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RESEARCH ARTICLE

An integral formulation for the global error of Lie Trotter splitting scheme

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ABSTRACT

An ordinary differential equation (ODE) can be split into simpler sub equations and each of the sub equations is solved subsequently by a numerical method. Such a procedure involves splitting error and numerical error caused by the time stepping methods applied to sub equations. The aim of the paper is to present an integral formula for the global error expansion of a splitting procedure combined with any numerical ODE solver.

1. Introduction

Consider an autonomous ODE system in a real Banach space

$$\frac{du}{dt} = (A+B)u, \qquad u(0) = u_0, \tag{1}$$

where A and B are Lie operators allowing us to write the formal solution as

$$u(t) = \varphi_t^{A+B} u_0 = e^{t(A+B)} u_0 = \sum_{k=0}^{\infty} \frac{t^k}{k!}(A+B)^k u_0, \tag{2}$$

The solutions of sub equations

$$\frac{du}{dt} = Au \qquad \text{and} \qquad \frac{du}{dt} = Bu, \tag{3}$$

can be merged within a small time step h by

$$u_{n+1} = e^{hb_1 B} e^{ha_1 A} e^{hb_2 B} \dots e^{ha_m A} e^{hb_{m+1} B} u_n,$$

or equivalently,

$$u_{n+1} = (\varphi^B_{hb_{m+1}} \circ \varphi^A_{ha_m} \circ \dots \varphi^B_{hb_2} \circ \varphi^A_{ha_1} \circ \varphi^B_{hb_1}) u_n,$$

where u_n and u_{n+1} are approximations at $t = t_n$ and $t = t_{n+1}$ with $h = t_{n+1} - t_n$. The reverse orders of A and B as well as a_i and b_i should be noticed. This happens when one applies Lie transforms to their corresponding maps. This phenomena is termed as *Vertauschungssatz* in the literature [1]. One of the sub problems in (3) (or both) can be solved numerically. When a splitting procedure and a numerical solver are of p^{th} and r^{th} order respectively, we are interested in the integral form of the leading term of the global error.

Although it is very classical subject of numerical analysis, the global error analysis of the numerical solvers for ODEs has been discussed by Viswanath [2] and Iserles [3] in different aspects. Viswanath employed Lyapunov's exponents to express error patterns of numerical solvers for hyperbolic problems. However, Iserles presented a way of deriving an asymptotic formula for the global error in the numerical solution of highly oscillatory problems.

Error bound for splitting schemes is an active research area. The splitting of bounded operators was analyzed in [1, 4]. Jahnke and Lubich [5] found error bounds for the Strang splitting in the presence of unbounded operators, which corresponds to splitting a time dependent PDE without discretization of space operators. Hansen and Ostermann [6] also presented error analysis of splitting schemes for unbounded operators in the content of semigroup theory. Apart from the above mentioned approaches, Csomos and Farago [7] discussed the interaction of the error caused by numerical methods employed for sub problems and splitting schemes. Our main task is to give clear integral representation of this interaction. In this work, we propose to approximate the global error in terms of the local errors and the discrete flow by a Riemann integral.

2. Preliminaries

We would like to explain some of notations which will be used in the later sections. Consider the initial value problem

$$\mathbf{y}' = f(t, \mathbf{y}), \qquad \mathbf{y}(t_0) = \mathbf{y}_0, \tag{4}$$

where $\mathbf{y}_0 \in \mathbb{R}^m$ and $f : \mathbb{R}^+ \times \mathbb{R}^m \to \mathbb{R}^m$ is continuous. When a small perturbation is introduced to the initial value $\mathbf{y}_0$, for the perturbed solution $\tilde{\mathbf{y}}(t)$, the error $\mathbf{e}(t) = \mathbf{y}(t) - \tilde{\mathbf{y}}(t)$, evolves with [3,8]

$$e(t) = \Psi(t)\Psi^{-1}(c)e(c) + \mathcal{O}(e(c)^2), t > c > 0, \tag{5}$$

where $\Psi(t)$ satisfies the variational equation

$$\Psi'(t) = J(t)\Psi(t), \qquad \Psi(0) = I, \tag{6}$$

where $J(t) = \dfrac{\partial f}{\partial \mathbf{y}}$. In order to use exponentials in defining flows we firstly express (4) an autonomous system as

$$\frac{dt_1}{dt} = 1, \tag{7}$$

$$\frac{d\mathbf{y}}{dt} = f(t_1, \mathbf{y}), \tag{8}$$

and then define a Lie operator as follows

$$L = \frac{\partial}{\partial t_1} + f(t_1, \mathbf{y})\frac{\partial}{\partial \mathbf{y}}, \tag{9}$$

which enables us to express (4) as

$$\frac{du}{dt} = Lu, \qquad u(0) = u_0, \tag{10}$$

where $u = (t_1, y)^T$ and the formal solution is $u(t) = \varphi_t^L(u_0) = e^{tL}u_0$.

