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Asymptotic Factorization of Operators in Complex Time

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Operator splitting with complex fractional-steps, perhaps regarded as a mathematical curiosity, is shown to be a feasible tool for stable numerical solution of ordinary as well as partial differential equations. This result may appear surprising, as in Q. Sheng (*IMA J. Numer. Anal.* **112** (1989)) stability of a splitting is defined as equivalent to the presence of all-positive fractional steps. Equivalences between the classes of fractional-step operator splittings for autonomous nonlinear scalar differential equations and splittings for vector evolution equations which involve linear operators are established. The implication is that results for the well-investigated linear case can be applied over a larger class of problems. Further analysis reveals circumstances in which the splitting concept can be used to broaden the range of stability of algorithms which may be used for the numerical solution of ordinary differential equations. Thus, alternatives to the usual methods for stiff systems integration become available. © 1991 Academic Press, Inc.

INTRODUCTION

Operator splitting via the method of fractional steps has been widely envisaged as an approach to synthesis of numerical schemes for problems posed in spaces of higher dimension, by utilizing well-known algorithms strictly applicable in spaces of lower dimension. Classically, the majority of applications have been restricted to order of accuracy $P \leqslant 2$. However, with the advent [1] of essentially non-oscillatory (ENO) one-dimensional shock-capturing schemes of higher order accuracy ($P \leqslant 15$), strong interest in the capability for application to higher dimensional problems has arisen [2].

Investigation of the existence of higher order accurate, fractional-step operator splittings for evolution equations which involve linear operators has produced discouraging results: for third-order accuracy, no splittings exist which involve all-positive fractional steps [3]. However, the existence of third-order accurate splittings characterized by complex fractional steps has been theoretically predicted [4], although no specific examples are given.

Unfortunately, the idea of complex fractional steps perhaps has been regarded a mathematical curiosity, as no practical applications are known to the authors. Therefore, one objective of the present paper is to derive some of the complex split-

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tings whose existence is suggested in [4]; to establish that they can be practically applied in numerical solution of differential equations; and to provide evidence that these numerical calculations are stable.

Stable calculation in such manner has not previously been anticipated. Indeed, in Ref. [3], stability is defined as being equivalent to the presence of all-positive fractional steps.

A second objective is to explore equivalences between families of splittings for diverse kinds of evolution equations. It is established that third-order accurate, fractional-step splitings for equations which involve only linear operators are also applicable to a class of scalar nonlinear differential equations. This allows broader application of the more readily obtained operator factorizations of linear equations [3, 4].

Finally, a scheme is revealed by which operator splitting can be used to broaden the range of stability of algorithms for the numerical solution of ordinary differential equations. It is shown that the scheme provides alternatives to the classical methods for stiff systems integration. Some highly accurate splittings are derived, whose order of accuracy is $N = 3, 4, 5$. These splittings are used to demonstrate the concept.

A Method of Undetermined Fractional Steps

There is now considered the problem of finding fractional-step operator splittings for the class of evolution equations

$$\frac{\partial u}{\partial t} = A(u) + B(u)$$
$$u(-, t_0) = u_0(-). \tag{1}$$

Here, u is an $n \times 1$ vector, and A, B are mutually non-commutative general linear operators which commute with the time derivative operator. It is remarked that Eq. (1) can represent systems of either ordinary or partial linear differential equations, as well as more general kinds of evolution equations.

The equations

$$\frac{\partial v}{\partial t} = A(v), \qquad \frac{\partial w}{\partial t} = B(w) \tag{2}$$

are referred to as the natural spliting associated with (1). It is assumed that the Cauchy initial-value problems for Eqs. (1)–(2) are well posed, over some finite time interval of length τ, on which there exist operators L_x, L_y which are third-order approximations to the transfer functions of the Cauchy problem for Eqs. (2).

