in \mathbb{C} \ \forall\ \beta\},$$

where S is the stability domain of the time discretization method being used; for further details, see [9]. For the system (5), we have

$$\Delta t \hat{L}_\phi^N(\beta) = p(\beta) + \mathrm{i}q(\beta),$$
$$p(\beta) = 2(2s + \phi c)\sin^2(\beta/2), \quad q(\beta) = c\sin\beta.$$

It can easily be verified that the region S_L is fully contained in an ellipse given by

$$\left(\frac{v}{\psi} + 1\right)^2 + \left(\frac{w}{c}\right)^2 = 1; \quad \psi = 2s + \phi c. \tag{6}$$

Furthermore, we have used the standard *theta-method* for the time integration, for which the stability-region is given by

$$S \equiv \left|\frac{1 + z(1-\theta)}{1 - z\theta}\right| \le 1, \quad z = x + \mathrm{i}y, \tag{7}$$

which is equivalent to $(1-2\theta)(x^2+y^2)+2x \le 0$. This implies that in a case $1-2\theta \neq 0$, S is a region inside a circle (including the boundary) defined as

$$(x + r)^2 + y^2 = r^2, \quad r = \frac{1}{1 - 2\theta}. \tag{8}$$

Since for von Neumann stability it is sufficient to prove $S_L \subseteq S$, from (6) and (8) we have

$$r \ge \max\{\psi, c, c^2/\psi\}. \tag{9}$$

Geometrically, the weight ϕ controls the length of horizontal axis of the ellipse (6), while the location of the center and the length of the radius of the circle (8) is controlled by θ. Moreover, in the case where ε is small, and $\phi = 0$ (which corresponds to pure central differencing), this may lead to a situation where the boundary of the ellipse (6) would lie outside the circle (8), resulting in an oscillatory computed solution. On the other hand, $\phi = 1$ (which corresponds to pure upwinding) may unnecessarily stretch the horizontal axis of the ellipse (6), causing damping in the computed solution. Thus, an optimal value of ϕ should be between 0 and 1, and should be positive, ensuring that ψ is positive. This implies that the ellipse (6) which is a cover of the eigenvalues associated with spatial discretization, should also be entirely in the left half-plane.

In general, it is desirable to have a time integration method whose stability region contains the entire left half-plane. Then one may take any time step for (5), provided that all the eigenvalues have negative real parts, as is often the case in practice [5, §8.3]. In our case, the region of stability given by (7) will be in left half-plane if and only if $1 - 2\theta \geq 0$. This suggests that

$$\theta \leq 1/2. \tag{10}$$

3.3 Using stability analysis

Following the standard von Neumann analysis, the amplification factor G can be found by substituting $\Phi_j^n = G^n e^{ij\beta}, \beta = \xi \Delta x$ in (3), and it is given as

$$G = \frac{A_2 e^{-i\beta} + B_2 + C_2 e^{i\beta}}{A_1 e^{-i\beta} + B_1 + C_1 e^{i\beta}}.$$

It can easily be checked that the requirement for stability, namely $|G| \leq 1$ for all β, leads to the following bounds:

$$(1 - 2\theta)c^2 - \psi \leq 0, \quad \text{and} \quad \psi\big((1 - 2\theta)\psi - 1\big) \leq 0. \tag{11}$$

Given (4), we have $\psi > 0$, and so the inequalities in (11) are automatically satisfied if $\theta \geq 1/2$. Thus *any scheme is unconditionally stable for* $\theta \geq 1/2$. For $\theta < 1/2$, the method is stable providing that

$$(1 - 2\theta)c^2 \leq \psi \leq (1 - 2\theta)^{-1}. \tag{12}$$

This can be rewritten more usefully as a sharp bound on Δt ensuring the stability of the method:

$$\Delta t \leq \frac{1}{1 - 2\theta} \min \left[\frac{2\varepsilon}{a^2} + \phi \frac{\Delta x}{a}, \left(\frac{2\varepsilon}{\Delta x^2} + \frac{\phi a}{\Delta x} \right)^{-1} \right].$$

For example, if $\theta = 0$ and $\phi = 0$ (forward Euler with central differencing), then one should take $\Delta t \leq \min(2\varepsilon/a^2, \Delta x^2/\varepsilon)$.

