JOURNAL OF COMPUTATIONAL PHYSICS 67, 472–478 (1986)

Note

On Operator Splitting for Unsteady Boundary Value Problems

INTRODUCTION

In this article we consider the initial value problem

$$\frac{\partial u}{\partial t}=\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+H; \qquad t>0, \quad -\infty<x, \quad y<\infty, \tag{1}$$

$$u(0, x, y)=u_0(x, y). \tag{2}$$

Here u, F, G, H are $m \times 1$ vectors, and

$$F(u)=f_1(u)+f_2\left(u, \frac{\partial u}{\partial x}\right), \tag{3a}$$

$$G(u)=g_1(u)+g_2\left(u, \frac{\partial u}{\partial x}\right). \tag{3b}$$

We shall assume that u_0 belongs to the class of functions, D, which are sufficiently smooth that (1)–(2) has a unique, strong solution $u(x, y, t)$, which for $0 \leqq t \leqq T$ is in the class C^{P+1} of functions possessing continuous partial derivatives $D^{\alpha}u$ of order through $p+1$, for some $p \geqq 2$.

In [1], MacCormack uses a frozen Jacobian (locally linearized) analysis and a gain matrix approach to argue that a certain operator splitting of the two-dimensional, conservation form, Navier–Stokes equations (which have the form of Eq. (1)) is second-order accurate. Here we establish that MacCormacks intuitive result, which through the above approach can rigorously be shown valid only for linear systems, is also true in the presence of nonlinearity. Additional second-order splittings are obtained, for the case in which derivative-free source terms are present in the fluid dynamics equations. Some discussion of operator optimality is given.

0021-9991/86 $3.00

Evolution Operator

Under the above assumptions, there exists an operator [2] $E^{\tau} = E(\tau, t)$ with the property that

$$U^{n+1} = E^{\tau} U^{n}, \tag{4}$$

where $U^n = u(x, y, t)$, $U^{n+1} = u(x, y, t + \tau)$. Although the applications normally call for discrete values on a space lattice, for convenience of analysis we prefer x, y in (4) to be variable.

Approximate Factorization

A major problem of modern numerical analysis is the discovery of operator products

$$L^{\tau} = \prod_{j=1}^{M} L^{\tau_j} \tag{5}$$

which to pth order accuracy approximate the operator of Eq. (4); i.e.,

$$U^{N+1} = E^{\tau} U^{n} = L^{\tau} U^{n} + O(\tau^{p+1}). \tag{5}$$

Here, we shall be concerned with the case $p = 2$.

Regimen

For economy of machine implementation the operators L^{τ_j} are to be the simplest possible. In practice they provide second-order accurate approximations to solutions of certain equations which are associated with Eq. (1), through the natural splitting

$$\frac{\partial v}{\partial t} = \frac{\partial F}{\partial x}(v), \tag{6a}$$

$$\frac{\partial w}{\partial t} = \frac{\partial G}{\partial y}(w), \tag{6b}$$

$$\frac{\partial Q}{\partial t} = H(Q, x, y). \tag{6c}$$

The corresponding approximation operators for Eqs. (6) we denote by

$$\left.\begin{aligned} V^{n+1} &= L_x V^n \quad &(7a)\\ w^{n+1} &= L_y w^n \quad &(7b)\\ Q^{n+1} &= L_s Q^n \quad &(7c)\end{aligned}\right\} + O(\tau^3).$$

The method of operator splitting was originated by Peaceman and Rachford [3], in deriving a variant of the alternating direction (ADI) method which lends itself to the use of cyclic acceleration parameters for accelerating convergence. In seeking numerical solutions of (1), the curse of dimensionality may be avoided through splittings such as provided by Eqs. (5)–(7), often with improved time-step restrictions. Moreover, advantage can be taken of the long and successful history of research results concerning efficient numerical schemes for solving equations such as (6). Particularly of note are the advantages of MacCormack's method for the Navier–Stokes equations [1], and of certain higher order shock capturing schemes for the Euler equations [4, 5].

