ACCUMULATION OF GLOBAL ERROR IN LIE GROUP METHODS FOR LINEAR ORDINARY DIFFERENTIAL EQUATIONS*

BOJAN OREL[†]

Abstract. In this paper we will investigate how the local errors accumulate to the global error in Lie group methods for linear ODEs. The concept of the local and global errors has to be redefined to fit in the framework of Lie groups and algebras. Formulas for tracking the global error are proposed and demonstrated on numerical examples.

Key words. ordinary differential equations, Lie group methods, global error, local error

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1. Introduction. Among all properties that come with the numerical solution of the initial value problem in ordinary differential equations (ODEs), small global error is usually the most important. If the global error of the computed solution is small enough on the interval of interest, other properties of the solution, such as correct asymptotic behavior, conservation of invariants, or retaining the geometric structure, become less important.

In this paper, we will focus on the case when the global error is small. The reason for this is at least twofold: first, as the numerical solution is close to the exact solution, we expect to observe similar dynamics of both solutions, while the behavior of the global error can be more unpredictable, when the distance between both solutions becomes larger. Second, the global error estimate can be used for the step-size control and large global error indicates that the step-size control failed. How large the global error can be before it is too large depends on the problem we are solving. In this paper we will consider the global error too large, if the exact and numerical solutions at a certain value of the independent variable cannot be covered with the same coordinate chart of the solution manifold.

The global error at a certain point t is usually a consequence of *local errors* committed at each step from the initial point up to t. How the local errors are accumulating into the global error depends on the differential equation, on the numerical method, and on the step-size selection. While we have some control over the size of the local errors during the process of solving an ODE, the global errors are usually beyond our reach.

The connection between global and local errors and possible methods for controlling the global error directly has inspired a lot of research in recent years. Highham [10] analyzed the connection between the error tolerance and the global error in the case of Runge-Kutta methods. Dormand et al. [6] proposed global embedding Runge-Kutta schemes for step-size control based on the estimation of the global error. Calvo et al. [1] studied methods for the global error estimation in the presence of the step-size selection mechanism for Runge-Kutta methods. Stuart [25] analyzed tolerance proportionality of the global error in Runge-Kutta methods. Viswanath [26] was concerned with situations where the usual exponential growth of the global error can be replaced by a less pessimistic one. Onumanyi et al. [22] studied global error estimates for the finite difference methods for initial and boundary value problems. Kulikov and Shindin were concerned with estimates for the local and global errors of linear multi-step methods with constant coefficients and fixed step-size in [17], and linear multi-step methods combined with Hermite type interpolation in [18]. Cao and Petzold [3]

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[†]Faculty of Computer and Information Science, University of Ljubljana, Tržaška 25, 1000 Ljubljana, Slovenia (bojan.orel@fri.uni-lj.si).

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proposed a method for the estimation of the global error, based on the approximate condition number, calculated from the solutions of the adjoint system of ODEs. Hundsdorfer [11] considered improved bounds for the global error for the solution of stiff ODEs computed by general linear methods. Chan and Murua [4] found out that the global errors of the solutions of periodic and integrable Hamiltonian problems grow linearly when solved by extrapolated symplectic or symmetric methods. Estep [7] obtained improved global error estimates, both a priori and a posteriori, for finite element methods and constructed an effective theory for global error control. Iserles [13] developed an integral formula for the leading term in a global error expansion of an arbitrary time stepping method, based on the variational equation, and applied this formula to highly oscillating ODEs. Niesen [21] combined the Alekseev-Gröbner lemma with the theory of modified equations to obtain an a priori estimate for the global error of Runge-Kutta methods. Schiff and Schnider [24] developed a method for error estimation for the computations in Lie groups.

In this paper, we will study the global error of Lie group methods for solving linear ODEs of Lie type. Section 2 is devoted to Lie group methods. In Section 3 the definition of the local and global errors in the Lie group setting is proposed and a recursive formula for the global error is given. The corresponding relations from the Lie algebra viewpoint are described in Section 4. In Section 5 the problem of tracking the global error is studied. Some numerical examples that confirm our theory are given in Section 6. The last section contains some conclusions and open questions.