With $\tau_k = h_k \tau$ and $u^n = u(-, t_n)$, asymptotic factorizations of the transfer operator for solutions of (1) are to be investigated, which are of the fractional-step form

$$u^{n+1} = L_x^{\tau_s} \cdots L_y^{\tau_2} L_x^{\tau_1} u^n + O(\tau^4). \tag{3}$$

A method of undetermined fractional steps (UFS) which reveals restrictions on the τ_j is now given. For linear equations, this method is equivalent to the approach [4] of truncated exponential operator expansions. However, the approach [4] does not generalize to nonlinear equations, whereas the present method does. This is because truncations of the operator expansion

$$u(t+\tau) = \exp(\tau Q)\, u(t) = (I + \tau Q + (\tau Q)^2/2 + \cdots)\, u(t) \tag{4}$$

afford a valid approximation to the transfer function of equations such as (2) only when Q is a linear operator. However, when Q is nonlinear, one need only replace powers $Q^n(u)$ with formal derivatives $D^{(n)}u(t)$ obtained from the evolution equation which is under consideration. There results nth order canonical approximation operators

$$u(t+\tau) = P_n(\tau D)\, u(t) + O(\tau^{n+1}), \tag{5}$$

where

$$P_n(x) = 1 + x + \cdots + x^n/n! \tag{6}$$

Referring to Eq. (3), define fractional steps $\tau_j = h_j \tau$, and let

$$L_x^{\tau_j} = P_n(\tau_j A), \qquad L_y^{\tau_k} = P_n(\tau_k B). \tag{7}$$

When (7) is substituted in (3), terms of order $n+1$ are neglected, and coefficients of like operators are equated with those of the expansion

$$u(t+\tau) = P_n(\tau(A+B))\, u(t) + O(\tau^{n+1}) \tag{8}$$

there results a system of determining equations for any existent fractional-step splitting whose order of accuracy is n.

It is to be noted that if too few operator factors are attempted in Eq. (3), insufficient terms may result to equate coefficients of like operators. When the product (3) is not operator poor, there may result extraneous determining equations; one must discard equations which are either repeated or which are functionally dependent upon others. There results a *minimal generating set* (MGS) of determining equations for the appropriate fractional steps of a splitting for the linear system (1). Sheng [3] shows, in a slightly more general context, that all-positive solutions to the MGS do not occur, if n is larger than two. By examination of the MGS, it has been verified independently by the authors that no all-positive solutions occur, for linear splittings having eight or fewer operator factors.

ASYMPTOTIC FACTORIZATION OF ORDINARY DIFFERENTIAL OPERATORS

In this section the method of UFS is used to obtain fractional-step asymptotic factorizations of the form (3) for the transfer function of the initial-value problem

$$\frac{du}{dt} = a(u) + b(u), \qquad u(t_0) = u_0. \tag{9}$$

The equivalence of systems (9) and (1) under the operation of asymptotic factorization by equation splitting is then established. Some particular splittings which may be used for either system are obtained. It is shown in the sequel that the splittings obtained in this section may be used to enhance the stability of classical algorithms for numerical integration of ordinary differential equations. The feasibility of using complex fractional steps is also investigated.

Let L_x, L_y be third-order approximations to the initial-value problems which result from the natural splitting of (9) which separates $a(u), b(u)$. Employing the UFS method, there results the following minimal generating set of equations which determine six-factor, third-order fractional step splittings of the form (3) for (9):

$$h_1 + h_3 + h_5 = 1 \tag{10}$$

$$h_2 + h_4 + h_6 = 1 \tag{11}$$

$$h_1 h_2 + (h_1 + h_3)(h_4 + h_6) + h_5 h_6 = \tfrac{1}{2} \tag{12}$$

$$h_2 h_3 (h_4 + h_6) + h_5 h_6 (h_2 + h_4) = \tfrac{1}{6} \tag{13}$$

$$h_1 h_2 (h_3 + h_5) + (h_1 + h_3) h_4 h_5 = \tfrac{1}{6}. \tag{14}$$

By setting $h_6 = 0$ there is obtained the minimal generating set of determining equations for five-factor, third-order splittings. If now h_5, h_6 both vanish, the resulting system (10)–(14) is inconsistent; no third-order, four-factor splittings for problem (9) exist.

