EXTRAPOLATION METHODS IN LIE GROUPS

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ABSTRACT. The numerical solution of differential equations on Lie groups by extrapolation methods is investigated. The main principles of extrapolation for ordinary differential equations are extended on the general case of differential equations in noncommutative Lie groups. An asymptotic expansion of the global error is given. A symmetric method is given and quadratic asymptotic expansion of the global error is proved. The theoretical results are verified by numerical experiments.

KEY WORDS: Lie group, geometric integration, extrapolation methods.

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1. INTRODUCTION

We are concerned with the numerical solution of initial value problems for differential equations in a Lie group G. Such a differential equation in a Lie group is given by

$$y' = f(y)|_y, \quad f : G \to \mathfrak{g}. \tag{1}$$

The solution is a curve $y : [t_0, t_e] \to G$. Equation (1) says that the tangent vector $y'(t) \in TG|_{y(t)}$ on the curve y equals the vector field $f(y(t))$ at the point $y(t)$. The vector field $f(y(t))$ is given by the map $f : G \to \mathfrak{g}$ from the Lie group into the Lie algebra. In this paper we consider the Lie algebra as the set of right invariant vectorfields, i.e., we have $f(y)|_z = dR_z(f(y)|_e)$ where dR_z is the differential of right translation.

For the matrix group $G = GL(n)$ we adopt the notation $y(t) = Y(t)$ and $f(y)|_e = A(Y)$. Equation (1) becomes

$$Y'(t) = A(Y(t)) \cdot Y(t).$$

There are naturally several differences between differential equations in $\mathbb{R}^n$ and in Lie groups. The differences are best understood if we consider an affine manifold and the corresponding set of translations as a special case (the linear, commutative case) of a Lie group with corresponding Lie algebra. The Lie group (affine manifold) $\mathbb{R}^n$ has the set of translations as Lie algebra, and this is isomorphic to $\mathbb{R}^n$. In the nonlinear case, the Lie algebra may be viewed as a set of transformations, too, namely the flow of right invariant vector fields. In general this set of transformations is not isomorphic to the Lie group.

The last point is clearly the main difference between differential equations in $\mathbb{R}^n$ and in a Lie group: in $\mathbb{R}^n$ the Lie group can be identified with the Lie algebra — but in the general nonlinear noncommutative case they can not be identified. The distance between two elements of the Lie group can only be measured in the Lie algebra – it is a real valued vector space; the Lie group is no real valued vector space. Therefore we have to represent the error in the numerical solution by the flow of right invariant vectorfields.

Our method will produce a solution that stays automatically in the Lie group under the following proposition: We approximate the flow of the differential equation by an element of the Lie algebra. This element of the Lie algebra is computed as a linear combination of function calls $f(y)$ at points $y \in G$ and lie brackets of these function calls. Such a method maintains automatically every invariant subgroup of the differential equation.

Differential equations on Lie groups occur in several applications. The motion of multibody systems occuring in robotics [3] can be viewed this way. Further applications are found in molecular dynamics [2] and numerical linear algebra [1].

Differential equations on Lie groups have been investigated by several authors. Munthe-Kaas developed a class of Runge-Kutte methods on Lie groups. He has shown that the Butcher theory applies to commutative groups [4]. He gives correction functions for general Runge-Kutta methods to be applied on noncommutative Lie groups [5, 6]. Iserles, Marthinsen and Nørsett [7] consider linear differential equations with time dependent coefficients as differential equations in Lie groups. They develop an integration scheme that is based upon the magnus series expansion of the exact solution. Calvo, Iserles and Zanna investigate isospectral flows [12].