2. Lie group methods. Let \mathcal{G} be a matrix Lie group, \mathfrak{g} its Lie algebra and $a : \mathbb{R} \times \mathcal{G} \to \mathfrak{g}$. The solution of the differential equation,

$$(2.1) Y' = a(t, Y)Y,$$

that satisfies the initial condition, $y(t_0) = y_0 \in \mathcal{G}$, is a function $y : \mathbb{R} \to \mathcal{G}$. Differential equations such as (2.1) are important in many different application areas; see [14].

Classical numerical methods such as Runge-Kutta and linear multi-step methods can be used to solve the equation (2.1) by embedding it in some Euclidean space \mathbb{R}^N , but its numerical solutions as a rule do not stay on \mathcal{G} [2]. This failure of classical methods to respect the structure of \mathcal{G} is the main reason that recently many new methods were proposed to overcome this difficulty, such as the Crouch-Grossman method [5], the Magnus method [15, 19], the Runge-Kutta-Munthe-Kaas method [20], and the Fer method [8, 12, 27].

All of these Lie group methods share a similar pattern: equation (2.1) is pushed to the corresponding Lie algebra \mathfrak{g} , solved there, and the solution is pulled back to the Lie group \mathcal{G} via the exponential map. It is true that the corresponding ODE in the Lie algebra \mathfrak{g} (the *dexpinv* equation; see [14]) is more complicated than (2.1), but this disadvantage is more than compensated for by the fact that \mathfrak{g} is a linear space, hence the numerical solution will stay in \mathfrak{g} and the exponential map will pull it back to \mathcal{G} .

In this paper we will consider numerical methods of the form

$$Y_{n+1} = e^{\hat{\sigma}(Y_n)} Y_n,$$

which includes the Magnus and Runge-Kutta-Munthe-Kaas methods for the solution of (2.1). The Crouch-Grossman and Fer methods can be formally brought to the same form by the Baker-Campbell-Hausdorff formula if the step-size is not too large. All these numerical methods generate a sequence Y_n of elements in \mathcal{G} , such that for a given sequence of real numbers,

$$(2.3) t_0 < t_1 < \dots < t_n < \dots,$$

 Y_i approximates the value of the true solution at t_i . We will assume that the step-sizes, $h_n =: t_n - t_{n-1}, n = 1, 2, ...$, are small enough so that the exact solution satisfies a similar relation,

(2.4)
$$Y(t_{n+1}) = e^{\sigma(Y(t_n))}Y(t_n).$$

Sometimes the mapping $\Phi_n : G \to G$ defined by $\Phi_n(X) = e^{\sigma(Y(t_n))}X$ is called the *exact* flow and the mapping $\Psi_n(X)$, defined by $\Psi_n(X) = e^{\hat{\sigma}(Y_n)}X$, the numerical flow. Note that the flow in equations (2.2) and (2.4) depends explicitly only on the starting point $(Y_n$ or $Y(t_n)$). The dependence of the flow on the independent variable t and the time-step is implicitly described by the index n and the the sequence of time-points (2.3).

3. Local and global errors. The global error is usually defined as a difference between the numerical and exact solution $Y_n - Y(t_n)$; cf. [9]. Since in the Lie group subtraction (and even addition) is not defined, we have to begin differently.

DEFINITION 3.1. The global error after the *n*-th step of the numerical method is the unique element $G_n \in \mathcal{G}$ such that $Y_n = G_n Y(t_n)$.

Also the usual definition of the local error cannot be literally extended to the Lie group setting.

DEFINITION 3.2. The local error at the (n + 1)st step is the unique element $L_{n+1} \in \mathcal{G}$ that satisfies the equation,

$$e^{\hat{\sigma}(Y_n)} = L_{n+1}e^{\sigma(Y_n)}.$$

REMARK 3.3. The global and local errors of Definitions 3.1 and 3.2 are close to unit elements in the Lie group. When addition is the group operation, both errors are close to zero; see Example 3.5.

In order to explore the dependence of the global error on the local errors, we commence with the definition of the global error after the (n + 1)st step: $G_{n+1}Y(t_{n+1}) = Y_{n+1}$. With the definition of the exact flow (2.4) and the numerical flow (2.2), we obtain

$$G_{n+1}e^{\sigma(Y(t_n))}Y(t_n) = e^{\hat{\sigma}(Y_n)}Y_n$$

Taking into account the definition of the global error at the *n*th step and the definition of the local error at the (n + 1)st step,

$$G_{n+1}e^{\sigma(Y(t_n))}Y(t_n) = L_{n+1}e^{\sigma(Y_n)}G_nY(t_n).$$

Right multiplying both sides of this relation by $(Y(t_n))^{-1}e^{-\sigma(Y(t_n))}$, we obtain the following result.

