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# ON THE NUMERICAL SOLUTION OF THE THREE-DIMENSIONAL ADVECTION-DIFFUSION EQUATION

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A new approach is proposed for the numerical solution of three-dimensional advection-diffusion equations, which arise, among others, in air pollution modelling. The technique is based on directional operator splitting, which results in one-dimensional advection-diffusion equations. Then upstream-type difference approximations are applied for the first-order derivatives and non-standard difference approximations for the second-order derivatives. This approach leads to significant qualitative improvements in the behaviour of the numerical solutions.

#### Introduction

The investigation of advection-diffusion equations in higher dimensions is of great importance. The atmospheric flows and heat transfer processes as well as the concentration changes of pollutants are commonly described by a set of partial differential equations, which are mathematical formulations of one or more of the conservation laws of physics. These include the equations of momentum, mass and energy conservation, which involve advection and diffusion terms as a main constituent. Advection-diffusion equations take the form

$$\frac{\partial \xi}{\partial t} + v_1 \frac{\partial \xi}{\partial x_1} + v_2 \frac{\partial \xi}{\partial x_2} + v_3 \frac{\partial \xi}{\partial x_3} = F + \frac{\partial}{\partial x_1} \left( \mu_1 \frac{\partial \xi}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( \mu_2 \frac{\partial \xi}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left( \mu_3 \frac{\partial \xi}{\partial x_3} \right), \tag{1.1}$$

where  $\mu_i$  and  $v_i$  are the eddy viscosity and the velocity component of the fluid, respectively, in the direction  $x_i$  (i=1,2,3), and F is the source/sink of the quantity  $\xi$ . The terms  $v_i(\partial \xi/\partial x_i)$  are usually called advection (or sometimes convection) terms, and describe the transportation of the quantity  $\xi$  by the velocity field. The terms  $\partial(\mu_i\,\partial \xi/\partial x_i)/\partial x_i$  are called diffusion (or sometimes viscous) terms, and express the spreading of quantity  $\xi$  by the process of turbulent diffusion. The equation is usually provided with appropriately defined initial and boundary conditions.

Since analytical solutions of advection-diffusion problems cannot usually be found, we have to solve them numerically. However, the numerical treatment of equations of the form (1.1) is a highly complicated task. The main reasons for this are the following:

- the equations are nonlinear;
- due to changes in the input parameters the equations can change the type (hyperbolic, parabolic or elliptic);
- the size of the discretized problem can be very large in a real-life physical model.

Therefore, choosing a sufficiently accurate as well as efficient numerical method for solving advection-diffusion problems is not an easy task. In this case the application of operator splitting seems a good alternative. In [1] Prusov et

al. suggest a new finite-difference method for the one-dimensional convection-diffusion equation. Our aim is to extend this method to higher dimensions by using operator splitting based on directional decomposition.

The structure of the paper is as follows. In Section 2 we propose possible splitting algorithms for problems of the form (1.1). In Section 3 we deal with the numerical solution of the sub-problems obtained by splitting. We close the paper with some useful remarks and a summary of the results.

#### 1. Solving the three-dimensional advection-diffusion equation by operator splitting

The aim of operator splitting is to replace an initial value problem with a sequence of simpler problems, for which accurate as well as efficient solvers available in standard program packages exist [2, 3]. The mathematical background of operator splitting can be sketched as follows. Let S denote a normed space and consider the abstract initial value problem

$$\frac{dw(t)}{dt} = Aw(t) = (A_1 + A_2)w(t), \quad t \in [0, T]$$

$$w(0) = w_0,$$
(2.1)

where  $w(t) \in \mathbf{S}$ ,  $t \in [0,T]$  is the unknown function, and A is a given operator  $\mathbf{S} \to \mathbf{S}$ , which can be decomposed into a sum of two "simpler" operators  $A_1$  and  $A_2$ . (By "simpler" we mean that the corresponding initial-value problems are easier to treat numerically than the original problem.) The simplest kind of operator splitting is the so-called sequential splitting, where we solve the following sequence of initial value problems:

$$\frac{dw_k^{(1)}(t)}{dt} = A_1 w_k^{(1)}(t), \quad t \in ((k-1)\tau, k\tau] 
 w_k^{(1)}((k-1)\tau) = w_{sp}((k-1)\tau),$$
(2.2)

and

$$\frac{dw_k^{(2)}(t)}{dt} = A_2 w_k^{(2)}(t), \quad t \in ((k-1)\tau, k\tau] 
w_k^{(2)}((k-1)\tau) = w_k^{(1)}(k\tau), 
w_{sp}(k\tau) = w_k^{(2)}(k\tau)$$
(2.3)

for k = 1, 2, ..., n, where  $\tau = T/n$  is the splitting time step, and  $w_{sp}(0) = w_0$ . This scheme can be extended to more than two sub-operators in a natural way.

Another possibility is the Marchuk-Strang splitting [4], defined by the following algorithm:

$$\frac{dw_k^{(1)}(t)}{dt} = A_1 w_k^{(1)}(t), \quad t \in ((k-1)\tau, (k-0.5)\tau]$$

$$w_k^{(1)}((k-1)\tau) = w_{sp}((k-1)\tau), \tag{2.4}$$

$$\frac{dw_k^{(2)}(t)}{dt} = A_2 w_k^{(2)}(t), \quad t \in ((k-1)\tau, k\tau] 
w_k^{(2)}((k-1)\tau) = w_k^{(1)}((k-0.5)\tau),$$
(2.5)

$$\frac{dw_k^{(3)}(t)}{dt} = A_1 w_k^{(3)}(t), \quad t \in ((k-0.5)\tau, k\tau] 
 w_k^{(3)}((k-0.5)\tau) = w_k^{(2)}(k\tau) 
 w_{sp}(k\tau) = w_k^{(3)}(k\tau)$$
(2.6)

for k = 1, 2, ..., n, where  $w_{sp}(0) = w_0$ .

Obviously, there are several ways to define the sub-operators  $A_i$  in a splitting procedure. We can choose the sub-operators on a physical base, e.g., we can separate the advection and diffusion terms in Eq. (2.1) (physical

decomposition) [5]. Another possibility is to separate the  $x_1$ -,  $x_2$ - and  $x_3$ -derivatives in the equation (directional decomposition) [6]. For the three-dimensional advection-diffusion problem the physical decomposition would lead to advection problems, which are of hyperbolic type, and diffusion problems, which are of parabolic type. This would cause us difficulties in defining appropriate boundary conditions for the sub-problems. Therefore, we recommend the latter one, which results in three one-dimensional advection-diffusion problems at each time step. Particularly, if we apply the sequential splitting, the detailed algorithm will read as follows:

$$\frac{\partial \xi_k^{(1)}(t)}{\partial t} = -v_1 \frac{\partial \xi_k^{(1)}}{\partial x_1} + \frac{\partial}{\partial x_1} \left( \mu_1 \frac{\partial x_k^{(1)}}{\partial x_1} \right) + F_{x_1}, \quad t \in ((k-1)\tau, k\tau]$$

$$\xi_k^{(1)}((k-1)\tau) = \xi_{sp}((k-1)\tau), \tag{2.7}$$

$$\frac{\partial \xi_{k}^{(2)}(t)}{\partial t} = -v_{2} \frac{\partial \xi_{k}^{(2)}}{\partial x_{2}} + \frac{\partial}{\partial x_{2}} \left( \mu_{2} \frac{\partial x_{k}^{(2)}}{\partial x_{2}} \right) + F_{x_{2}}, \quad t \in ((k-1)\tau, k\tau]$$

$$\xi_{k}^{(2)}((k-1)\tau) = \xi_{k-1}^{(1)}(k\tau), \tag{2.8}$$

$$\frac{\partial \xi_{k}^{(3)}(t)}{\partial t} = -v_{3} \frac{\partial \xi_{k}^{(3)}}{\partial x_{3}} + \frac{\partial}{\partial x_{3}} \left( \mu_{3} \frac{\partial x_{k}^{(3)}}{\partial x_{3}} \right) + F_{x_{3}}, \quad t \in ((k-1)\tau, k\tau]$$

$$\xi_{k}^{(3)}((k-1)\tau) = \xi_{k-1}^{(2)}(k\tau),$$

$$\xi_{sp}(k\tau) = \xi_{k}^{(3)}(k\tau)$$
(2.9)

for k = 1, 2, ..., n, where  $\xi_{sp}(0) = \xi_0$ . If the original problem is defined over a bounded spatial domain, the equations (2.7)-(2.9) are also provided with appropriately defined boundary conditions.

