Riv. Mat. Univ. Parma (6) **2*** (1999), 235-243

A. V. BOBYLEV and T. OHWADA (*)

On the generalization of Strang's splitting scheme (**)

1 - Introduction

The splitting algorithm is widely employed in the numerical analysis of the initial value problem of the form:

$$\frac{\partial f(\xi, t)}{\partial t} = A[f] + B[f], \qquad \xi \in R^d, \qquad t > 0, \tag{1}$$
$$f(\xi, 0) = f_0(\xi),$$

where A and B are (linear or nonlinear) operators acting from a Banach space F to F, $f \in F$, and $f_0 \in F$. For brevity we assume that the operators act on ξ variables only (autonomous case). The splitting scheme solves approximately the problem (1) on a small interval $t \in [0, \Delta t]$ in the following way. Equation (1) is split into two equations:

$$\frac{dy}{dt} = A(y), \qquad y(0) = f_0, \qquad 0 \leq t \leq \Delta t, \tag{2}$$
$$\frac{dz}{dt} = B(z), \qquad z(0) = y(\Delta t), \quad 0 \leq t \leq \Delta t,$$

and the approximate solution of problem (1) is obtained as

$$f(., \Delta t) \approx z(\Delta t). \tag{3}$$

(*) Department of Engineering Sciences, Physics and Mathematics, Karlstad University, Universitetgatan 1, 651 88 Karlstad, Sweden; Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Kyoto 606-8501, Japan.
(**) Received September 27, 1999. AMS classification 65 G 99, 76 P 05.

For the case where A and B are differential operators, the error of the splitting scheme has been investigated by Strang together with the modification for the improvement of accuracy (Strang's splitting) [**1**]. The evolution equations of the form (1) are widely studied by physicists, engineers, and mathematicians, e.g., Boltzmann equation, Fokker-Planck equation, and Vlasov-Poisson equation, which are employed in the analysis of rarefied gas flows, neutron transport, and s emiconductor device modeling, etc. Many of such equations have operators other than differential ones and Strang's result is not sufficient for general cases. As for the Boltzmann equation, one of the authors (O) discussed the accuracy of the splitting method and developed higher order schemes from the discussion [**2**]. It is inefficient to discuss the accuracy of the method for each equation, however. Instead of doing this, in the present study, we will consider the abstract Cauchy problem (1) and examine the accuracy of the splitting method for general evolution equations. As an immediate consequence of the discussion, we will show that the accuracy in time is improved from first order to second order by a simple modification. This is the generalization of Strang's result for PDEs. The accuracy of Strang's splitting method is also demonstrated numerically in a Cauchy problem for the BGK equation, which is widely employed as a model equation of the Boltzmann equation.

2 - Error of splitting method

For the brevity, we express the solution of an abstract Cauchy problem

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = P(Y)\,, \qquad Y\big|_{t=0} = Y_0 \in F\,, \tag{4}$$

as

$$Y(t) = S_P^t(Y_0)\,. \tag{5}$$

The splitting method for the case of $P = A + B$ is nothing more than the following approximation of the operator $S_{A+B}^{\Delta t}$:

$$S_{A+B}^{\Delta t} \approx S_B^{\Delta t} S_A^{\Delta t}\,. \tag{6}$$

In the following, we first consider the simplest case of linear operators, and then, proceed to the general case of nonlinear operators.

2.1 - *Linear operators*

When A and B are linear operators, then we can write (by definition) $P(x) = \widehat{P}x$. In this case, $S_P^{\Delta t} = \exp(\Delta t \widehat{P})$. Then the error of the splitting method is evaluated as follows:

$$\widehat{\delta}(\Delta t) = \exp[\Delta t(\widehat{A} + \widehat{B})] - e^{\Delta t \widehat{B}} e^{\Delta t \widehat{A}}$$

$$(7) \qquad = \left\{\widehat{I} + \Delta t(\widehat{A} + \widehat{B}) + \frac{\Delta t^2}{2}(\widehat{A} + \widehat{B})^2 + O(\Delta t^3)\right\}$$