THEOREM 3.4. The global error obtained by using the numerical method (2.2) to solve the equation (2.1) with the exact solution (2.4) satisfies the recurrence relation,

(3.1)
$$G_{n+1} = L_{n+1}e^{\sigma(Y_n)}G_n e^{-\sigma(Y(t_n))}.$$

EXAMPLE 3.5. For $G = \mathbb{R}^d$, d a positive integer, and with addition as the group operation, we have the classical setting for the ODEs,

(3.2)
$$y' = f(t, y), \quad y(t_0) = y_0,$$

with $y : \mathbb{R} \to \mathbb{R}^d$ and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$. Now the definition for the global error (Definition 3.1) reduces to the familiar one (see for example [9]) $G_n = y_n - y(t_n)$ and the local error (Definition 3.2) to $L_{n+1} = e^{\hat{\sigma}(y_n)} - e^{\sigma(y_n)}$. The numerical flow is in this setting usually

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FIG. 3.1. The relation between the global errors at t_n and at t_{n+1} and the local error at t_{n+1} (A slice of the Lady Windermere's fan [9]).

denoted by $y_{n+1} = y_n + \widehat{\Phi}(y_n)$ and the exact flow by $y(t_{n+1}) = y(t_n) + \Phi(y(t_n))$. Note that both $\widehat{\Phi}(y_n)$ and $\Phi(y(t_n))$ explicitly depend on the value of the corresponding solution $(y_n \text{ or } y(t_n))$ even when equation (3.2) is linear. Equation (3.1) for the classical setting reads

$$G_{n+1} = L_{n+1} + G_n + \Phi(y_n) - \Phi(y(t_n));$$

see Figure 3.1. Under the assumption that the differential equation (3.2) satisfies the Lipschitz condition, the classical a priori bound for the global error [9, Theorem II.3] follows.

4. Local and global errors in the Lie algebra. In this section we will restrict our attention to linear differential equations of Lie type,

$$(4.1) Y' = a(t)Y.$$

For linear equations the exact flow $e^{\sigma(Y(t_n))}$ in (2.4) and the numerical flow $e^{\hat{\sigma}(Y_n)}$ in (2.2) do not depend on the solution value Y, so we will use the short-hand notation e^{σ_n} and $e^{\hat{\sigma}_n}$, respectively.

To analyze the qualitative behavior of the numerical methods on the Lie group \mathcal{G} as the step-size approaches 0, we have to exploit the properties of the corresponding Lie algebra \mathfrak{g} . Let us start this section by outlining the precise meaning of the phrase *order of approximation*. Suppose that two maps A and \tilde{A} from \mathbb{R} to \mathcal{G} are given.

DEFINITION 4.1. $\tilde{A}(h)$ is an order p approximant to A(h) as $h \to 0$ if and only if there exists an element $\bar{g} \in \mathfrak{g}$, different from 0 and independent of h (called the principle error term), such that $\tilde{A}(h) = G(h)A(h)$ with

$$G(h) = e^{g(h)}$$
 and $g(h) = \overline{g}h^p + \mathcal{O}(h^{p+1}).$

For the remainder of this section we will assume that the step-sizes are constant $h =: h_n$ for all n = 1, 2, ... To find a sufficient condition for an order of a numerical method, we

will first consider the behavior of the numerical method for $h \to 0$ and for some fixed $N \in \mathbb{N}$ (consequently $t_N \to t_0$). For each $n \leq N + 1$, there exists some $g_n \in \mathfrak{g}$ such that

$$(4.2) G_n = e^{g_n}.$$

and some $l_n \in \mathfrak{g}$ such that

$$(4.3) L_n = e^{l_n}.$$

Now the result of Theorem 3.4 can be rephrased as

(4.4)
$$G_{n+1} = e^{g_{n+1}} = e^{l_{n+1}} e^{\sigma_n} e^{g_n} e^{-\sigma_n}.$$

In the proof of our result below we need the Baker-Campbell-Hausdorff (BCH) formula from [14], which serves to define bch(F, G) := H.