Several numerical methods have been constructed for the solution of the resulting one-dimensional advection-diffusion problems [7-12]. Recently, finite element [13] and spectral methods are very popular [14]. There are also many finite difference schemes that can be considered according to the number of spatial grid points involved, the number of time-levels used, and whether they are explicit or implicit in nature [15–42].

Standard three-point finite difference methods of approximating spatial derivatives can work well for smooth solutions, but they fail when severe gradients or discontinuities are present, which are common in the shock wave problems [17-21]. Lower-order accurate finite difference methods, such as upstream-type finite differences, can be a remedy for the numerical oscillations and dispersions. However, they have a large amount of "numerical viscosity" that smoothes the solution in much the same way that physical viscosity would, but to an extent that is unrealistic by several orders of magnitude [20]. Standard four-point finite difference methods are good in their higher-order accuracy and in reducing numerical smearing effects [21]. But, they are plagued by their generation of spurious oscillations or overshoots in the neighbourhood discontinuities and lack accuracy [17, 18]. Total variation stable finite difference schemes (TVD) [10, 11] guarantee oscillation-free solutions but they are limited to second-order accuracy. Higher-order accurate TVD schemes are attractive for problems with long computational time or with required higher accuracy solutions [11]. But, the objection to the standard higher-order schemes comes from the additional nodes necessary to achieve the higher-order accuracy. This precludes the use of implicit methods since the obtained matrix is not of threediagonal form, and it is necessary to use fictitious nodes for the boundary conditions. Also, they do not allow easily for non-uniform grids, unless at the expense of the order of accuracy. On the other hand, the compact schemes that treat functions and their derivatives as unknowns at the grid nodes, like the scheme [31], are fourth-order accurate, and compact in the sense that they reduce to three-diagonal form. The compact schemes generally consist of finite difference schemes which involve two or three grid points. The three-point schemes fall into two classes. The first class consists of methods which are fourth-order accurate for uniform grids, such as schemes [26–28], the operator compact implicit scheme [26-28] and the Hermite finite difference method [29]. The second class consists of methods that allow variable grids such as the cubic spline methods [30–33], and the Hermite finite difference method [34, 35]. In [36, 37] a compact fourth-order finite difference scheme was introduced with three nodal points for the convection-diffusion equations. This scheme does not seem to suffer excessively from spurious oscillatory behaviour or numerical viscosity.

The disadvantage of the above higher-order compact schemes involving three nodal points is that the boundary conditions are no longer sufficient and they do not allow easily for non-uniform grids, unless at the expense of the order of accuracy. Another disadvantage of some compact schemes is the complexity of the resulting nonlinear finite difference equations and the associated difficulty in solving them efficiently. On the other hand, the compact scheme with two nodal points is fourth-order accurate even for non-uniform spatial grids, and no fictitious points, neither extra formulas are needed for Dirichlet boundary conditions [38]. The discretization of the convective term might be done in a number of ways [39, 40]. The Ellam scheme is probably one of the best known convective schemes [41].

In the next section we present a non-standard finite-difference method for the solution of the sub-problems obtained by splitting (2.7)-(2.9).