The purpose of this note is to provide rigorous proof, in the general nonlinear case, of the second-order accuracy of a splitting considered in reference [1]. There, MacCormack justifies second-order accuracy by means of a frozen Jacobian analysis and a gain matrix approach. Thus, his method rigorously establishes the result only in the case of a linear system. In addition we consider the problem of obtaining second-order splittings for systems characterized by presence of derivative-free source terms, as in axis-symmetric geometries. Some discussions of the optimality of the splitting approach is given.

Three Factor, Second-Order Accurate Splittings

In reference [6], Strang proves a result on operator splitting, which is somewhat more general, but whose content is essentially, the following:

Splitting Theorem 1.

Suppose operators L_x^τ, L_y^τ are known, which provide, as in Eqs. (7a), (7b), *second-order accurate updates for solutions of Eqs.* (6a), (6b). *Then, either of the composition operators defined by*

$$U^{n+1} = (L_x^{\tau/2} L_y^{\tau} L_x^{\tau/2})\, U^n \tag{8a}$$

and

$$U^{n+1} = (L_y^{\tau/2} L_x^{\tau} L_y^{\tau/2})\, U^n \tag{8b}$$

provides a second-order accurate, three-factor splitting for the equation

$$\frac{\partial u}{\partial t} = \frac{\partial F(u)}{\partial x} + \frac{\partial G(u)}{\partial y}. \tag{9}$$

Comment 1. Using the methods of Strang [6], we can show that no two-factor splitting which employs individually second-order accurate operators can, over one step, yield a second-order splitting for Eq. (9). Thus, among the class of operators which are second-order accurate over one step, Eqs. (8a), (8b), are optimal, in terms of the number of operators applied.

Comment 2. The results of Strang are general enough to encompass splittings for equations such as

$$\frac{\partial u}{\partial t} = C(t, x, y, u, D^{\alpha} u), \tag{10}$$

where $D^{\alpha} u$ are derivatives of arbitrary order. The equation

$$C = a + b \tag{11}$$

signifies an arbitrary splitting, subject only to the restriction that there exist operators L_a^{τ}, L_b^{τ} which provide second-order updates for the equations

$$\frac{\partial v}{\partial t} = a \tag{12a}$$

and

$$\frac{\partial w}{\partial t} = b. \tag{12b}$$

Some complications emerge when C is an explicit function of t; however, these shall not concern us, as we shall not require explicit time dependence of C.

Four-Factor Second-Order Accurate Splitting

Now, observe that if the operator sequence of (8a), (8b) is applied twice, six operator applications are necessary to advance a 2τ time increment. MacCormack [1] seems to have been first to note that a more economical second-order update, over time increment 2τ, can be obtained. He considers cyclical applications of the operator sequence

$$U^{n+1} = (L_x^{\tau} L_y^{\tau} L_y^{\tau} L_x^{\tau})\, U^n. \tag{13}$$

His justification of second-order accuracy we shall sketch, as follows: Consider a Fourier mode

$$U(x, y, t) = A(t)\, e^{i(\lambda x + \eta y)}. \tag{14}$$

By applying the operator sequence in (13) to the Fourier mode of (14), with frozen Jacobian matrices J_F, J_G, it emerges [1] that (13) produces a gain matrix

$$g_x g_y g_y g_x \tag{15}$$

which differs only by third order terms from the exact gain matrix obtained when (14) is substituted in Eq. (9). Thus, (13) has been rigorously justified second-order accurate only for linear systems (9), with otherwise locally linearized second-order accuracy.

However, by approximately factoring the full-step (middle) operators in (8a), (8b), we now show that MacCormack's cyclically reversed sequence (13) is, in general, second-order accurate, subject only to the restrictions required for proving Strang's splitting theorem.