LEMMA 4.2 (Baker-Campbell-Hausdorff). For sufficiently small $t \ge 0$, we have

$$\exp(tF)\exp(tG) = \exp(tH),$$

where H = bch(F, G) can be constructed from iterated commutators of F and G. The first few terms are

(4.5)
$$H = F + G + \frac{t}{2}[F,G] + \frac{t^2}{12}([F,[F,G]] + [G,[G,F]]) + \mathcal{O}(t^3).$$

LEMMA 4.3. For the linear differential equation, Y' = a(t)Y, $Y(t_0) = Y_0$, and the numerical solution, obtained by a method for which the local error has the property that for each n there exists some \bar{l}_n , different from 0 and independent of h, such that $l_n = \bar{l}_n h^{p+1} + O(h^{p+2})$, with fixed step-size, Y_n is an order p approximant to $Y(t_n)$ and

$$g_{n+1} = h^{p+1} \sum_{i=1}^{n+1} \bar{l}_i + \mathcal{O}(h^{p+2}).$$

Proof. First we observe that the exact and numerical flow are both of order 1 with respect to h, i.e., $\sigma(Y_n) = \mathcal{O}(h)$ and $\hat{\sigma}(Y_n) = \mathcal{O}(h)$. Since, for a linear differential equation, the flow is independent of Y, so $\sigma(Y_n) = \sigma(Y(t_n)) := \sigma_n$.

We will prove the lemma by induction. For the exact initial condition the global error after the first step equals $g_1 = l_1 = h^p \bar{l}_1 + \mathcal{O}(h^{p+1})$.

Next suppose that for some $n \leq N$ the relation $g_n = h^p \bar{g}_n + \mathcal{O}(h^{p+1})$ holds. Then, by applying repeatedly the BCH formula (4.5) to (4.4),

$$G_{n+1} = \underbrace{e^{l_{n+1}}e^{\sigma_n}}_{= e^{h^p \bar{l}_{n+1} + \sigma_n + \mathcal{O}(h^{p+1})}} \underbrace{e^{g_n e^{-\sigma_n}}}_{e^{h^p \bar{g}_n - \sigma_n + \mathcal{O}(h^{p+1})}}_{= e^{h^p (\bar{l}_{n+1} + \bar{g}_n) + \mathcal{O}(h^{p+1})}.$$

From this recursion the statement of the lemma follows easily. \Box

REMARK 4.4. In the proof of Lemma 4.3, we have tacitly assumed that the exact and numerical solution for all points of interest belong to the same coordinate chart of the group G.

More interesting than the behavior of the global error G_n for fixed n as $h \to 0$ is the behavior of G_n as $h \to 0$ and nh = T is fixed (hence $n \to \infty$). The length T of the interval

should be small enough so that the exact and the numerical solution will stay on the same coordinate chart of G for all $t \in [t_0, t_0 + T]$. Let the basic mesh be defined by the sequence of time-points $t_i = t_0 + \frac{i}{n}T$. From Lemma 4.3 it is clear that

$$g_n = \frac{T}{n} \left(h^p \sum_{i=1}^n \bar{l}_i + \mathcal{O}(h^{p+1}) \right).$$

Introducing the average principal local error term \tilde{l}_n as

$$\tilde{l}_n = \frac{1}{n} \sum_{i=1}^n \bar{l}_i,$$

this can be simplified to

$$g_n = h^p T \tilde{l}_n + \mathcal{O}(h^{p+1}).$$

The existence of the limit $\tilde{l} = \lim_{h \to 0} \tilde{l}_n$ is guaranteed if the principal local error terms, \bar{l}_i , corresponding to the point $t_i = t_0 + \frac{i}{n}T$ smoothly depend on i as $n \to \infty$. Thus we have proved the following result.

THEOREM 4.5. For fixed T > 0 let h > 0 be small enough so that the local error L_{n+1} , the global errors G_n and G_{n+1} , and the numerical flow e^{σ_n} belong to the same coordinate chart of G for every $t_n \in [t_0, t_0 + T]$. The numerical solution of a linear differential equation $Y' = a(t)Y, Y(t_0) = Y_0$ at the fixed point $t_0 + T$ by the numerical method (2.2) with the local error of order p+1 (as in Lemma 4.3) with equal step-sizes is an order p approximation to the exact solution $Y(t_0 + T)$.

On the basis of this result the following definition is justified.