We restrict our investigations to matrix Lie groups. There is no loss in generality in this approach as long as we are concerned with finite dimensional groups because of Ados theorem:

Theorem 1.1. *Let $\mathfrak{g}$ be a finite dimensional Lie algebra. Then $\mathfrak{g}$ is isomorphic to a subalgebra of $\mathfrak{gl}(n)$ for some n.*

The main tool for our analysis is the Baker-Campbell-Hausdorff formula (BCH-formula, see [14] for details)

(2)
$$\operatorname{Exp}(X)\operatorname{Exp}(Y) = \operatorname{Exp}\left(\sum_{i=1}^{\infty} c_i(X,Y)\right) \text{ with}$$

(3)
$$\begin{aligned} c_1(X,Y) &= X + Y, \\ (n+1)c_{n+1}(X,Y) &= \frac{1}{2}[X - Y, c_n(X,Y)] \\ &\quad + \sum_{1\le p\le n/2} K_{2p} \sum_{\substack{k_1,\dots,k_{2p}>0 \\ k_1+\dots+k_{2p}=n}} [c_{k_1}(X,Y),[\dots,[c_{k_{2p}}(X,Y),X+Y]\dots], \end{aligned}$$

where Exp is the matrix exponential. The series above converges absolutely in a neighborhood of zero. The matrix exponential corresponds to the exponential map in the more abstract setting of general Lie groups.

Furthermore the flow of rightinvariant (resp. leftinvariant) vectorfields is given by multiplication from the left (resp. right) with the matrix exponential. Therefore we will use the same notation for both.

2. Local and global error

We extend the wellknown concepts of local and global error from the theory of ordinary differential equations to differential equations on Lie groups. Most definitions extend straightforwardly by replacing additions by the flow of vector fields, but care has been taken to guarantee the basic lemmata from the theory of ordinary differential equations.

Definition 2.1. *A one-step method for the differential equation* (1) *on a Lie group computes an approximation* y_{n+1} *for* $y(t_{n+1})$ *via*

$$y_{n+1} = \mathrm{Exp}(h\Phi(t_n, y_n, h; f))y_n. \tag{4}$$

The function Φ *is called the increment function.*

We say shortly Φ to denote the one-step method with increment function Φ.

Definition 2.2. *A one-step method is called C-stable on the equation* (1)*, if there exist constants* $C, L, h_0 > 0$ *such that for* $h \leq h_0$ *and initial values* $\eta, \tilde{\eta}$ *with*

$$\tilde{\eta} = \mathrm{Exp}(k)\eta, \quad k \in \mathfrak{g}, \|k\| \leq Ch, C > 0,$$

there exists $k^* \in \mathfrak{g}$ *with*

$$\begin{aligned} \mathrm{Exp}(h\Phi(t, \tilde{y}, h; f))\tilde{\eta} &= \mathrm{Exp}(k^*)\,\mathrm{Exp}(h\Phi(t, y, h; f))\eta \\ \|k^*\| &\leq (1 + Ch)\|k\|. \end{aligned}$$

Definition 2.3. *The local error* $le(t, y, h)$ *of a one-step method is defined as*

$$y_{n+1} = \mathrm{Exp}(le(t_n, y_n, h))y(t_n + h) \tag{5}$$

where y_{n+1} *is the numerical solution after one step with stepsize* h *and initial value* $y_n = y(t_n)$ *at* $t = t_n$.

If the flow of the exact solution is given by $y(t+h) = \mathrm{Exp}(h\nu(t, y(t), h))y(t)$ and the leading term of the local error is given by $d_{p+1}(t)h^{p+1}$ then the increment function satisfies

$$h\Phi(t, y(t), h) = h\nu(t, y(t), h) + d_{p+1}(t)h^{p+1} + \mathcal{O}\left(h^{p+2}\right) \tag{6}$$

Definition 2.4. *The global error* $e(t, h)$ *of the one-step method* Φ *(applied with initial value* $y_0 = y(t_0)$*) is given by*

$$y_n = \mathrm{Exp}(e(t_n, h))y(t_n) \tag{7}$$

We can formulate the main theorem of this section:

Theorem 2.5. *Let* Φ *be a C-stable one-step method. If the local error satisfies*

$$le(t, y(t), h) = \mathcal{O}\left(h^{p+1}\right)$$

then the global error satisfies

$$e(t, h) = \mathcal{O}\left(h^{p}\right).$$

Proof. The proof is straightforwardly obtained by adapting the Lady Windermere's Fan technique from ordinary differential equations. We consider sequences $y_i^{(k)}$ of numerical solutions starting with $y_k^{(k)} = y(t_k)$. The assumption on the local error gives

$$y_k^{(k-1)} = \mathrm{Exp}(\mathcal{O}\left(h^{p+1}\right))y_k^{(k)}.$$

With C-stability we have

$$y_n^{(k-1)} = \operatorname{Exp}(\mathcal{O}\left(h^{p+1}\right))y_n^{(k)}$$
$$y_n = \left(\prod_{k=1}^{n} \operatorname{Exp}(\mathcal{O}\left(h^{p+1}\right))\right) y(t_n)$$