It is noted that the UFS method when applied to the linear equation (1) generates a system of 14 equations in six unknowns. This system may be reduced to Eq. (10)–14), by throwing out equations which are linear combinations of, or functionally dependent upon, the above minimal set. In the parlance of Strang [5], as regards the algebra involved, it is every man for himself.

As Eqs. (10)–(14) represent the same minimal generating set of equations which is obtained when the UFS method is applied to the problem of determining six-factor fractional-step splittings for system (1), the following theorem is established:

THEOREM I. An equivalence class of approximate factorizations. *A necessary and sufficient condition that third-order, five- or six-factor fractional-step splittings of* (9) *exist is that the linear system* (1) *have third-order, five- or six-factor splittings whose fractional steps also serve system* (9). *Thus, the initial-value problems* (1) *and* (9) *are equivalent, as regards fractional-step splitting.*

Splitting in Complex Time

According to Theorem I, the splittings for (1), (9) are revealed once an exhaustive analysis of Eqs. (10)–(14) is accomplished. Unfortunately, system (10)–(14) possesses no solutions which provide splittings having all-positive fractional-steps. Only complex solutions are available when $h_6 = 0$; if h_6 does not vanish, factorizations having either complex or mixed positive–negative fractiona steps exist. A solution of (10)–(14) which provides a non-standard five-factor splitting for both Eq. (9) and its linear equivalent (1) is the following:

$$h_1 = \frac{3 + i\sqrt{3}}{12}, \qquad h_3 = \frac{1}{2}, \qquad h_4 = \frac{1}{6}(3 - i\sqrt{3})$$
$$h_2 = \frac{3 + i\sqrt{3}}{6}, \qquad h_5 = \frac{1}{12}(3 - i\sqrt{3}). \tag{15}$$

At first glance it might appear that complex-time operator factorization has small merit. Depending upon the approximation operators L_x, L_y, this could be the case; for example, ENO schemes [1] are not known to be adaptable to complex time. However, as may be seen by the numerical experiments reported in the sequel, finite-differencing can produce operators which are so adaptable. The general rule is that any real functions involved must admit an analytic continuation whose complex values are machine calculable, and the numerical algorithm must be compatible with generalization to complex functions.

Mixed Positive–Negative Steps

Any reluctance to abide with complex fractional-step splittings for the linear equations (1) requires one to consider more than five factors in the splitting, if third-order accuracy is desired. It has been verified independently by the authors that no all-positive step, third-order accurate splitting having less than nine factors can exist. Reference [3] shows that no all-positive step splitings of any sort exists, whose order of accuracy exceeds two. For completeness, there is now indicated the existence of one six-factor, third-order mixed positive–negative fractional step splitting for systems (1), (9):

$$h_6 = \tfrac{7}{24}, \qquad h_5 = \tfrac{24}{17}, \qquad h_4 = -\tfrac{1}{24}, \qquad h_3 = -\tfrac{2}{3}, \qquad h_2 = \tfrac{3}{4}, \qquad h_1 = \tfrac{13}{51}. \tag{16}$$

Eight-Factor Splittings

The minimal generating set of determining equations for up to eight-factor splittings of Eq. (1) is given by:

$$h_1 + h_3 + h_5 + h_7 = 1 \tag{17}$$

$$h_2 + h_4 + h_6 + h_8 = 1 \tag{18}$$

$$h_1 + h_3(1 - h_2) + h_5(h_6 + h_8) + h_7 h_8 = \tfrac{1}{2} \tag{19}$$

$$h_1 h_2(1 - h_1) + (h_1 + h_3) h_4(h_5 + h_7) + h_6 h_7(1 - h_7) = \tfrac{1}{6} \tag{20}$$

$$h_2 h_3(1 - h_2) + (h_2 + h_4) h_5(h_6 + h_8) + h_7 h_8(1 - h_8) = \tfrac{1}{6}. \tag{21}$$

A Stiff Systems Applications of Operator Splitting

Consider now a quasi-linear vector system

$$\frac{du}{dt} = Au + f(u) \tag{22a}$$

$$u(0) = u_0 \tag{22b}$$

System (22) shall be called *linearly stiff* provided the matrix A has widely separated eigenvalues, each having negative real part, whereas the nonlinear system obtained when A is set to zero is not a stiff system. Much research has been devoted to numerical methods for efficiently solving stiff linear systems.