DEFINITION 4.6. The numerical method (2.2) has order p iff there exists an element $\bar{l}_n \in \mathfrak{g}$, different from 0 and independent of h, such that the local error satisfies

$$L_n = e^{l_n} \quad \text{with} \quad l_n = \bar{l}_n h^{p+1} + \mathcal{O}(h^{p+2}).$$

5. Tracking the global error. To compute the size of the global error, we will exploit the result stated in Theorem 3.4,

(5.1)
$$G_{n+1} = L_{n+1} e^{\sigma(Y_n)} G_n e^{-\sigma(Y(t_n))}.$$

This equation enables us to follow the global error from one step to another, if we are able to compute a reliable estimation of the local error L_{n+1} . From the definition of the local error

$$L_{n+1} = e^{l_{n+1}} = e^{\hat{\sigma}_n} e^{-\sigma_n}.$$

Before applying the Baker-Campbell-Hausdorff formula, we should notice the connection between σ_n and $\hat{\sigma}_n$: for the method of order p there is $\delta_n \in \mathfrak{g}$ with $\delta_n = \mathcal{O}(h^{p+1})$, such that $\hat{\sigma}_n = \sigma_n + \delta_n$. Therefore,

(5.2)
$$e^{l_{n+1}} = e^{\sigma_n + \delta_n} e^{-\sigma_n} = e^{\delta_n - [\delta_n, \sigma_n]/2 + \mathcal{O}(h^{p+3})}.$$

Thus the cost of the tracking the global error according to formulas (3.1) and (5.2) amounts to one additional commutator and two additional exponents, provided we have at our disposal an approximation of the exact flow σ_n , which is at least 2 orders more accurate than $\hat{\sigma}_n$.

Such an approximation can be computed either as

- 1. numerical flow of the method of order p + 2, or
- 2. using one step of Richardson's extrapolation [23], or
- 3. using k steps of pth order method with step-size h/k for some $k \ge 4$, or
- 4. some other appropriate way.

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FIG. 6.1. The numerical solution of the Airy equation (6.1) on the whole interval [0, 200] (above) and on interval [195, 200] (below).

6. Examples.

Airy equation. We applied the technique for tracking the global error to the Airy equation,

(6.1)
$$Y' = a \cdot Y; \quad a = \begin{bmatrix} 0 & 1 \\ -t & 0 \end{bmatrix}; \quad Y : \mathbb{R} \to \mathbb{R}^2,$$

with initial condition Y(0) = I (the identity matrix), solved by the Magnus method. Since the trace of a is 0, the matrix $a \in \mathfrak{sl}(2, \mathbb{R})$ (Lie algebra consisting of all 2×2 real matrices with vanishing trace) and the solution $Y(t) \in SL(2, \mathbb{R})$ (special linear group, consisting of 2×2 real matrices with determinant equal to 1) for all t, provided the initial value $Y(0) = Y_0 \in SL(2, \mathbb{R})$.

 $TABLE \ 6.1$ The accuracy of the global error estimate for the Airy equation on the interval [0,1000].

step-size	$\max \log(Y_n(Y(t_n)^{-1})) $	$\max \log(G_n) $
2^{-3}	$1.7 \cdot 10^{-1}$	$2.1 \cdot 10^{0}$
2^{-4}	$1.5 \cdot 10^{-4}$	$1.6 \cdot 10^{-4}$
2^{-5}	$8.2 \cdot 10^{-6}$	$8.8 \cdot 10^{-6}$
2^{-6}	$5.0 \cdot 10^{-7}$	$5.1 \cdot 10^{-7}$
2^{-7}	$3.1 \cdot 10^{-8}$	$3.1 \cdot 10^{-8}$
2^{-8}	$2.0 \cdot 10^{-9}$	$1.9 \cdot 10^{-9}$



FIG. 6.2. True (solid) and estimated (dashed) errors for the Airy equation, computed by a fourth order Magnus method with step-size $h = 2^{-4}$ on [0, 200]. Only the interval [195, 200] is shown.

We computed the solution by a fourth order Magnus method using the σ_n computed by a sixth order Magnus method as an approximant for the exact flow and estimated the global error of the fourth order numerical solution using formulas (3.1) and (5.2). The numerical solution is plotted in Figure 6.1, above on the whole interval [0, 200], below only on the interval [195, 200]. The estimated global error was then compared to the exact global error.