With the BCH-formula the assertion follows. □

3. Asymptotic expansion of the global error

We start with a one-step method in a Lie group for the differential equation

$$y' = f(y)|_y .$$

The method is given by an incrementation function Φ via

$$y_{n+1} = \operatorname{Exp}(h\Phi(t_n, y_n, h))y_n. \tag{8}$$

Theorem 3.1. *The numerical solution computed by an one-step method Φ of order p with stepsize h possesses an asymptotic expansion of the form*

$$y_n = \operatorname{Exp}(h^p e_p(t_n)) \operatorname{Exp}(h^{p+1} e_{p+1}(t_n)) \dots \operatorname{Exp}(h^N e_N(t_n)) \operatorname{Exp}(\mathcal{O}\left(h^{N+1}\right))y(t_n), \tag{9}$$

where $y(t_n)$ is the exact solution at t_n and e_i are smooth mappings $[t_0, t_e] \to \mathfrak{g}$.

Proof. We construct a sequence of approximations $y_n^{(i)}$ of order $p+i$ which satisfy

$$y_n^{(0)} = y_n \tag{10}$$
$$y_n^{(i+1)} = \operatorname{Exp}(-h^{p+i} e_{p+i}(t_n))y_n^{(i)}. \tag{11}$$

To guarantee order $p+i$ for $y_n^{(i)}$ we investigate the one-step methods $\Phi^{(i)}$ that generate the $y_n^{(i)}$:

$$\begin{aligned}
\operatorname{Exp}(h\Phi^{(i+1)}(t_n, y_n^{(i+1)}, h))y_n^{(i+1)} &= y_{n+1}^{(i+1)} \\
&= \operatorname{Exp}(-h^{p+i} e_{p+i}(t_n+h))y_{n+1}^{(i)} \\
&= \operatorname{Exp}(-h^{p+i} e_{p+i}(t_n+h)) \operatorname{Exp}(h\Phi^{(i)}(t_n, y_n^{(i)}, h))y_n^{(i)} \\
&= \operatorname{Exp}(-h^{p+i} e_{p+i}(t_n+h)) \\
&\quad \cdot \operatorname{Exp}(h\Phi^{(i)}(t_n, \operatorname{Exp}(h^{p+i} e_{p+i}(t_n)y_n^{(i+1)}, h))) \\
&\quad \cdot \operatorname{Exp}(h^{p+i} e_{p+i}(t_n))y_n^{(i+1)}.
\end{aligned}$$

This gives recursive expressions for $\Phi^{(i)}$:

$$\Phi^{(0)} = \Phi \tag{12}$$
$$\operatorname{Exp}(h\Phi^{(i+1)}(t, y, h)) = \operatorname{Exp}(-h^{p+i} e_{p+i}(t+h)) \cdot \tag{13}$$
$$\operatorname{Exp}(h\Phi^{(i)}(t, \operatorname{Exp}(h^{p+i} e_{p+i}(t))y, h)) \operatorname{Exp}(h^{p+i} e_{p+i}(t)). \tag{14}$$

We show that e_{p+i} can be choosen in such a way that $\Phi^{(i+1)}$ has order $p+i+1$. It is sufficient to do this for $i=0$. Let the local error of the method be

$$le(t, y(t), h) = d_{p+1} h^{p+1} + \mathcal{O}\left(h^{p+2}\right).$$

We expand Φ in a Taylor series by the BCH-formula:

$$\begin{aligned} h\Phi^{(1)}(t,y(t),h) =& - h^p e_p(t+h) + h\Phi(t, \mathrm{Exp}(h^p e_p(t))y(t),h) + h^p e_p(t) \\ &+ \frac{1}{2}([-h^p e_p(t+h), h\Phi(\dots)] + [-h^p e_p(t+h), h^p e_p(t)] + [h\Phi(\dots), h^p e_p(t)]) \\ &+ \mathcal{O}\left(h^{p+2}\right) \\ =& - h^{p+1} e_p'(t) + h\Phi(t, \mathrm{Exp}(h^p e_p(t))y(t),h) \\ &+ [h\Phi(t, \mathrm{Exp}(h^p e_p(t))y(t),h), h^p e_p(t)] + \mathcal{O}\left(h^{p+2}\right) \\ =& - h^{p+1} e_p'(t) + h\Phi(t, \mathrm{Exp}(h^p e_p(t))y(t),h) + [hf(y(t)), h^p e_p(t)] \\ &+ \mathcal{O}\left(h^{p+2}\right) \end{aligned}$$

Because the method Φ is of order at least 1, we have $\Phi(t,y,h) = f(y) + \mathcal{O}(h)$. We consider Φ as a function of $y \in G$ under the flow of the right invariant vectorfield $h^p e_p(t)$ and expand it in a Lie series:

$$\begin{aligned} \Phi(t, \mathrm{Exp}(h^p e_p(t))y(t),h) =& \Phi(t,y(t),h) + h^p e_p(t)[\Phi(t,\cdot,h)]|_{y(t)} + \mathcal{O}\left(h^{2p}\right) \\ =& \Phi(t,y(t),h) + h^p e_p(t)[f]|_{y(t)} + \mathcal{O}\left(h^{p+1}\right). \end{aligned}$$

Using (6) we obtain:

$$h\Phi^{(1)}(t,y(t),h) = h\nu(t,y(t),h) + d_{p+1}(t)h^{p+1} - e_p'(t)h^{p+1} \tag{15}$$

$$+ e_p(t)[f]|_{y(t)} h^{p+1} + [f(y(t)), e_p(t)]h^{p+1} + \mathcal{O}\left(h^{p+2}\right) \tag{16}$$

The method $\Phi^{(1)}$ is of order $p+1$ if we choose e_p as the solution of the initial value problem

$$e_p'(t) = e_p(t)[f]|_{y(t)} + [f(y(t)), e_p(t)] + d_{p+1}(t) \tag{17}$$

$$e_p(0) = 0. \tag{18}$$

This procedure can be repeated to have $\Phi^{(i)}$ of order $p+i$ for $i > 1$. Note that we assume the local error of $\Phi^{(i-1)}$ being $\mathcal{O}\left(h^{p+i-1}\right)$ for initial values on the exact solution only. This is exactly what we have proved for $\Phi^{(i)}$ in the case $i = 0$.

Further the C-stability of $\Phi^{(i)}$ is implied by the C-stability of Φ. This gives order $p+N$ for $\Phi^{(n)}$ and the asserted expansion of the global error. □

4. Extrapolation for one-step methods

Let be given a one-step method Φ for the differential equation (1).

We compute approximations $y_{n+1,i}$ with n_i steps with stepsizes $h_i = H/n_i$. We denote the increment function in the j-th step by $\Phi_{i,j}$. We denote the corresponding increment function for all these n_i steps by Φ_i. It is given by

$$\mathrm{Exp}(H\Phi_i) = \mathrm{Exp}(h_i\Phi_{i,n_i}) \dots \mathrm{Exp}(h_i\Phi_{i,1}).$$

For our extrapolation procedure it is necessary to compute this increment function up to sufficient accuracy.

We apply the BCH-formula on the asymptotic expansion of the global error

$$\mathrm{Exp}(H\Phi_i) = \mathrm{Exp}(h_i^p e_p(t_{n+1})) \dots \mathrm{Exp}(h_i^p e_p(t_{n+1}))\, \mathrm{Exp}(\mathcal{O}\left(H^{N+1}\right))\, \mathrm{Exp}(H\nu(t,y_n,H))$$

to get

$$H\Phi_i = H\nu(t, y_n, H) + h_i^p e_p(t_{n+1}) + \sum_{k=p+1}^{N} h_i^k \tilde{e}_k(t_{n+1}) + \mathcal{O}\left(H^{N+1}\right),$$

where the commutators of the BCH-formula are contained either in the $h^k\tilde{e}_k$ terms or in the $\mathcal{O}\left(h^{N+1}\right)$ term. It is clear once the Φ_i are computed up to a sufficient order we can extrapolate as in the case of ordinary differential equations.