Suppose L^τ is second-order accurate for the equation

$$\frac{\partial z}{\partial t} = g(x, y, D^\alpha z). \tag{16}$$

Then, to within terms of third order, it is required that

$$L^\tau z = z + \tau g(x, y, D^\alpha z) + \frac{\tau^2}{2} \sum_\alpha B_\alpha \cdot D^\alpha g, \tag{17}$$

where B_α are the Jacobian matrices of g with respect to the derivatives $D^\alpha z$. Thus,

$$L^\tau(L^\tau z) = L^\tau z + \tau g(x, y, D^\alpha z + \tau D^\alpha g) + \frac{\tau^2}{2} \sum_\alpha B_\alpha \cdot D^\alpha g + O(\tau^3). \tag{18}$$

Expanding the second term in the right member, we see that

$$L^\tau(L^\tau z) = L^\tau z + \tau g(x, y, D^\alpha z) + \tfrac{3}{2}\tau^2 \sum_\alpha B_\alpha \cdot D^\alpha g + O(\tau^3). \tag{19}$$

This becomes, not surprisingly,

$$L^\tau(L^\tau z) = L^{2\tau} z + O(\tau^3). \tag{20}$$

Hence, by applying (20) to Strang's results (8a), (8b), we see that MacCormack's cyclically reversed sequence (13) is second order accurate, over time increment 2τ, for general nonlinear systems of the form (9).

Splitting in the Presence of Source Terms

In recent research concerning second-order accurate shock-capturing algorithms for the Euler equations, interest is focused upon the problem of splitting Eq. (1) for the case in which nonzero $H(u, x, y)$ is present in (1). Carofano [7], following MacCormacks [1] results for the two-dimensional case, intuitively employs the splitting

$$U^{n+2} = (L_x^\tau L_y^\tau L_s^\tau L_s^\tau L_y^\tau L_x^\tau)\, U^n, \tag{21}$$

where L_s^τ is a second-order operator for Eq. (6c). We now discuss optimality for (21), and rigorously establish second-order accuracy.

In view of Comments 1 and 2, it is unlikely that a three-factor product of individually second-order operators can be found, which over one step with time increment, τ, provides a second-order update for (1). What can be done, rigorously, is to consider splittings which pair up any two of the quantities F, G, H against the other. Typically, the splitting

$$a = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y}, \qquad b = H, \qquad C = a + b \tag{22}$$

together with results similar to Eq. (8) obtainable by applying Strang's general result (Comment 2), establishes that

$$U^{n+1} = [L_s^{\tau/2}(L_x^{\tau/2} L_y^\tau L_x^{\tau/2})\, L_s^{\tau/2}]\, U^n \tag{23a}$$

and

$$U^{n+1} = L_s^{\tau/2}(L_y^{\tau/2} L_x^\tau L_y^{\tau/2})\, L_s^{\tau/2} U^n \tag{23b}$$

both provide five-factor, best possible in number, second-order accurate splittings, over one step of increment τ, for the Eq. (1) with source terms present. Among other possibilities similarly obtained, the factorization

$$U^{n+1} = [L_x^{\tau/2}(L_y^{\tau/2} L_s^\tau L_y^{\tau/2})\, L_x^{\tau/2}]\, U^n \tag{24}$$

shall be of particular interest.

It is clear that an approximate factorization of L_s^τ in (24) can be used to establish second-order accuracy for the Carofano splitting of Eq. (21), when $\tau/2$ is replaced by τ. Hence, Eqs. (21), (23), (24) provide equivalent second-order accurate splittings of Eq. (1) in the presence of source terms. Equation (24), applied over time increment 2τ, should be most efficient, but at the expense of cyclically modifying the time-step.

Comment 3. Our final comment is that, in terms of the optimal number of operators, Strang's splitting of Eq. (8), over time increment 2τ, is still one operator evaluation more efficient than is the MacCormack version of Eq. (13). However, in many cases stability restrictions or special problem idiosyncracies may mandate other priorities.

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Received: September 6, 1985; revised: February 24. 1986

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