$$- \left\{\widehat{I} + \Delta t \widehat{B} + \frac{\Delta t^2}{2}\widehat{B}^2 + O(\Delta t^3)\right\}\left\{\widehat{I} + \Delta t \widehat{A} + \frac{\Delta t^2}{2}\widehat{A}^2 + O(\Delta t^3)\right\},$$

where $\widehat{I}$ denotes identity. A direct calculation leads to the formula

$$(8) \qquad \widehat{\delta}(\Delta t) = \frac{\Delta t^2}{2}[\widehat{A}, \widehat{B}] + O(\Delta t^3),$$

where

$$[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$$

denotes the commutator of the two linear operators. Hence, in the linear case, the simple splitting scheme (2) is second order accurate only in the special case of commuting operators.

2.2 - *General case*

Let us now consider the general case of nonlinear operators. Then we need to assume that both of the operators A and B have continuous second derivatives. That is, there exist bounded linear operators $\widehat{A}'_x$ and $\widehat{B}'_x$ and bilinear operators $\widehat{A}''_x$ and $\widehat{B}''_x$ such that

$$\lim_{s \to 0} \frac{A(x + sh) - A(x)}{s} = \widehat{A}'_x(h), \qquad \lim_{s \to 0} \frac{B(x + sh) - B(x)}{s} = \widehat{B}'_x(h),$$

$$\lim_{s \to 0} \frac{\widehat{A}'_{x + sh'}(h) - \widehat{A}'_x(h)}{s} = \widehat{A}''_x[h, h'], \qquad \lim_{s \to 0} \frac{\widehat{B}'_{x + sh'}(h) - \widehat{B}'_x(h)}{s} = \widehat{B}''_x[h, h'],$$

and $\widehat{A}''_x$ and $\widehat{B}''_x$ ($\widehat{A}'_x$ and $\widehat{B}'_x$ also) are continuous with respect to x.

If P has a continuous second derivative $\widehat{P}''_x$, the solution of (4) is expressed as

$$Y(\Delta t) = Y_0 + \Delta t P(Y_0) + \frac{\Delta t^2}{2} \widehat{P}'_{Y_0} P(Y_0) + \frac{\Delta t^3}{6} \{\widehat{P}''_{Y_0}[P(Y_0), P(Y_0)] + \widehat{P}'_{Y_0} \widehat{P}'_{Y_0} P(Y_0)\} + o(\Delta t^3). \tag{9}$$

Therefore the solution of (1) is expressed as

$$S^{\Delta t}_{A+B}(f_0) = f_0 + \Delta t[A(f_0) + B(f_0)] + \frac{\Delta t^2}{2} [\widehat{A}'_{f_0} + \widehat{B}'_{f_0}][A(f_0) + B(f_0)] + O(\Delta t^3). \tag{10}$$

On the other hand, the solution of (2) is expressed as

$$\begin{aligned} y(\Delta t) &= S^{\Delta t}_A (f_0) = f_0 + \Delta t A(f_0) + \frac{\Delta t^2}{2} \widehat{A}'_{f_0} A(f_0) + O(\Delta t^3), \\ z(\Delta t) &= S^{\Delta t}_B [y(\Delta t)] = y(\Delta t) + \Delta t B[y(\Delta t)] + \frac{\Delta t^2}{2} \widehat{B}'_{y(\Delta t)} B[y(\Delta t)] + O(\Delta t^3). \end{aligned} \tag{11}$$