#### 2. A finite-difference scheme for the one-dimensional advection-diffusion problem

Consider the one-dimensional advection-diffusion equation

$$\frac{\partial \xi}{\partial t} + v \frac{\partial \xi}{\partial x} = \frac{\partial}{\partial x} \left( \mu \frac{\partial \xi}{\partial x} \right) + F, \quad \mu \ge 0, \quad 0 \le x \le l, \quad t > 0$$
 (3.1)

with initial condition

$$\xi(x,0) = \eta(x), \quad 0 \le x \le l \tag{3.2}$$

and Dirichlet boundary conditions

$$\xi(0,t) = \alpha(t), \quad \xi(l,t) = \beta(t) \quad t > 0, \tag{3.3}$$

where v(x,t),  $\mu(x,t)$ ,  $\eta(x)$ ,  $\alpha(t)$  and  $\beta(t)$  are known functions, while the function  $\xi(x,t)$  is unknown. Let us divide the spatial interval [0,l] of the problem into J equal parts with division points  $x_0 < x_1 < ... < x_{J-1} < x_J$ , and denote the length of the j-th sub-interval by  $h_j$ . Besides, divide [0,T] into N equal parts by points  $t^n = nTN^{-1}$ , n = 0,1,...,N, with time step  $\tau$ . We define the grid  $\Omega = \{(x_j,t^n), j=0,1,...J, n=0,1,...N\}$ , and denote by  $\xi_j^n$  the approximation of  $\xi(x_j,t^n)$ .

Integrating Eq. (3.1) at  $x_i$  from  $t^n$  to  $t^{n+1}$  yields

$$\xi_{j}^{n+1} = \xi_{j}^{n} - \int_{t^{n}}^{t^{n+1}} \left[ v \frac{\partial \xi}{\partial x} - \frac{\partial}{\partial x} \left( \mu \frac{\partial \xi}{\partial x} \right) - F \right]_{j} dt$$
 (3.4)

Approximating the integral on the right-hand side by the mean-value theorem, we obtain

$$\xi_{j}^{n+1} = \xi_{j}^{n} - \tau \left[ v \frac{\partial \xi}{\partial x} - \frac{\partial}{\partial x} \left( \mu \frac{\partial \xi}{\partial x} \right) - F \right]_{j}^{t=\theta}, \tag{3.2}$$

where  $t^n < \theta < t^{n+1}$ . For the approximation of the derivatives  $\left(\partial \xi/\partial x\right)_j^{t=\theta}$  and  $\left[\partial \left(\mu \, \partial \xi/\partial x\right)/\partial x\right]_j^{t=\theta}$  we will use the following difference relations:

$$\left(\frac{\partial \xi}{\partial x}\right)_{j}^{t=\theta} = \frac{1}{h_{j-1} + h_{j}} \left[ h_{j-1} \frac{\xi_{j+1} - \xi_{j}}{h_{j}} + h_{j} \frac{\xi_{j} - \xi_{j-1}}{h_{j-1}} \right]^{t=\theta} - \frac{h_{j-1} h_{j}}{6} \left( \frac{\partial^{3} \xi}{\partial x^{3}} \right)^{t=\theta}, \quad (3.3a)$$

$$\left[ \frac{\partial}{\partial x} \left( \mu \frac{\partial \xi}{\partial x} \right) \right]_{j}^{t=\theta} = \frac{1}{h_{j-1} + h_{j}} \left[ \left( \mu_{j+1} + \mu_{j} \right) \frac{\xi_{j+1} - \xi_{j}}{h_{j}} - \left( \mu_{j} + \mu_{j-1} \right) \frac{\xi_{j} - \xi_{j-1}}{h_{j-1}} \right]^{t=\theta} - \frac{h_{j} - h_{j-1}}{3} \left( \frac{\partial^{3} \xi}{\partial x^{3}} \right)^{t=\theta} \quad (3.4a)$$

The unilateral difference expressions  $(\xi_{j+1}-\xi_j)/h_j$  and  $(\xi_j-\xi_{j-1})/h_{j-1}$  in (3.3a) and (3.4a) will be taken at different time levels (n and n+1). For construction of approximations only by two points it is natural for physical reasons to have on the (n+1)-th layer a point  $x_j$  as central, and to select the second one from that side from where  $\xi$  is transferred by advection to the central point. It is easy to see that the created difference scheme (3.3a) and (3.4a) has an approximation error of the first order in  $\tau$ . In this manner we gain the following form:

• for v > 0

$$\left(\frac{\partial \xi}{\partial x}\right)_{j}^{t=\theta} \approx \frac{1}{h_{j-1} + h_{j}} \left[ h_{j-1} \frac{\xi_{j+1}^{n} - \xi_{j}^{n}}{h_{j}} + h_{j} \frac{\xi_{j}^{n+1} - \xi_{j-1}^{n+1}}{h_{j-1}} \right] + \tau \frac{\partial^{2} \xi}{\partial t \partial x} \bigg|_{j}^{t=\theta},$$
(3.3b)

$$\left[\frac{\partial}{\partial x}\left(\mu\frac{\partial\xi}{\partial x}\right)\right]_{j}^{t=\theta} \approx \frac{1}{h_{j-1}+h_{j}}\left[\left(\mu_{j+1}+\mu_{j}\right)\frac{\xi_{j+1}^{n}-\xi_{j}^{n}}{h_{j}}-\left(\mu_{j}+\mu_{j-1}\right)\frac{\xi_{j}^{n+1}-\xi_{j-1}^{n+1}}{h_{j-1}}\right]+\tau\frac{\partial^{2}\xi}{\partial t\partial x}\bigg|_{j}^{t=\theta}; (3.4b)$$

• for v < 0

$$\left. \left( \frac{\partial \xi}{\partial x} \right) \right|_{j}^{t=\theta} \approx \frac{1}{h_{j-1} + h_{j}} \left[ h_{j-1} \frac{\xi_{j+1}^{n+1} - \xi_{j}^{n+1}}{h_{j}} + h_{j} \frac{\xi_{j}^{n} - \xi_{j-1}^{n}}{h_{j-1}} \right] + \left. \tau \frac{\partial^{2} \xi}{\partial t \partial x} \right|_{j}^{t=\theta}, \tag{3.3c}$$

$$\left[\frac{\partial}{\partial x}\left(\mu\frac{\partial\xi}{\partial x}\right)\right]_{j}^{t=\theta} \approx \frac{1}{h_{j-1} + h_{j}}\left[\left(\mu_{j+1} + \mu_{j}\right)\frac{\xi_{j+1}^{n+1} - \xi_{j}^{n+1}}{h_{j}} - \left(\mu_{j} + \mu_{j-1}\right)\frac{\xi_{j}^{n} - \xi_{j-1}^{n}}{h_{j-1}}\right] + \tau\frac{\partial^{2}\xi}{\partial t\partial x}\Big|_{j}^{t=\theta}$$
(3.4c)

Substituting (3.3b), (3.4b) or (3.3c), (3.4c) in (3.2) we will receive a difference scheme for the one-dimensional advection-diffusion problem (3.1) in the following form:

• for v > 0

$$\frac{\xi_{j}^{n+1} - \xi_{j}^{n}}{\tau} + \frac{1}{h_{j-1} + h_{j}} \left[ h_{j-1} v_{j}^{n} \frac{\xi_{j+1}^{n} - \xi_{j}^{n}}{h_{j}} + h_{j} v_{j}^{n+1} \frac{\xi_{j}^{n+1} - \xi_{j-1}^{n+1}}{h_{j-1}} \right] - \frac{1}{h_{j-1} + h_{j}} \left[ \left( \mu_{j+1}^{n} + \mu_{j}^{n} \right) \frac{\xi_{j+1}^{n} - \xi_{j}^{n}}{h_{j}} - \left( \mu_{j}^{n+1} + \mu_{j-1}^{n+1} \right) \frac{\xi_{j}^{n+1} - \xi_{j-1}^{n+1}}{h_{j-1}} \right] - F_{j}^{n} = 0,$$

$$j = 1, 2, ..., J - 1, \quad n = 0, 1, ...,$$

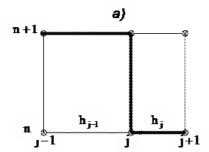
$$\xi_{j}^{0} = \eta(x_{j}), \quad j = 0, 1, ..., J,$$
(3.5a)