An idea for treating the stiffness of the composite system (22) is to associate with the stiff linear part its exact transfer operator L_x, while an approximate operator L_y is associated with the non-stiff, nonlinear part. The total system is now solved with some approximate operator composite of L_x, L_y of the form (3). Through use of this device, and when a non-stiff numerical integration scheme is involved, larger time increments than the non-split system allows can now be employed, the size of which is dictated only by the nonlinear part of Eq. (22). Of course, the trade-off is that the efficiency gained in step-size must not be completely offset by the inefficiency in operation count which arises from the splitting. For those whose interest is reliable numerical output without consideration of stiffness, this approach should be ideal.

This method has the flexibility of allowing the order of accuracy of the numerical integration scheme which is used on the nonlinear part to be, consistently, as high as is compatible with the accuracy of the splitting. Here, it is remarked that many stiff integration packages vary the order of accuracy of the scheme used as the solution progresses, in order to remain in the stable regime. Since the exact linear transfer operator is $\exp(A\tau)$, which is absolutely stable if A has left half-plane eigenvalues, the stability of the present scheme is dictated by the (assumed small) eigenvalues inherent in the nonlinear part of Eq. (22). The resulting numerical integration algorithms shall be called *essentially absolutely stable*, as the small eigenvalues of the well-behaved nonlinear part pose no real threat to stability.

A Scalar Numerical Example

Consider now a simplified linearly-stiff problem, arising in the heory of nonlinear oscillations, which serves to illustrate the features of the method:

$$\frac{du}{dt} = -50u + \cos(u), \qquad u(0) = Pi/2. \tag{23}$$

The solution of Eq. (23) exhibits boundary-layer behaviour near $t = 0$, quickly damping monotonicly to the steady solution (see Fig. 1), which is approximately $u = 0.019996$. If Eq. (23) is solved numerically employing a third-order accurate

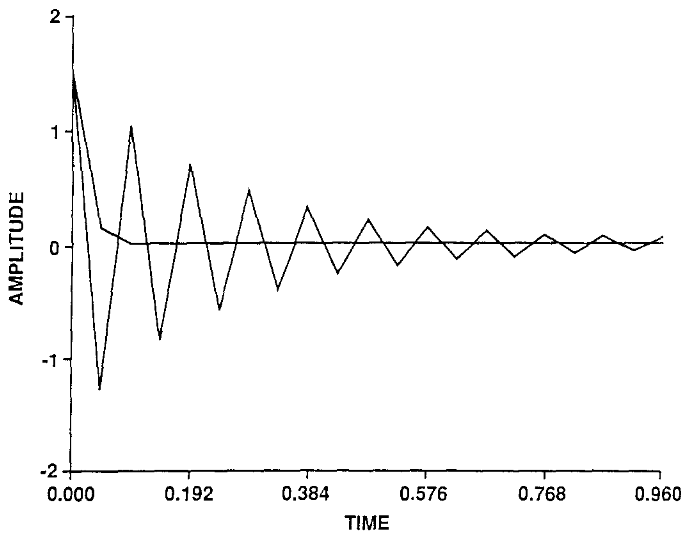

FIG. 1. No splitting versus Strangs second-order accurate splitting.

Runge–Kutta scheme, the time-step stability restriction is, approximately, $\tau < 0.04$. With $\tau = 0.045$, the numerical solution oscillates, due to the stability, and is highly inaccurate. However, with the same Runge–Kutta scheme and the same time-step, but applying Strang's second-order accurate splitting [5], the numerical solution converges monotonically, in seven steps, essentially as near as it can get thereafter to the steady solution (see Fig. 1). Hence, the splitting approach eliminates the stability problem; stepsize is now dictated by the truncation error of the scheme. A broadening of the range of stability for the Runge–Kutta method has been achieved via the spliting technique. Figure 2 illustrates the broadening of stability attainable by using the five-factor, third-order complex splitting of Eq. (15), the use of which is allowed by Theorem I.