It remains to compute the Φ_i. This can be done by the BCH-formula again, where the commutators have to be included up to the desired order. We say that a simple Lie bracket is a commutator of first order, where an iterated commutator like $[X, [Y, Z]]$ is called a commutator of second order, and so on.

In order to extrapolate up to order p we must compute $h\Phi_i$ up to order p. Because $\Phi_{i,j} = f(y_n) + \mathcal{O}(H)$ we have

$$\begin{aligned} [h_i\Phi_{i,j}, h_i\Phi_{i,l}] &= \mathcal{O}\left(H^3\right) \\ [h_i\Phi_{i,j_1}, \ldots, h_i\Phi_{i,j_k}] &= \mathcal{O}\left(H^{k+1}\right). \end{aligned}$$

So in general we have to compute the iterated commutators up to order $p-2$. There is a special case to be mentioned — the commutators of order 2 occuring in the BCH formula:

$$[X, X, Y] + [Y, Y, X] = [X - Y, [X, Y]] = [X - Y, [X - Y, Y]].$$

Because we have $X, Y = \mathcal{O}(H)$ but $X - Y = \mathcal{O}(H^2)$, we only need to include commutators up to order 1 for a method of order 4.

If we interprete the commutators as correction functions, we see that we have a similar structure in the correction function as in the RK-MK methods. There are no corrections neccessary for order 2, we need commutators of at least first order for order 3 and higher.

To implement the extrapolation procedure we use the harmonic sequence $n_i = i$. There are no corrections needed for $h\Phi_1$. We get $h\Phi_2$ by the BCH-formula, applied on $h\Phi_{2,2}$ and $h\Phi_{2,1}$, where only commutators up to order $p-2$ have to be included. To compute the $h_i\Phi_i$ we iterate the procedure for the computation of $h_2\Phi_2$ above.

5. Symmetric methods and quadratic expansion

Extrapolation is even more powerful when the basic method possesses an quadratic expansion of the global error. The GBS algorithm uses the explicit midpoint rule for extrapolation. This method is symmetric and therefore possesses a quadratic expansion of the global error. The same is valid in Lie groups.

We show that the explicit midpoint rule is symmetric. The explicit midpoint rule on Lie groups is given by

$$\begin{aligned} y_1 &= \mathrm{Exp}(hf(y_0))y_0 \\ y_{n+1} &= \mathrm{Exp}(2hf(y_n))y_{n-1} \end{aligned} \tag{19}$$

Our proof is an adaptation of Stetters [13] proof of the symmetry of the explict midpoint rule for ordinary differential equations. Let

$$u_k = y_{2k} \tag{20}$$

$$v_k = \mathrm{Exp}(-hf(u_k))y_{2k+1}. \tag{21}$$

We write the explicit midpoint rule as a one-step method with stepsize $H = 2h$ for the doubled system

$$u = f(v)|_u, \quad u(t_0) = y_0 \tag{22}$$
$$v = f(u)|_v, \quad v(t_0) = y_0. \tag{23}$$

This one-step method is given by

$$Y_1 = \mathrm{Exp}(H/2 f(u_n)) v_n \tag{24}$$
$$u_{n+1} = \mathrm{Exp}(H f(Y_1)) u_n \tag{25}$$
$$v_{n+1} = \mathrm{Exp}(H/2 f(u_{n+1})) Y_1. \tag{26}$$

This can simply be solved for u_n, v_n:

$$\begin{aligned} Y_1 &= \mathrm{Exp}(-H/2 f(u_{n+1})) v_{n+1} \\ u_n &= \mathrm{Exp}(-H f(Y_1)) u_{n+1} \\ v_n &= \mathrm{Exp}(-H/2 f(u_n)) Y_1 \end{aligned}$$

The result is the same as obtained by applying the method formally with stepsize $-H$ on initial values u_{n+1}, v_{n+1}. We have proved:

Theorem 5.1. *Thus the explicit midpoint rule* (19) *is symmetric.*

It remains to check that the asymptotic expansion of an adjoint method is obtaind by substituting h by $-h$. Then the odd powers of h in the asymptotic expansion of symmetric methods would vanish.