Note that it can easily be verified that (12) and (9) are the same conditions, but derived using two different approaches.

4 Optimal values of the parameters

In this section we obtain optimal values of the parameters using a notion of *equivalent differential equation* and the standard truncation error analysis.

Using the modified equation approach descried by Warming and Hyett [8], we can obtain *the modified partial differential equation* equivalent to the scheme (2), written as:

$$\frac{\partial \Phi}{\partial t} + a \frac{\partial \Phi}{\partial x} - \varepsilon \frac{\partial^2 \Phi}{\partial x^2} + \sum_{q=2}^{\infty} \frac{a \Delta x^{q-1}}{q!} \kappa_q(c, s) \frac{\partial^q \Phi}{\partial x^q} = 0.$$

This difference scheme is first-order accurate if $\kappa_2 \neq 0$, and is p^{th}-order accurate if $\kappa_q = 0, q = 2, \ldots, p$, and $\kappa_{p+1} \neq 0$. The first two leading terms in the truncation

error are associated with numerical dissipation and dispersion, respectively [4, §9.2]. Thus, by setting these two terms equal to zero, one may obtain a higher order scheme. In the process, an optimal value of each of the parameters, θ and ϕ can also be obtained. The desired coefficients are:

$$\kappa_2 = \phi - c(1-2\theta), \qquad \kappa_3 = 1 - 6s - c^2 + 6s\theta + 3\theta\psi + 3c^2\theta,$$

giving optimal value of the parameters:

$$\phi = c(1-2\theta), \qquad \theta = \frac{3(c^2+2s) \pm \sqrt{3(2c^2+c^4+12s^2)}}{6c^2}. \tag{13}$$

This expression leads to two possible values for θ and ϕ. In view of (10) and (4), we take the smaller of the two values for θ in (13), thus giving the optimal values of the parameters:

$$\phi_{\text{opt}} = c(1-2\theta), \qquad \theta_{\text{opt}} = \frac{3(c^2+2s) - \sqrt{3(2c^2+c^4+12s^2)}}{6c^2}. \tag{14}$$

For $\theta \neq 0$ the scheme (3) is implicit in nature, and at each step one must solve a linear system of equations. It can be easily verified that the matrix on the left-hand side of (3), is diagonally dominant providing that

$$|2(1+\theta\psi)| \geq |-\theta(c+\psi)| + |\theta(c-\psi)|.$$

This will be the case for the optimal value of the weights θ_{opt} and ϕ_{opt} given in (14), ensuring that the system is easily solved.

Remark 2. The bound (4) may be combined with (14) to obtain another useful relation in terms of c and s, given as

$$c^4 - c^2 + 12s^2 \geq 0. \tag{15}$$

Moreover, by combining (12) and (14), we have

$$c^4 - c^2 + 12s^2 \leq 2s\sqrt{3(2c^2+c^4+12s^2)}. \tag{16}$$

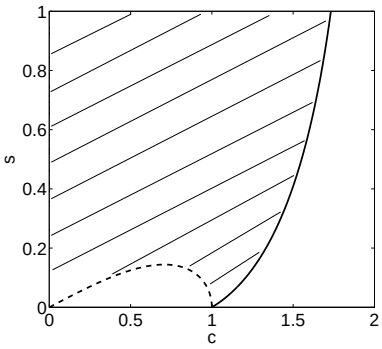

Fig. 1. The regions of stability and no-oscillations in c-s plane. The boundaries of the stability region (16), and no-oscillation region (15) are shown by solid line, and $\{- - -\}$, respectively. Any combination of $(\Delta x, \Delta t, \varepsilon, a)$ that falls into the shaded region would produce a von Neumann stable solution satisfying necessary conditions to be non-oscillatory.