3. Motivation

The local error ($\mathfrak{le}$) of a numerical method $u_{n+1} = R_{\Delta t}(u_n)$ with step size Δt for the initial value problem

$$\frac{du}{dt} = Lu, \qquad u(t_i) = u_i, \tag{11}$$

is given by

$$\Delta t^{r+1}\mathfrak{le}(u_n) = R_{\Delta t}(u_n) - \varphi_{\Delta t}^L(u_n) + \mathcal{O}(\Delta t^{r+2}). \tag{12}$$

The global error is defined as

$$\begin{aligned} e_{n+1} &= u_{n+1} - u(t_{n+1}),\\ &= R_{\Delta t}(u_n) - \varphi_{\Delta t}^L(u(t_n)). \end{aligned}$$

Therefore

$$\begin{aligned} e_{n+1} =&\Delta t^{r+1}\mathfrak{le}(u_n) + \varphi_{\Delta t}^L(u_n) - \varphi_{\Delta t}^L(u(t_n))\\ &+ \mathcal{O}(\Delta t^{r+2}). \end{aligned} \tag{13}$$

The difference $\varphi_{\Delta t}^L(u_n) - \varphi_{\Delta t}^L(u(t_n))$ can be interpreted as the time evolution of a small perturbation to initial condition $u(t_n)$ within a time interval of which length is Δt. As a result of this interpretation and considering (5), one obtains

$$\begin{aligned} \varphi_{\Delta t}^L(u_n) - \varphi_{\Delta t}^L(u(t_n)) =&\Psi(t_{n+1})\Psi^{-1}(t_n)e_n\\ &+ \mathcal{O}(\|e_n^2\|), \end{aligned} \tag{14}$$

where $\Psi(t)$ is the solution of variational equation of the corresponding initial value problem. Therefore the first order difference equation for global error is given by

$$\begin{aligned} e_{n+1} =&e_n\Psi(t_{n+1})\Psi^{-1}(t_n) + \Delta t^{r+1}\mathfrak{le}(u(t_n))\\ &+ \mathcal{O}(\Delta t^{r+2}). \end{aligned} \tag{15}$$

A careful reader notices that $u(t_n)$ is substituted in the term $\mathfrak{le}$ instead of u_n. It might be assumed that the difference is included in the term $\mathcal{O}(\Delta t^{r+2})$ as Iserles pointed out in [3].

Assuming $e_i = 0$, the solution of the linear difference equation is

$$e_n = \Delta t^{r+1}\Psi(t_n)\sum_{k=i}^{f-1}\Psi^{-1}(t_{k+1})(\mathfrak{le}(u(t_k)) + \mathcal{O}(\Delta t^{r+2})). \quad (16)$$

For $t_f - t_i = h = m\Delta t$, the error can be written in the integral form

$$e(t_f) = \Delta t^r\Psi(t_f)\int_{t_i}^{t_f}\Psi^{-1}(\tau+\Delta t)\mathfrak{le}(u(\tau))d\tau + \mathcal{O}(\Delta t^{r+1}).$$

As an example, we derive the global error of Euler method for the linear problem

$$\frac{du}{dt} = -\frac{1}{t+1}u(t), \qquad u(t_i) = u_i. \quad (17)$$

We will find an estimation for the actual error at $t_f = t_i + h$ with time step $\Delta t = \frac{h}{m}$. It is known that local error coefficient for Euler method (in terms of Lie Operator)

$$\mathfrak{le}(u(t)) = -1/2L^2(u(t)) = -\frac{u(t)}{(t+1)^2}. \quad (18)$$

The variational flow is determined by solving

$$\frac{d\Psi}{dt} = J(t)\Psi, \qquad \Psi(t_i) = 1, \quad (19)$$

where $J(t) = -\dfrac{1}{t+1}$. Therefore,

$$e(t_f) = \Delta t\Psi(t_f)\int_{t_i}^{t_f}\Psi(\tau+\Delta t)^{-1}\mathfrak{le}(u(t))d\tau + \mathcal{O}(\Delta t^2), \quad (20)$$

$$e(t_f) = \Delta t\frac{t_i+1}{t_f+1}\int_{t_i}^{t_f}\frac{\tau+1+\Delta t}{t_i+1}\left(\frac{-u(\tau)}{(\tau+1)^2}\right)d\tau + \mathcal{O}(\Delta t^2), \quad (21)$$

where $u(\tau) = u_i\dfrac{t_i+1}{\tau+1}$. Finally, one obtains the formula

$$e(t_f) \approx u_i\Delta t\left(\frac{1+t_i}{1+t_f}\right)\left(-1/2\,\frac{(\Delta t+2+2\,t_i)}{(1+t_i)^2} + 1/2\,\frac{(\Delta t+2+2\,t_f)}{(1+t_f)^2}\right), \quad (22)$$

that predicts the global error at $t = t_f$ in terms of initial value u_i at $t = t_i$ and step size Δt.