Noting

$$B[f_0 + \Delta t A(f_0) + \dots] = B(f_0) + \Delta t \widehat{B}'_{f_0} A(f_0) + O(\Delta t^2), \tag{12}$$

and

$$\widehat{B}'_{y(\Delta t)} B[y(\Delta t)] = \widehat{B}'_{f_0} B(f_0) + \Delta t\{\widehat{B}''_{f_0}[B(f_0), B(f_0)] + \widehat{B}'_{f_0} \widehat{B}'_{f_0} B(f_0)\} + o(\Delta t), \tag{13}$$

we have

$$S^{\Delta t}_B [S^{\Delta}_A t(f_0)] = f_0 + \Delta t[A(f_0) + B(f_0)] + \frac{\Delta t^2}{2} [\widehat{B}'_{f_0} B(f_0) + \widehat{A}'_{f_0} A(f_0) + 2\, \widehat{B}'_{f_0} A(f_0)] + O(\Delta t^3). \tag{14}$$

Hence, we obtain

$$S^{\Delta t}_{A+B}(f_0) - S^{\Delta t}_B [S^{\Delta t}_A (f_0)] = \frac{\Delta t^2}{2} \{\widehat{A}'_{f_0} B(f_0) - \widehat{B}'_{f_0} A(f_0)\} + O(\Delta t^3). \tag{15}$$

We remark that $\widehat{A}'_{f_0} \equiv \widehat{A}$ and $\widehat{B}'_{f_0} \equiv \widehat{B}$ if A and B are linear operators. That is, the formula (8) is obtained from Eq. (15).

3 - Strang's splitting

We note that the leading error term (15) is antisymmetric with respect to operators A and B. This simple observation leads immediately to the «symmetric splitting» formula

$$S_{A+B}^{\Delta t}(f_0) = S_B^{\Delta t/2}\{S_A^{\Delta t}[S_B^{\Delta t/2}(f_0)]\} + O(\Delta t^3), \tag{16}$$

which was first proposed by Strang [**1**] for PDEs. We can show now that this second order accurate formula is valid for any operators A and B which have continuous second derivatives. This is easily seen from

$$S_B^{\Delta t/2}\{S_A^{\Delta t}[S_B^{\Delta t/2}(f_0)]\} = S_B^{\Delta t/2}\big[S_A^{\Delta t/2}\{S_A^{\Delta t/2}[S_B^{\Delta t/2}(f_0)]\}\big], \tag{17}$$

Eq. (15), and

$$S_{A+B}^{\Delta t}(f_0) - S_A^{\Delta t}[S_B^{\Delta t}(f_0)] = -\frac{\Delta t^2}{2}\{\widehat{A}'_{f_0}B(f_0) - \widehat{B}'_{f_0}A(f_0)\} + O(\Delta t^3). \tag{18}$$

Equation (18) is obtained from Eq. (15) by changing A to B and vice versa. Similarly, we have another Strang's formula:

$$S_{A+B}^{\Delta t}(f_0) = S_A^{\Delta t/2}\{S_B^{\Delta t}[S_A^{\Delta t/2}(f_0)]\} + O(\Delta t^3). \tag{19}$$

Finally we notice a simple analogy between the above splitting formulas and usual quadrature formulas for integrals. If $u(t) \in C_2[0, 1]$, then standard rectangular formulas yield

$$\int_0^1 u(t)\,\mathrm{d}t = S_K(h) + O(h), \qquad h = \frac{1}{N} \to 0,$$

where

$$S_K(h) = h \sum_{n=K}^{N-1+K} u(nh), \qquad K = 0, 1.$$

On the other hand, the simple averaging of the two formulas leads to the trapezoidal rule

$$\int_0^1 u(t)\,\mathrm{d}t = S_2(h) + O(h^2), \qquad S_2 = \frac{S_0 + S_1}{2},$$

which has the second order of approximation. A similarity of this formula with

Strang's splitting formulas is quite obvious. It is remarkable that in both cases one can obtain a higher order of approximation almost without changing the computational procedure.

