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by

Arne Marthinsen and Brynjulf Owren

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Address: Department of Mathematical Sciences, Norwegian University of Science and Technology,
N-7034 Trondheim, Norway.

Quadrature Methods Based on the Cayley Transform*

Arne Marthinsen† Brynjulf Owren‡

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Abstract

Integration of Lie type equations on matrix Lie groups using Magnus series methods has recently been proposed by Iserles and Nørsett. The methods use the exponential mapping, whose computation may be very costly. In this paper a smaller class of Lie groups is considered, for which the exponential mapping can be replaced by e.g. the Cayley transform or the diagonal Padé approximants. Particular methods are being derived, and numerical experiments that illustrate and verify properties of the new methods are included.

AMS Subject Classification: 65L06, 34A50

Key Words: geometric integration, numerical integration of ordinary differential equations on manifolds, numerical analysis, quadratic Lie groups

1 Introduction

The linear matrix differential equation in $\mathbb{R}^{n\times n}$,

$$y' = a(t)y, \quad a, y : \mathbb{R} \to \mathbb{R}^{n\times n}, \tag{1}$$

was studied by Magnus [11] in 1954. He provided a representation of the solution as the matrix exponential of an expansion in terms of iterated matrix commutators and integrals. The expansion was obtained by assuming that, in some neighborhood of $y_0 \in \mathbb{R}^{n\times n}$, there is a function $\sigma : \mathbb{R} \to \mathbb{R}^{n\times n}$ such that $y(t) = \exp(\sigma(t))y_0$. The differential equation obtained in this new variable can be solved for instance by Picard iteration, and what results is the Magnus expansion.

Recently Moan [13] considered ways of turning the Magnus expansion into a useful numerical method for solving (1), and a successful solution was discovered later by Iserles and Nørsett [8], who found a remarkably cheap way of approximating the integrals involved in the Magnus expansion.

In equation (1) we can let $y \in \mathbb{R}^n$ and use the same approach. Furthermore, we may consider the equation

$$y' = a(t)\cdot y - y \cdot a(t) = [a(t), y], \quad y(t), a(t) \in \mathbb{R}^{n\times n}. \tag{2}$$

In this case, the representation $y(t) = \exp(\sigma(t))y_0\exp(-\sigma(t))$ leads again to the Magnus expansion for $\sigma(t)$.

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†Email: `Arne.Marthinsen@math.ntnu.no`, WWW: `http://www.math.ntnu.no/~arnema/`