The adjoint method of Φ is implicitly given by

$$y_n = \mathrm{Exp}(-h\Phi(t_n + h, \tilde{y}_{n+1}, -h)) \tilde{y}_{n+1}, \text{i.e.,} \tag{27}$$
$$\tilde{y}_{n+1} = \mathrm{Exp}(h\Phi(t_n + h, \tilde{y}_{n+1}, -h)) y_n \tag{28}$$

We assume the local error of Φ to be $le(t, y(t), h) = d_{p+1}(t) h^{p+1} + \mathcal{O}\left(h^{p+2}\right)$. We substitute h by $-h$ and then t by $t + h$ in equation (6):

$$\begin{aligned} -h\Phi(t+h, y(t+h), -h) &= -\, h\nu(t+h, y(t+h), -h) + d_{p+1}(t+h)(-h)^{p+1} + \mathcal{O}\left(h^{p+2}\right) \\ \mathrm{Exp}(h\Phi(t+h, y(t+h), -h) y_n &= \mathrm{Exp}(-d_{p+1}(t)(-h)^{p+1} + \mathcal{O}\left(h^{p+2}\right)) \\ &\quad \cdot \mathrm{Exp}(h\nu(t+h, y(t+h), -h)) y_n \\ &= \mathrm{Exp}(-d_{p+1}(t)(-h)^{p+1} + \mathcal{O}\left(h^{p+2}\right)) y(t+h) \end{aligned}$$

We see that $\tilde{y}_{n+1}$ is the fixed point of the equation (28). If we start the Iteration with $y(t+h)$ then the update after one step is $\mathrm{Exp}(-d_{p+1}(t)(-h)^{p+1} + \mathcal{O}\left(h^{p+2}\right))$. With a Banach Fixedpoint Theorem for Lie groups we conclude that the leading error term of the adjoint method is given by $d_{p+1}(t)(-1)^p h^{p+1}$.

Equation (17) implies that the leading term in the asymptotic expansion of the global error of the adjoint method is $(-1)^p e_p(t) h^p$.

Next we show that the adjoint of $\Phi^{(1)}$ is given by $\tilde{\Phi}^{(1)}$. We define $Y_2 = \mathrm{Exp}(h\tilde{\Phi}^{(1)}(t, Y_1, h)) Y_1$ and show that $Y_1 = \mathrm{Exp}(-h\Phi^{(1)}(t+h, Y_2, -h) Y_2$. Without loss of generality we choose

$Y_1 = \mathrm{Exp}(-(-h)^p e_p(t))y$. We have:

$$\begin{aligned} Y_2 &= \mathrm{Exp}(-h^p e_p(t+h))\,\mathrm{Exp}(h\tilde{\Phi}(t,y,h))y \\ \mathrm{Exp}(-h\Phi^{(1)}(t+h,Y_2,-h))y_2 &= \mathrm{Exp}(-h^p(-1)^p e_p(t))\,\mathrm{Exp}(-h\Phi(t+h,\mathrm{Exp}(h\tilde{\Phi}(t,y,h))y,-h)) \\ &\quad \cdot \mathrm{Exp}(h\tilde{\Phi}(t,y,h))y \\ &= \mathrm{Exp}(-h^p(-1)^p e_p(t))y = Y_1 \end{aligned}$$

which proofs that the diagram

$$\begin{array}{ccc} \Phi & \longrightarrow & \tilde{\Phi} \\ \downarrow & & \downarrow \\ \Phi^{(1)} & \longrightarrow & \tilde{\Phi^{(1)}} = \tilde{\Phi}^{(1)} \end{array}$$

commutes.

By iterating the procedure $\Phi^{(i)} \to \Phi^{(i+1)}$ we see that the asymptotic expansion of the adjoint method is obtained by replacing h by $-h$ in the asymptotic expansion of the original method. This gives:

Theorem 5.2. *A selfadjoint geometric method possesses an expansion of the global error in even powers of h.*

6. Extrapolation with the explicit midpoint-rule

The explicit midpoint-rule can be viewed as a symmetric one-step method for the approximations y_{2k}.