4 - Numerical example

In this section, we demonstrate the accuracy of Strang's splitting method numerically for the one-dimensional BGK equation. Let $f(x_1, \zeta_i, t)$ be the nondimensional distribution function, where x_i, ζ_i, and t are nondimensional space coordinates, molecular velocity, and time, respectively. The nondimensional BGK equation in the spatially one-dimensional case is expressed as

$$\begin{aligned}
&\frac{\partial f}{\partial t} = (A+B)(f),\\
&A(f) = -\zeta_1 \frac{\partial f}{\partial x_1},\\
&B(f) = \varrho\left[\frac{\varrho}{\pi^{3/2}T^{3/2}}\exp\left[-\frac{(\zeta_i - u_i)^2}{T}\right] - f\right],\\
&\varrho = \int f \, d\boldsymbol{\zeta},\\
&\varrho u_i = \int f \, d\boldsymbol{\zeta},\\
&T = \frac{2}{3\varrho}\int (\zeta_i - u_i)^2 f \, d\boldsymbol{\zeta},
\end{aligned} \tag{20}$$

where the integration is carried out over the whole velocity space (R^3). We consider the Cauchy problem of this equation from the initial condition

$$\begin{aligned}
&f(x_1, \zeta_i, 0) = \frac{1}{\pi^{3/2}\sqrt{a(x_1)}}\exp\left(-\frac{\zeta_1^2}{a(x_1)} - \zeta_2^2 - \zeta_3^2\right),\\
&a(x_1) = 1 + 4\exp(-5x_1^2).
\end{aligned} \tag{21}$$

The corresponding values of ϱ, u_i, and T are $\varrho = 1$, $u_i = (0, 0, 0)$, and $T = 1 + (4/3)\exp(-5x_1^2)$.

Owing to the symmetry of the problem, we have only to solve the problem for $x_1 > 0$. Furthermore, in the present case, $u_2 = u_3 = 0$ and the variables ζ_2 and ζ_3 can be eliminated by using Chu's method [3].

We solve the Cauchy problem (20) and (21) numerically by using Strang's splitting method, i.e., $S_A^{\Delta t/2} S_B^{\Delta t} S_A^{\Delta t/2}$. The computation by the conventional splitting method, $S_A^{\Delta t} S_B^{\Delta t}$, is a lso done for comparison. The condition of the computation is as follows. The computational region for x_1 is $0 \leqslant x_1 \leqslant 5$ and that for ζ_1 is $-10 \leqslant \zeta_1 \leqslant 10$; uniform mesh systems are employed for x_1 and ζ_1; the number of mesh points is 201 for x_1 and that for ζ_1 is 401; the computation is carried out until $t = 0.4$ for $\Delta t = 0.2,\ 0.1,\ 0.05,\ 0.025$.

Since the spatially homogeneous BGK equation is solved analytically [cf. the orthogonality condition (23)], no error is induced in the computation of $S_B^{\Delta t}\{f_0\}$. In the computation of $S_A^{\Delta t/2}\{f(x_1, \zeta_i)\} \equiv f(x_1 - \zeta_1 \Delta t/2, \zeta_i)$, a higher order interpolation with the truncation error of $O(\Delta x_1^7)$ is employed, where Δx_1 is the width of x_1 mesh and the truncation error is much less than Δt^3 for all cases of Δt. The analytical solution for the spatially homogeneous equation and the same interpolation are employed in the computation of conventional splitting method.

The values of ϱ and T for $(t, x_1) = (0.4, 0)$ are tabulated in Tables 1 and 2. From these tables, we find that the rate of convergence is 2nd order for Strang's splitting and first order for the conventional splitting.

Finally we remark on the error of conventional splitting for the BGK equation. The leading error of the conventional splitting, Eq. (18), is expressed as

$$\varepsilon(x_1, \zeta_i) = \frac{\Delta t^2}{2}\left[\zeta_1 \frac{\partial B(f_0)}{\partial x_1} + \widehat{B}'_{f_0}\left(-\zeta_1 \frac{\partial f_0}{\partial x_1}\right)\right], \tag{22}$$

TABLE 1. - The values of ϱ at $(t, x_1) = (0.4, 0)$.