The results of the experiments are summarized in Table 6.1. It is apparent that for reasonably small step-sizes, $h \le 2^{-4}$, the estimated error resembles the true global error remark ably well even on very long time intervals. It has to be noted that the difference between the true and the estimated errors for the smallest step-size, 2^{-8} , is inaccurate due to the limited precision. Figure 6.2 confirms the good agreement between the true and estimated global errors even on a very long interval with a relatively large step-size for a highly oscillatory solution of the Airy equation. Note also that the peaks in the global error correspond to the extreme values of the solution.

Coupled oscillator equation. Equations describing a system of four coupled oscillators [16], (6.2)

$$y' = \begin{bmatrix} 0 & t \sin \frac{\pi t}{4} & 0 & 0 \\ -t \sin \frac{\pi t}{4} & 0 & t \sin \frac{\pi t}{2} & 0 \\ 0 & -t \sin \frac{\pi t}{2} & 0 & t \sin \frac{3\pi t}{4} \\ 0 & 0 & -t \sin \frac{3\pi t}{4} & 0 \end{bmatrix} y, \qquad t \ge 0, \qquad y(0) = I,$$

present a considerable problem for classical ODE methods. Since the matrix of the system is skew-symmetric, the solution of this equation evolves in $SO(4, \mathbb{R})$, the special orthogonal group consisting of 4×4 real orthogonal matrices with determinant equal to 1.

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FIG. 6.3. True (solid) and estimated (dashed) errors for the coupled oscillator equation (6.2), computed by a fourth order Magnus method with step-size $h = 2^{-6}$ on [0, 40]. Only the interval [30, 40] is shown.

step-size	$\max \log(Y_n(Y(t_n)^{-1})) $	$\max \log(G_n) $
2^{-4}	$1.0 \cdot 10^{-2}$	$8.9 \cdot 10^{-2}$
2^{-5}	$6.6 \cdot 10^{-4}$	$5.9 \cdot 10^{-4}$
2^{-6}	$4.2 \cdot 10^{-5}$	$4.1 \cdot 10^{-5}$
2^{-7}	$2.6 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$
2^{-8}	$1.6 \cdot 10^{-7}$	$1.6 \cdot 10^{-7}$
2^{-9}	$1.0 \cdot 10^{-8}$	$1.0 \cdot 10^{-8}$
2^{-10}	$6.4 \cdot 10^{-10}$	$6.4 \cdot 10^{-10}$
2^{-11}	$4.0 \cdot 10^{-11}$	$4.0 \cdot 10^{-11}$

TABLE 6.2 The accuracy of the global error estimate for the coupled oscillator equation on the interval [0, 40].

The fourth order Magnus method was used to solve equation (6.2). The accurate solution and the approximant to the exact σ_n were computed by the Magnus method of order four with the step-size equal to one tenth of the step-size used to compute the numerical solution. The global error was estimated according to equations (3.1) and (5.2) and compared to the difference between the numerical (computed with step-size h) and accurate (computed with step-size h/10) solutions.

The results of numerical experiments with the system (6.2) are summarized in Table 6.2. It is easily observed from these data that the estimate of the global error follows closely the difference between the approximate and accurate solution for the step-sizes $h \le 2^{-4}$. Again, the inferior behavior of the global error estimate for the step-size $h = 2^{-11}$ is a consequence

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of limited precision. The good agreement between the true global error and its estimate is evident also from Figure 6.3.

7. Conclusions. We investigated the connection between global and local errors in Lie group methods for computing numerical solutions of linear ordinary differential equations. For this purpose, the terms *local* and *global error* had to be reformulated to fit the framework of the Lie group. The results for the global error are necessarily local. They are valid only in some neighborhood of the exact solution. It was shown that for linear differential equations, the corresponding Lie algebra can be used for quantitative error analysis, as long as the exact and the numerical solution belong to the same coordinate chart. It was shown how an approximation for the global error can be computed. This can be exploited in constructing an adaptive algorithm for solving ODEs with global error control.