5 Numerical experiments

To compare various representative methods within the framework of two-weight scheme for the model advection-diffusion problem (1), we consider a model predicting the transport of a Gaussian pulse with unit amplitude centered at $x = a$, given by

$$\Phi(x,0) = \exp\left(\frac{-(x-a)^2}{4\varepsilon}\right), \quad 0 \le x \le 2.$$

This problem is widely used for comparison of different numerical schemes for the advection-diffusion problem; see, e.g., [1, 6]. The exact solution to this problem is

$$\Phi(x,t) = \frac{1}{\sqrt{1+t}} \exp\left(\frac{-(x-(1+t)a)^2}{4\varepsilon(1+t)}\right), \quad 0 \le x \le 2, \quad t \ge 0.$$

The boundary conditions are taken from the exact solution.

In Table 1 we present a comparison between some commonly used methods and the scheme (14) for various values of N where we have taken the problem data as $a = .25$, $\varepsilon = 10^{-2}$ and $\Delta t = 2\Delta x$. The errors presented are the maximum point-wise errors at time $T = 2$.

Table 1. Comparison of various schemes for test problem with $\varepsilon = 10^{-2}$

N	Forward Euler Central Diff	Explicit Lax-Wendroff	Implicit Upwinding	Crank-Nicolson Central Diff	Optimal scheme (14)
64	2.45e+01	3.78e+04	8.95e-02	5.38e-03	4.48e-04
128	1.77e+33	8.11e+35	4.99e-02	1.33e-03	1.24e-04
256	1.65e+116	4.92e+118	2.65e-02	3.33e-04	3.17e-05
512	—	—	1.37e-02	8.32e-05	7.96e-06
1024	—	—	6.97e-03	2.08e-05	1.99e-06

We observe that, for all cases, the scheme (14) is superior to all of the others. Since we have taken $\Delta t = 2\Delta x$ there is nothing to ensure that the explicit schemes are stable, and indeed they fail entirely for some values of N.

To verify that there is nothing particularly advantageous for the scheme (14) in taking these parameters, we repeat the experiments for $\varepsilon = 10^{-4}$ and give the results in Table 2. Again we see that the method (14) yields a more accurate solution than the other schemes. In all cases, the methods are less accurate for $\varepsilon = 10^{-4}$ compared to $\varepsilon = 10^{-2}$; this is hardly surprising since a uniform mesh is used in all cases.

Table 2. Comparison of various schemes for test problem with $\varepsilon = 10^{-4}$

N	Forward Euler Central Diff	Explicit Lax-Wendroff	Implicit Upwinding	Crank-Nicolson Central Diff	Optimal scheme (14)
64	5.12e+00	3.29e-01	4.83e-01	3.77e-01	2.12e-01
128	4.97e+01	2.41e-01	4.50e-01	2.92e-01	9.92e-02
256	3.98e+02	1.29e-01	4.02e-01	2.17e-01	2.31e-02
512	5.02e+01	3.07e-02	3.39e-01	7.92e-02	3.07e-03
1024	6.56e-01	2.35e-03	2.66e-01	2.00e-02	2.54e-04

6 Conclusions

We have presented a two-weight scheme for a time dependent advection-diffusion problem. An optimal value of the weights involved have been obtained and their roles in the scheme have been geometrically interpreted. The supporting numerical results suggest that the method is promising.

There are several restrictions to note. Firstly, we have assumed that the coefficient of advection, a, is constant. We are in the process of relaxing this restriction for a more general case where $a = a(t)$. This only requires new values of ϕ and θ at each time step.

We also note that many studies of problems of the form (1) consider so-called *parameter robust methods*, (e.g., [7]), that perform well for arbitrarily small values of ε. However, due to the nature of our intended work related to enhancing certain existing hydrodynamics and solute transport models, we are restricted to using uniform meshes (and a range of values of ε that occur in applied problems). We do not claim that the method presented here is parameter robust. However, in the future we aim to extend the approach to allow for piecewise uniform meshes by employing domain decomposition techniques.

Finally, we note that the analysis presented here can be extended to higher dimensional analogous problems via standard ADI approaches; this is work in progress.

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