	$\Delta t = 0.2$	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.025$
Strang's splitting	0.74968	0.75199	0.75267	0.75282
Conventional splitting	0.76900	0.75964	0.75587	0.75428

TABLE 2. - The values of T at $(t, x_1) = (0.4, 0)$.

	$\Delta t = 0.2$	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.025$
Strang's splitting	1.30421	1.30615	1.30632	1.30636
Conventional splitting	1.35140	1.32958	1.31824	1.31236

where the operators B and $\widehat{B}'_{f_0}$ satisfy the orthogonality condition

$$\int \begin{pmatrix} 1 \\ \zeta_i \\ \zeta_j^2 \end{pmatrix} B(.)\, \mathrm{d}\boldsymbol{\zeta} = 0\,, \tag{23}$$

$$\int \begin{pmatrix} 1 \\ \zeta_i \\ \zeta_j^2 \end{pmatrix} \widehat{B}'_{f_0}(.)\, \mathrm{d}\boldsymbol{\zeta} = 0\,. \tag{24}$$

From this property, $\int \varepsilon(x_1, \zeta_i)\, \mathrm{d}\boldsymbol{\zeta} = 0$ but $\int \zeta_1 \varepsilon(x_1, \zeta_i)\, \mathrm{d}\boldsymbol{\zeta}$ and $\int \zeta_j^2 \varepsilon(x_1, \zeta_i)\, \mathrm{d}\boldsymbol{\zeta}$ are not equal to zero in general; the projection of ε onto ϱ is zero and that onto u_1 and that onto T are $O(\Delta t^2)$. Then, for $t = \Delta t$, the result for ϱ is better than that for T and u_1. However, the convergence rate of conventional splitting is first order even for ϱ. This is because the error of each time step is not accumulated as it is. That is, the error $\varepsilon(x_1, \zeta_i)$ becomes $\varepsilon(x_1 - (n-1)\zeta_1 \Delta t, \zeta_i) \sim (n-1)\Delta t \zeta_1 (\partial\varepsilon/\partial x_1)$ at $t = n\Delta t$ by the operation $(S_A^{\Delta t})^{n-1}$. Then, its projection onto ϱ is not zero and is $O[(n-1)\Delta t^3)$. Taking account of $(n-1) + (n-2) + \ldots + 1 \sim n^2/2$ and $n \sim 1/\Delta t$, we find that the amount of accumulated error for n time steps becomes $O(\Delta t)$ for ϱ. The same discussion is applied to the case of the original Boltzmann equation.

5 - Acknowledgements

The main part of the present study was done while one of the authors (A. V. B.) was staying at Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University as a fellow of Japan Society for the Promotion of Science (JSPS). The support from JSPS and the kind hospitality of the department are gratefully acknowledged by him. Both authors are grateful to Professor Y. Sone and Professor K. Aoki of the department for helpful discussions.

References

[1] G. Strang, *On the construction and comparison of difference schemes*, SIAM J. Numer. Anal. **5** (1968), 506-517.

[2] T. OHWADA, *Higher order approximation methods for the Boltzmann equation*, J. Comput. Phys. **139** (1998), 1-14.

[3] C. K. CHU, *Kinetic-theoretic description of the formation of a shock wave*, Phys. Fluids 8 (1965), 12.

Abstract

The accuracy of splitting method is investigated in an abstract Cauchy problem and is shown to be first order in time for general evolution equations except for a special case. A general formula for the leading term is obtained. It is also shown as an immediate consequence of the formula that the accuracy is improved from first order to second order by a simple modification. Such a modification was first proposed by Strang [*G. Strang, SIAM J. Numer. Anal.* **5** (1968), 506] *for PDEs. Thus, the Strang result is generalized in the present paper to the case of arbitrary evolution equations. In particular, it is valid for practically important case of integro-differential nonlinear kinetic equations and therefore there is no need to make additional error estimates in each particular case. The accuracy of generalized Strang's splitting method is demonstrated numerically for the BGK equation.*

* * *