REFERENCES

- M. CALVO, D. J. HIGHAM, J. I. MONTIJANO, AND L. RÁNDEZ, Global error estimation with adaptive explicit Runge-Kutta methods, IMA J. Numer. Anal., 16 (1996), pp. 47–63.
- [2] M. P. CALVO, A. ISERLES, AND A. ZANNA, Runge-Kutta methods on manifolds, in Numerical Analysis: A. R. Mitchell's 75th Birthday Volume, G. A. Watson and D. F. Griffiths, eds., World Scientific, Singapore, 1996, pp. 57–70.
- [3] Y. CAO AND L. PETZOLD, A posteriori error estimation and global error control for ordinary differential equations by the adjoint method, SIAM J. Sci. Comput., 26 (2004), pp. 359–374.
- [4] R. P. K. CHAN AND A. MURUA, Extrapolation of symplectic methods for Hamiltonian problems, Appl. Numer. Math., 34 (2000), pp. 189–205.
- [5] P. E. CROUCH AND R. GROSSMAN, Numerical integration of ordinary differential equations on manifolds, J. Nonlinear Sci., 3 (1993), pp. 1–33.
- [6] J. R. DORMAND, J. P. GILMORE, AND P. J. PRINCE, Globally embedded Runge-Kutta schemes, Ann. Numer. Math., 1 (1994), pp. 97–106.
- [7] D. ESTEP, A posteriori error bounds and global error control for approximation of ordinary differential equations, SIAM J. Numer. Anal., 32 (1995), pp. 1–48.
- [8] F. FER, *Résolution de l'équation matricielle* dU/dt = pU par produit infini d'exponentielles matricielles, Acad. Roy. Belg. Bull. Cl. Sci. (5), 44 (1958), pp. 818–829.
- [9] E. HAIRER, S. P. NØRSETT, AND G. WANNER, Solving Ordinary Differential Equations I, Springer, Berlin, 1987.
- [10] D. J. HIGHAM, The tolerance proportionality of adaptive ODE solvers, J. Comput. Appl. Math., 45 (1993), pp. 227–236.
- W. HUNDSDORFER, On the error of general linear methods for stiff dissipative differential equations, IMA J. Numer. Anal., 14 (1994), pp. 363–379.
- [12] A. ISERLES, Solving linear ordinary differential equations by exponentials of iterated commutators, Numer. Math., 45 (1984), pp. 183–199.
- [13] A. ISERLES, On the global error of discretization methods for highly-oscillatory ordinary differential equations, BIT, 42 (2002), pp. 561–599.
- [14] A. ISERLES, H. MUNTHE-KAAS, S. P. NØRSETT, AND A. ZANNA, Lie group mathods, Acta Numer, 9 (2000), pp. 215–365.
- [15] A. ISERLES AND S. P. NØRSETT, On the solution of linear differential equations in Lie groups, Phil. Trans. Royal Society A, 357 (1999), pp. 983–1020.
- [16] A. ISERLES, S. P. NØRSETT, AND A. F. RASMUSSEN, *Time-symmetry and high-order Magnus methods*, Appl. Numer. Math., 39 (2001), pp. 379–401.
- [17] G. Y. KULIKOV AND S. K. SHINDIN, On the efficient computation of asymptotically sharp estimates for local and global errors in multistep methods with constant coefficients, Zh. Vychisl. Mat. Mat. Fiz., 44 (2004), pp. 840–861.
- [18] ——, On multistep interpolation-type methods with automatic control of global error, Zh. Vychisl. Mat. Mat. Fiz., 44 (2004), pp. 1388–1409.
- [19] W. MAGNUS, On the exponential solution of differential equations for a linear operator, Comm. Pure Appl. Math., 7 (1954), pp. 649–673.
- [20] H. MUNTHE-KAAS, Runge-Kutta methods on Lie groups, BIT, 38 (1998), pp. 92–111.
- [21] J. NIESEN, A priori estimates for the global error committed by Runge-Kutta methods for a nonlinear oscillator, LMS J. Comput. Math., 6 (2003), pp. 18–28.

- [22] P. ONUMANYI, U. W. SIRISENA, AND S. N. JATOR, Continuous finite difference approximations for solving differential equations, Int. J. Comput. Math., 72 (1999), pp. 15–27.
- [23] B. OREL, Extrapolated magnus methods, BIT, 41 (2001), pp. 1089-1010.
- [24] J. SCHIFF AND S. SCHNIDER, Lie groups and error analysis, J. Lie Theory, 11 (2001), pp. 231–254.
- [25] A. M. STUART, Probabilistic and deterministic convergence proofs for software for initial value problems, Numer. Algorithms, 14 (1997), pp. 227–260.
- [26] D. VISWANATH, Global errors of numerical ODE solvers and Lyapunov's theory of stability, IMA J. Numer. Anal., 21 (2001), pp. 387–406.
- [27] A. ZANNA, On the numerical solution of isospectral flows, PhD thesis, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK, 1998.