4. Global error of Lie Trotter Splitting

In this section, the above mentioned procedure is modified to obtain the global error expansion of any splitting procedure combined with any ODE solver. For clarity, the derivation of the formulas are given for Lie-Trotter that is widely used in the literature. The extension to the higher splitting schemes can be done in a similar way. Another simplification is that one part is assumed to be solved exactly and the other part is solved numerically.

Consider the scheme

$$u_{n+1} = [R^A_{\Delta t}]^{(m)}(\varphi^B_h(u_n)), \quad (23)$$

indicating that the sub equation $u' = Bu$ is solved exactly in $[t_n, t_{n+1}]$ and the sub equation $u' = Au$ is solved by r^{th} order numerical method $R^A_{\Delta t}$ $(r > 1)$in $[t_n, t_{n+1}]$ with step size $\Delta t = \frac{h}{m}$ (m step in each sub interval). Such a procedure involves the following two local errors

$$\begin{aligned}\Delta t^r\mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u_n)) &= [R^A_{\Delta t}]^{(m)}(\varphi^B_h(u_n)) - \varphi^{A+B}_h(u_n) + \mathcal{O}(\Delta t^{r+1}),\\ h^2\mathfrak{le}_{\mathfrak{S}}(u_n) &= \varphi^A_h\circ\varphi^B_h(u_n) - \varphi^{A+B}_h(u_n) + \mathcal{O}(h^3),\end{aligned} \quad (24)$$

where $\mathfrak{le}_{\mathfrak{S}}(u_n) = \frac{1}{2}[B, A]$ is the coefficient of the leading term of the local splitting error (Lie Trotter in this case). $\mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u_n))$ should be considered as the global error of $R^A_{\Delta t}$ at $t_f = t_{n+1}$ starting from $t_i = t_n$ with step size Δt. This kind of global error terms of ODE solvers can be computed by method described in the motivation section. (See 20 in case of Euler method). The term $\mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u_n))$ also warns us to compute the error of the method $R^A_{\Delta t}$ at the point $\varphi^B_h(u_n)$ not at the point u_n. This is the key issue in the derivation error formulas for the splitting schemes.

Consider the partition $0 = t_0 < t_1 < t_2 < ... < T$ of the interval $[0, T]$. The global error is defined by

$$e_{n+1} = u_{n+1} - u(t_{n+1}) = [R^A_{\Delta t}]^{(m)} \circ \varphi^B_h(u_n) - \varphi^{(A+B)}_h(u(t_n)).$$

Adding and subtracting the terms $(\varphi^A_h \circ \varphi^B_h)(u_n)$ and $\varphi^{(A+B)}_h(u_n)$ yields

$$\begin{aligned} e_{n+1} =& [R^A_{\Delta t}]^{(m)} \circ \varphi^B_h(u_n) - (\varphi^A_h \circ \varphi^B_h)(u_n) \\ &+ (\varphi^A_h \circ \varphi^B_h)(u_n) - \varphi^{(A+B)}_h(u_n) \\ &+ \varphi^{(A+B)}_h(u_n) - \varphi^{(A+B)}_h(u(t_n)). \end{aligned}$$

Grouping the terms two by two and considering (24) and (14) one can write

$$\begin{aligned} e_{n+1} =& \Delta t^r \mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u_n)) + h^2 \mathfrak{le}_{\mathfrak{S}}(u_n) \\ &+ e_n \Psi(t_{n+1})\Psi^{-1}(t_n) + \mathcal{O}(h^3) + \mathcal{O}(\Delta t^{r+1}), \end{aligned} \tag{25}$$

where Ψ is the solution of variational equation that corresponds to the full equation (1).

