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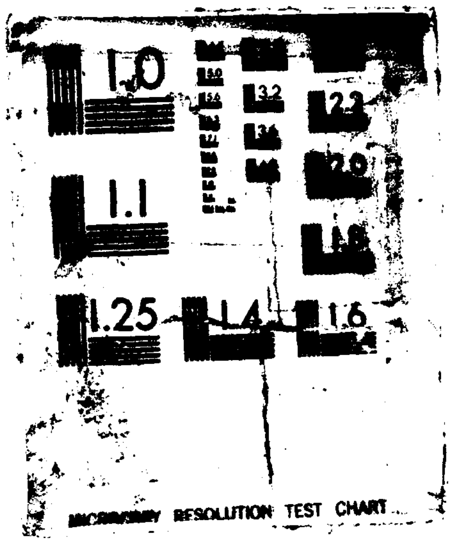
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MEMORANDUM REPORT BRL-MR-3605

ON OPERATOR SPLITTING FOR UNSTEADY BOUNDARY VALUE PROBLEMS

CHARLIE H. COOKE

JUNE 1987

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US ARMY BALLISTIC RESEARCH LABORATORY
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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 is second-order accurate. ~~Here we establish that~~ MacCormack's 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.

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I. INTRODUCTION

In this report we consider the initial value problem

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

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

Here u, F, G, H are m X 1 vectors, and

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

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

$$H = H(u,x,y). \tag{3c}$$

We shall assume that u_0 belongs to the class of functions, D, which are sufficiently smooth that Equations (1) and (2) have a unique, strong solution $u(x,y,t)$, which for $0 \le t \le T$ is in the class C^{p+1} of functions possessing continuous partial derivatives $D^{\alpha}u$ of order through p+1, for some $p \ge 2$. Thus, when Equation (1) is hyperbolic, u_0,T must be restricted such that no shock formation occurs in $0 \le t \le T$.

1. EVOLUTION OPERATOR

Under the above assumption, there exists an operator[1] $E^{\tau} = E(\tau,t)$ with the property that

$$U^{n+1} = E^{\tau}U^{n}, \quad 0 \le t \le t + \tau \le T \tag{4}$$

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 Equation (4) to be variable.

2. APPROXIMATE FACTORIZATION

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

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

which to p-th order accuracy approximate the operator of Equation (4); i.e.,

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

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

3. REGIMEN

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

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

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

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

The corresponding approximation operators for Equation (6) we denote by

$$v^{n+1} = L_x^{\tau}\, v^{n} \tag{7a}$$

$$\left.\begin{aligned} w^{n+1} &= L_y^{\tau} w^{n} \end{aligned}\right\} + O(\tau^3) \tag{7b}$$

$$Q^{n+1} = L_s^{\tau}\, Q^{n} \tag{7c}$$

The method of operator splitting was originated by Peaceman and Rachford,[2] in deriving a variant of the alternating direction (ADI) method which lends itself to the use of cyclic parameters for accelerating convergence. In seeking solutions of (1), the curse of dimensionality may be avoided through splittings such as provided by Equations (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 Equation (6). Particularly of note are the advantages of MacCormack's method for the Navier-stokes Equations,[3] and certain higher order shock capturing schemes for the Euler Equations.[4,5]

The purpose of this work is to provide rigorous proof, in the general nonlinear case, of the second-order accuracy of a splitting considered by MacCormack.[3] 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 discussion of the optimality of the splitting approach is given.

II. THREE-FACTOR, SECOND-ORDER ACCURATE SPLITTINGS

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

1. SPLITTING THEOREM 1

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

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

and

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

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

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

2. COMMENT 1

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

3. 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 do not concern us, as we shall not require explicit time dependence of C.

III. FOUR-FACTOR SECOND-ORDER ACCURATE SPLITTING

Now, observe that if the operator sequence of Equations (8a,b) is applied twice, six operator applications are necessary in order to advance a 2τ time increment. MacCormack[3] seems to have been first to notice that a more economical second-order update, over time increment 2τ, can be obtained. He considers cyclical applications of the operator sequence

$$U^{n+1} = (L^{\tau}{}_x L^{\tau}{}_y L^{\tau}{}_y L^{\tau}{}_x)U^n \tag{13}$$

His justification of second-order accuracy is sketched below:

Consider a Fourier mode

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

By applying the operator sequence in Equation (13) to the Fourier mode of Equation (14), with frozen Jacobian matrices J_F, J_G, it emerges[3] that Equation (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 Equation (14) is substituted in Equation (9). Thus, Equation (13) has been rigorously justified second-order accurate only for linear systems Equation (9), with otherwise locally-linearized second-order accuracy.

However, by approximately factoring the full-step (middle) operators in Equations (8a,b), we now show that MacCormack's cyclically reversed sequence Equation (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

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

This becomes, not surprisingly,

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

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

IV. 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 Equation (1) for the case in which nonzero H(u,x,y) is present in Equation (1). Carofano,[7] following MacCormack's[3] results for the two-dimensional case, intuitively employs the splitting

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

where L_s^{τ} is second-order operator for Equation (6c). We now discuss optimality for Equation (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 Equation (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

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

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

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

and

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

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

$$U^{n+1} = L_x^{\tau/2} (L_y^{\tau/2} L_s^{\tau} L_y^{\tau/2}) L_x^{\tau/2} U^n \qquad (24)$$

shall be of particular interest.

It is clear that an approximate factorization of L_s^{τ} in Equation (24 can be used to establish second-order accuracy for the Carofano splitting of Equation (21), when $\frac{\tau}{2}$ is replaced by τ. Hence, Equations (21, 23-24) provide equivalent second-order accurate splittings of Equation (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.

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

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