Splitting of Vector Nonlinear Systems

The behaviour characteristic of the previous example has also been experienced when numerically solving with a third-order accurate splitting the stiff systems test problem [6] given by

$$\frac{dx}{dt} = -2000x + 1000y + 1000, \qquad x(0) = 0 \tag{24}$$

$$\frac{dy}{dt} = x - y, \qquad y(0) = 0. \tag{25}$$

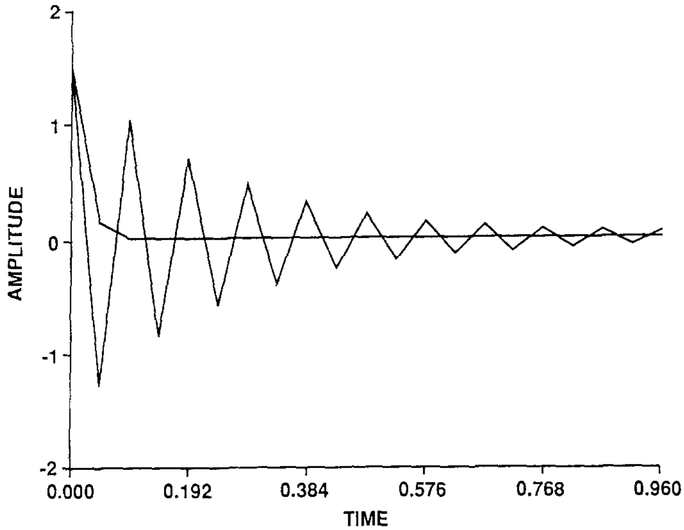

FIG. 2. No splitting versus complex third-order accurate splitting.

Solution of system (24)–(25) requires synthesis of new splittings, as will now be indicated. Consider vector nonlinear equations of the form

$$\frac{\partial u}{\partial t} = A(u) + C(u). \tag{26}$$

Here, $C(u) = c$ is a constant vector mapping defined on R_n, while A is any linear operator which commutes with the time differentiation operator and whose powers A^P, $P = 1, 2, ..., n$ do not annihilate C. In this event, all-positive-step, nth order accurate splittings of system (26) require only $n+1$ factors. Typical such splittings (refer to Eq. (3)) are now indicated:

A four-factor, third-order splitting,

$$h_1 = 0, \quad h_2 = \tfrac{1}{4}, \quad h_3 = \tfrac{2}{3}, \quad h_4 = \tfrac{3}{4}, \quad h_5 = \tfrac{1}{3}. \tag{27}$$

A five-factor, fourth-order splitting,

$$h_1 = 0, \quad h_2 = \tfrac{1}{6}, \quad h_3 = \tfrac{1}{2}, \quad h_4 = \tfrac{2}{3}, \quad h_5 = \tfrac{1}{2}, \quad h_6 = \tfrac{1}{6}. \tag{28}$$

A six-factor, fifth-order splitting,

$$h_1 = 0, \quad h_2 = \tfrac{1}{9}, \quad h_3 = (6 - \sqrt{6})/10, \quad h_4 = (16 + \sqrt{6})/36 \tag{29a}$$

$$h_5 = \sqrt{6}/5, \quad h_6 = (16 - \sqrt{6})/36, \quad h_7 = (4 - \sqrt{6})/10. \tag{29b}$$