Thus we take the even approximates y_{2k} for extrapolation. At first we give a method of order 4 by extrapolating once:

$$\begin{array}{l} k_0 = f(y_n) \\ \text{for } i = 1:2 \\ \quad Y_{i,1} = \mathrm{Exp}(H/2^i k_0)Y_{i,0} \\ \quad k_{i,1} = f(Y_{i,1}) \\ \text{end} \\ \text{for } j = 2:3 \\ \quad Y_{2,j} = \mathrm{Exp}(H/2k_{2,j-1})Y_{2,j-2} \\ \quad k_{2,j} = f(Y_{2,j}) \\ \text{end} \\ H\Phi_1 = Hk_{1,1} \\ H\Phi_2 = H/2k_{2,1} + H/2k_{2,3} + 1/2[H/2k_{2,1}, H/2k_{2,3}] \\ H\Phi = (4H\Phi_2 - H\Phi_1)/3 \\ y_{n+1} = \mathrm{Exp}(H\Phi)y_n \end{array}$$

To compute the approximation $H\Phi_2$ we have used the truncated BCH-formula

$$\mathrm{Exp}(H/2k_{2,3})\,\mathrm{Exp}(H/2k_{2,1}) = \mathrm{Exp}(H/2k_{2,3} + H/2k_{2,1} + H^2/8[k_{2,3}, k_{2,1}] + \mathcal{O}\left(H^5\right)).$$

The procedure above has order 4. It can be implemented with an effort of 4 matrix exponentiations per step by using $Y_{i,1} = \mathrm{Exp}(H/4k_0)\,\mathrm{Exp}(H/4k_0)y_n$. We need 5 function evaluations per step. In contrast to the RK-MK methods we need only one commutator here where a RK-MK method of order 4 needs commutators in the correction functions for the internal stages and for the final value.

The procedure above can be extended in a natural way to construct methods of higher order. We have to use the required number of terms in the BCH-formula to get the desired order, i.e., for order p we have to include commutators up to order $p-2$ as mentioned above.

7. Numerical Experiments

For our testing purposes we choose an equation that originates from [15]. The righthand side is simply given in matlab notation by

$$f(x) = diag(diag(x,+1),+1) - diag(diag(x,+1),-1).$$

The solution of this differential equation evolves in the Lie group $O(5)$, the group of orthogonal matrices of dimension 5. The Lie algebra of $O(5)$ is just isomorphic to the set of skew-symmetric matrices of dimension 5.

We have implemented the extrapolation procedure above with fixed order 4 and 6 in matlab. In table 7 we verify that the methods have order 4 resp. 6:

Order 4		
h	err	err/h^4
1.00e-01	1.1e-07	1.19e-03
7.14e-02	3.1e-09	1.19e-03
3.57e-02	1.9e-09	1.19e-03
2.56e-02	5.1e-10	1.19e-03
1.81e-02	1.2e-10	1.18e-03
1.29e-02	3.3e-11	1.18e-03
9.25e-03	8.7e-12	1.18e-03
6.62e-03	2.3e-12	1.20e-03
4.73e-03	8.3e-13	1.65e-03

Order 6		
h	err	err/h^6
5.00e-01	2.7e-07	1.7e-05
3.33e-01	2.4e-08	1.7e-05
2.50e-01	4.3e-09	1.7e-05
2.00e-01	1.1e-09	1.7e-05
1.42e-01	1.5e-10	1.8e-05
1.00e-01	1.8e-11	1.8e-05
7.14e-02	2.4e-12	1.8e-05
5.00e-02	2.9e-13	1.8e-05
3.57e-02	4.0e-14	1.9e-05

We see clearly order 4 resp. 6 until the solution reaches a level of accuracy that is beyond the accuracy of the reference solution.