$$\xi_0^n = \alpha(t^n), \ \xi_J^n = \beta(t^n), \ n = 0, 1, \dots N.$$

• for v < 0

$$\begin{split} &\frac{\xi_{j}^{n+1}-\xi_{j}^{n}}{\tau}+\frac{1}{h_{j-1}+h_{j}}\Bigg[h_{j-1}v_{j}^{n+1}\frac{\xi_{j+1}^{n+1}-\xi_{j}^{n+1}}{h_{j}}+h_{j}v_{j}^{n}\frac{\xi_{j}^{n}-\xi_{j-1}^{n}}{h_{j-1}}\Bigg]-\\ &-\frac{1}{h_{j-1}+h_{j}}\Bigg[\Big(\mu_{j+1}^{n+1}+\mu_{j}^{n+1}\Big)\frac{\xi_{j+1}^{n+1}-\xi_{j}^{n+1}}{h_{j}}-\Big(\mu_{j}^{n}+\mu_{j-1}^{n}\Big)\frac{\xi_{j}^{n}-\xi_{j-1}^{n}}{h_{j-1}}\Bigg]-F_{j}^{n}=0\,, \quad (3.5b)\\ &j=J-1,J-2,...,2,1,\quad n=0,1,...,\\ &\xi_{j}^{0}=\eta\Big(x_{j}\Big),\quad j=0,1,...,J\,\,,\\ &\xi_{0}^{n}=\alpha\Big(t^{n}\Big),\quad \xi_{J}^{n}=\beta\Big(t^{n}\Big),\quad n=0,1,...\,N. \end{split}$$

The templates corresponding to the scheme (3.5) are shown in Figures 1a and 1b.



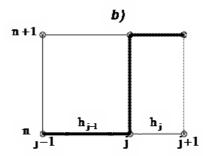


Fig. 1. Templates of difference networks: a) of the scheme (3.5a); b) of the scheme (3.5b)

In this manner for the solution of the advection-diffusion problem (3.1)–(3.3) we have received a clone of the so-called "running computation scheme" usually used for the solution of one-dimensional wave equations of the first order (see, for example [42]). Therefore, in spite of the fact that the scheme (3.5) is formally implicit, it is easily solved in an explicit way.

### 3. Remarks

A thorough theoretical analysis of the finite-difference method introduced in Section 3 and some simple numerical experiments demonstrating stability and convergence properties of the scheme can be found in [1]. It has been shown that this scheme possesses some good properties of both the explicit and implicit difference schemes. It is as economic as an explicit scheme and is stable on any permissible grids as an implicit scheme.

The problem of convective diffusion is an example of problems for which the application of the implicit scheme (3.5) is really justified. As it is known, the stability condition for the explicit schemes demands that  $\tau$  should decrease as  $h^2$ . This requirement necessitates the application of a much greater number of time steps than it is dictated by reasons of accuracy only. Besides, it can happen that the differences  $\xi_j^{n+1} - \xi_j^n$ , j = 0,1,...,J become as small as disturbances arising as a result of round-off errors. The implicit scheme (3.5) is free from this lack as it is unconditionally stable and has an approximation error of equal order in  $\tau$  and t0. Therefore, if there is a necessity for increasing the accuracy of the numerical solution, it is possible to achieve it at the expense of decreasing  $\tau$ 1 and t2 in equal measure.

From (3.3) and (3.4) it follows that the scheme can reach almost second order of accuracy, intrinsic to central difference schemes for spatial derivatives by using small time steps, or when the field of the gradient  $\partial \xi/\partial x$  of the transferred value  $\xi$  varies smoothly.

#### 4. Summary

We considered the three-dimensional advection-diffusion problem on a bounded domain with Dirichlet boundary conditions. A splitting scheme based on directional decomposition was proposed for the solution. This procedure allows us to replace the three-dimensional problem with three simpler, one-dimensional advection-diffusion problems at each time step of the numerical integration. We proposed a non-standard finite-difference method for the solution of the one-dimensional sub-problems. This method unites the advantages of explicit and implicit schemes.

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