After approximating the solution of this difference equation as a Riemann integral, the global error in the integral form is computed by

$$\begin{aligned} e(T) =& h\Psi(T) \int_0^T \Psi^{-1}(t+h)\{\frac{\Delta t^r}{h} \mathfrak{le}_{\mathfrak{R}}\left(\varphi^B_h(u(t))\right) \\ &+ \frac{1}{2}[B,A]\} dt + \mathcal{O}(h^2) + \mathcal{O}(\Delta t^{r+1} h^{-1}). \end{aligned} \tag{26}$$

5. Numerical Example

In this section, we will show the sharpness of the estimation of the global errors given by (26). As a test equation we choose

$$\frac{du}{dt} = -\frac{u(t)}{t+1} - u^2(t), \qquad u(0) = 1, \tag{27}$$

with exact solution

$$u(t) = \frac{1}{(ln(t+1)+1)(t+1)},$$

The sub equations

$$\frac{du}{dt} = -\frac{u(t)}{t+1}, \qquad u(0) = u_0,$$

and

$$\frac{du}{dt} = -u^2(t), \qquad u(0) = u_0,$$

have the exact solutions $u_A(t) = \dfrac{u_0}{t+1}$ and $u_B(t) = \dfrac{u_0}{1+tu_0}$, respectively. One also needs the variational flows of the equations (27) which can be given as

$$\Psi_{full}(t) = \frac{1}{(ln(t+1)+1)^2(t+1)}. \tag{28}$$

When the part A is solved by first order Euler method with step size $\Delta t = \frac{h}{m}$ in $[t_n, t_{n+1}]$ and part B proceeds in time by its exact flow, the numerical scheme is written as

$$u_{n+1} = [R^A_{\Delta t}]^{(m)} \circ \varphi^B_h(u_n). \tag{29}$$

Firstly the term $\mathfrak{le}_{\mathfrak{R}}\left(\varphi^B_h(u(t))\right)$ that is, the global error of Euler time stepping at $t+h$ starting from t with initial condition $\varphi^B_h(u(t))$ is needed. Luckily, the desired error formula, but with initial condition u_i, has been already derived in (22). Just only taking $t_i = t$, $t_f = t+h$ and $u_i = \varphi^B_h(u(t)) = \dfrac{u(t)}{1+hu(t)}$, one should see

$$\begin{aligned} \Delta t \mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u(t))) &= [R^A_{\Delta t}]^{(m)}(\varphi^B_h(u(t))) \\ &\quad -(\varphi^A_h \circ \varphi^B_h)(u(t)), \\ &= \frac{u(t)(1+t)}{2(1+hu(t))(1+t+h)}\left(\frac{(\Delta t+2+2\tau)}{-(1+t)^2} + \frac{(\Delta t+2+2t+h)}{(1+t+h)^2}\right). \end{aligned}$$

On the other hand, the leading coefficient of Lie Trotter splitting for (27) is found to be

$$\mathfrak{le}_{\mathfrak{s}}(u(t)) = \frac{1}{2}[B,A]u(t) = -\frac{1}{2}\frac{u(t)^2}{t+1}. \tag{30}$$

Finally, computing the integral (26) yields the estimation

$$\begin{aligned} e(T) \approx& h\Psi_{full}(T) \int_0^T \Psi^{-1}_{full}(\tau+h) \\ &\left\{\frac{1}{m}\mathfrak{le}_{\mathfrak{R}}(\varphi^B_h(u(\tau))) + \mathfrak{le}_{\mathfrak{S}}(u(\tau))\right\} d\tau. \end{aligned} \tag{31}$$

Table I presents the sharpness of the estimation (31) for various Δt and h at final $T = 20$.

Table 1. Comparison of actual errors and estimated errors of Lie Trotter at $T = 20$.

	$h=0.1$ Δt=0.01	$h=0.1$ Δt=0.001	$h=0.01$ Δt=0.001	$h=0.01$ Δt=0.0001
Actual error	-1.909e-4	-1.445e-4	-1.899e-5	-1.438e-5
Estimated error	-1.621e-4	-1.575e-4	-1.409e-5	-1.404e-5

6. Remarks and Conclusion

Splitting methods are becoming more and more popular among practitioners of numerical methods for differential equations. These methods provide separate treatments of simpler sub equations comparing to whole problem. However, the interaction of the errors caused by splitting procedure and time stepping methods applied to sub problems should be considered because the interaction might lead to order reduction in the long time run. Such a derived formula enables us to estimate error behavior of a method so that suitable solvers are employed. We choose a simple test problem to give a clear description of the integral formula. However in most of the applied problems, exact flows of full equation and sub equations are not available. In this case, derived formulas can be used to obtain reasonable error bounds by taking appropriate norms of the given expressions. However, in case of long time integration, asymptotic solutions and asymptotics expansions of the corresponding integrals that can be computed by some perturbation methods such as WKB give the long time error behaviors of the numerical methods. Indeed, the presented formulas are derived in search of suitable splitting algorithms for the long time integration of highly oscillatory non linear equations.

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