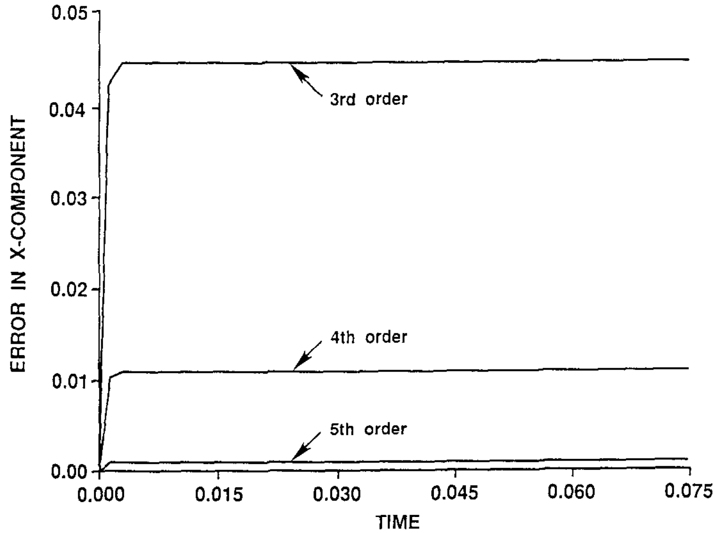

FIG. 3. Comparison of splitting accuracy.

The stiff system (24)–(25) has eigenvalues

$$R = -1000.5 - \sqrt{1{,}000{,}000.25} \tag{30a}$$

$$S = -1000.5 + \sqrt{1{,}000{,}000.25}. \tag{30b}$$

The x-component of the solution exhibits boundary layer behaviour near $t = 0$, whereas the y-component is of slow growth.

Numerical solution of (24)–(25) has been accomplished using Runge–Kutta integration of order $n = 3, 4, 5$ and the higher order, fractional-step splittings of Eqs. (27)–(29). Figure 3 exhibits the expected broadening in the range of stability which is achieved by the splitting. Also as expected, a better approximation is achieved by using the higher order splittings.

It is expected that the method can be applied to stiff systems, in general, through periodic extraction of a stiff linear part Ju, where J is the Jacobian matrix evaluated at some fixed instant. However, this may be an expensive operation.

Complex-Time Splitting of a Partial Differential Equation

Some numerical experiments are now presented which verify the increased accuracy of the corresponding operator splitting (15), as compared to that of the second-order splittings of Strang [5]. The problem under consideration is

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + u - u^2 = 0, \tag{31a}$$

$$u(x, 0) = \exp(x), \qquad -1 < x < 1 \tag{31b}$$

which has the solution $u = \exp(x - t)$.

TABLE I

Comparison of Splitting Accuracy

Exact solution	Strangs 3-factor	All-positive 4-factor	Complex 5-factor
0.9801986733	0.9801987089	0.9801986733	0.9801986733
1.0202013400	1.0202013814	1.0202013401	1.0202013401
1.0619365465	1.0618365946	1.0618365466	1.0618365466
1.1051709181	1.1051709739	1.1051709181	1.1051709181
1.1502737989	1.1502738637	1.1502737989	1.1502737989
1.1972173631	1.1972174385	1.1972173631	1.1972173632
1.2460767306	1.2460768183	1.2460767306	1.2460767307
1.2969300867	1.2969301888	1.2969300867	1.2969300868
1.3498588076	1.3498589265	1.3498588076	1.3498588077
1.4049475906	1.4049477291	1.4049475906	1.4049475907
1.4622845894	1.4622847509	1.4622845894	1.4622845896
1.5219615556	1.5219617438	1.5219615556	1.5219615558
1.5840739850	1.5840742045	1.5840739849	1.5840739851

By employing third-order backward differences on the space derivatives in Eq. (31), there is obtained a vector system of form similar to Eq. (9). This system is split such that L_x, L_y produce third-order accurate Runge–Kutta approximations to the systems derived from (31) which involve only time derivative and, respectively, the source term or space derivative in (31). The five-factor, complex-time fractional-step splitting of Eq. (15) is applied to this vector system of finite difference equations. Problem (31) is also solved numerically using a third-order, four-factor splitting [7] which employs all-positive fractional steps.

Table I shows a comparison of results for numerical solution of (31) obtained by Strang's second-order splitting [5], versus the third-order, all-positive step splitting of [7], and the complex-time splitting (15). There appears to be essentially four more correct digits in numerical results from the higher-order splittings. The stepsize $\tau = 0.001$ was used, and results after 20 cycles are shown. The accuracy is not affected when a large number of cycles is employed; thus, it is concluded by numerical experimant that the complex-time splitting is stable.

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