Next we compare the methods with the matlab built-in integrators ode23 and ode45:

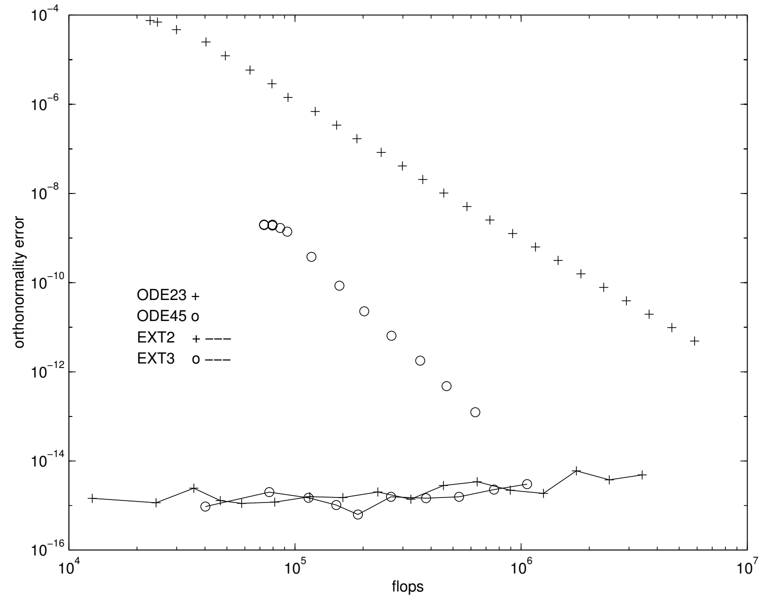

FIGURE 1.

The geometric extrapolation methods are presented by lines, where the low order method is denoted by additional crosses and the high order method is denoted by additional small circles. The low order matlab code ODE23 is based on a Runge-Kutta-Fehlberg formula of order 3 with an embedded method of order 2 for stepsize control. The high order matlab method ODE45 is based on DOPRI5. It is denoted by small circles. In Figure 1 the orthogonality error $\|x^T x - I\|$ is displayed. Our methods retain orthogonality up to machine accuracy, where as the numerical solutions computed by the Runge-Kutta methods drift off the manifold $O(5)$. It is clear that a price has to be paid, but this price is surprisingly low.

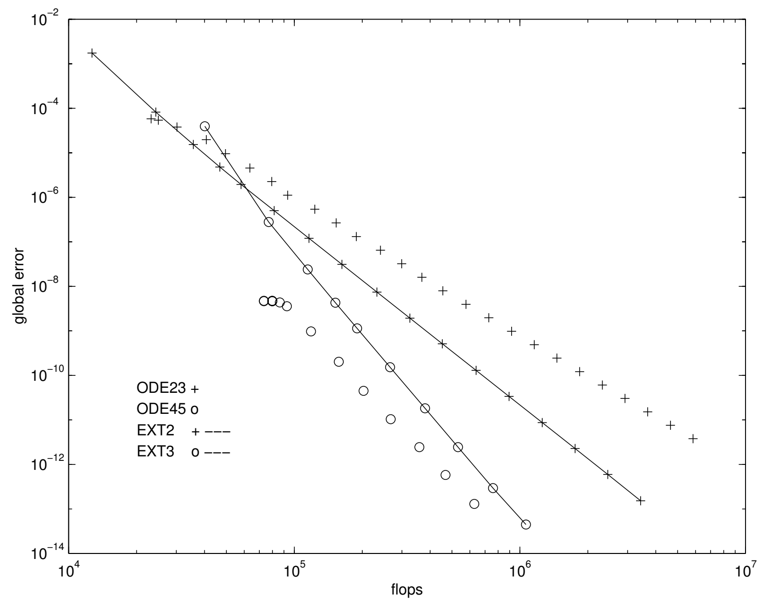

FIGURE 2.

In Figure 2 the efficiency of the geometric extrapolation methods in comparision with ODE23 and ODE45 is displayed.

The performance of the high order extrapolation method is almost comparable to ODE45. Both extrapolation methods beat the low order matlab code. We have to take into account that our extrapolation methods maintain orthogonality perfectly whereas the Runge-Kutta methods allow a drift off the manifold in the magnitude of the given error tolerance. Under the latter aspect the extrapolation methods perform very well.

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