‡Email: `Brynjulf.Owren@math.ntnu.no`, WWW: `http://www.math.ntnu.no/~bryn/`

All the examples above can be treated in a unified way by introducing the notion of a Lie algebra action on a manifold $\mathcal{M}$. For relevant background material on Lie groups and Lie algebras, see for instance Olver [15] or Marsden and Ratiu [12]. The work by Munthe-Kaas [14] and Engø [5] describe the use of Lie group and Lie algebra actions for solving ordinary differential equations (ODEs) on manifolds in a more general framework than what we consider in this paper. In the examples above, one can think of the representation of the solution as a special instance of an action by the Lie algebra $\mathfrak{gl}(n)$, which consists of the vector space $\mathbb{R}^{n\times n}$ furnished with the matrix commutator as Lie bracket. Thus, the action $\lambda : \mathfrak{gl}(n) \times \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ is given as $\lambda(v, y_0) = \exp(v)\cdot y_0$ in the case (1) and $\lambda(v, y_0) = \exp(v)\cdot y_0 \cdot \exp(-v)$ for (2). The above approach is made more powerful by allowing the action to be defined on a subalgebra of $\mathfrak{gl}(n)$, meaning a subspace $\mathfrak{g}$ of $\mathfrak{gl}(n)$ which is closed under matrix commutation. Examples of such subalgebras are the set of skew-symmetric $n \times n$ matrices, $\mathfrak{so}(n)$, and the set of trace-free matrices, $\mathfrak{sl}(n)$. The action splits $\mathbb{R}^{n\times n}$ into orbits: $\mathcal{O}_x = \{y \in \mathbb{R}^{n\times n} : y = \lambda(v, x), v \in \mathfrak{g}\}$. For the equation (1), by using the corresponding action by the Lie algebra $\mathfrak{so}(n)$, one finds that two matrices y and z belongs to the same orbit if and only if $z^T z = y^T y$. Similarly, acting by $\mathfrak{sl}(n)$ we see that two matrices belonging to the same orbit have the same determinant. If we replace $\mathbb{R}^{n\times n}$ by $\mathbb{R}^n$ and let the action be matrix-vector multiplication, we obtain, when $\mathfrak{g} = \mathfrak{so}(n)$, that $u, v \in \mathbb{R}^n$ belong to the same orbit if $\|u\|_2 = \|v\|_2$. However, acting by $\mathfrak{sl}(n)$, only two orbits result: $\{0\}$ and $\mathbb{R}^n\backslash\{0\}$. For equation (2), the isospectral case with $\mathcal{M} = \mathrm{Sym(n)}$ (symmetric $n\times n$ matrices) and $\mathfrak{g} = \mathfrak{so}(n)$ has been much studied, see e.g. Zanna [17]. Such $\lambda : \mathfrak{so}(n) \times \mathrm{Sym}(n) \to \mathrm{Sym}(n)$ is well-defined since $Q = \exp(v)$ is orthogonal whenever $v \in \mathfrak{so}(n)$, so $\exp(-v) = Q^T$. Moreover, since the action is a similarity transform, matrices in the same orbit share the same set of eigenvalues. The exact solution of the differential equations (1) and (2) evolves inside the particular orbit to which the initial value belongs. This may not be the case for a numerical approximation resulting from a classical method being applied directly to the equation. However, with the new representation, it suffices that the numerical approximation or truncated expansion, say $\tilde{\sigma}$, belongs to the linear space $\mathfrak{g}$ and we obtain $\tilde{y} = \lambda(\tilde{\sigma}, y_0) \in \mathcal{O}_{y_0}$. Thus, this provides us with a powerful tool for conserving first integrals.

Note that the formulation of ODE methods through Lie algebra actions on manifolds is not restricted to Lie algebras which are subalgebras of $\mathfrak{gl}(n)$. The Lie algebra may be considered to be an abstract object, and the action must simply allow us to express the ODE on the manifold through the formula (see Munthe-Kaas [14] for details)

$$y' = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \lambda\big(sf(t,y), y\big).$$

In particular, the problem defined by equation (1) fits into this framework if we let the Lie algebra be any subalgebra of $\mathfrak{gl}(n)$ or $\mathfrak{gl}(n)$ itself, and use the Lie algebra action $\lambda(v,p) = \phi(v)\cdot p$ where $\phi : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ is such that $\phi(v)$ is invertible and satisfies

$$\left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \phi(sv) = v. \tag{3}$$

We get

$$y' = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \big(\phi(sa(t))\cdot y\big) = a(t)y.$$

In the same way, we may consider the Lie algebra $\mathbb{R}^n$ where all brackets are set to zero and impose the action $\lambda(v,p) = p + v$. This corresponds to the traditional setting of classical methods. We now get

$$y' = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \big(y + sa(t)\big) = a(t),$$

i.e. a classical quadrature problem in euclidean space. It is hence natural to view problems of type (1) as *quadrature problems* in a generalised setting. Although this problem is easier to solve than the general problem, when a also depends on y, it is harder than classical quadrature problems since the right hand side depends on y.

The actions described above are well-known and tested for many problems. But an issue which is often raised, is the fact that computation of matrix exponentials is fairly expensive. For instance, if the general MATLAB function `expm` is used, it typically costs $20-30\ n^3$ flops to exponentiate an $n \times n$ matrix. Additional difficulties arise from the fact that the action should either be computed exactly or be replaced by an approximation which is such that $y \approx \lambda(v, x)$ belongs to the same orbit as x. Such approximations have been developed by Celledoni and Iserles [1, 2]. Another approach consists in looking for actions λ which do not involve computation of the exponential. In searching for good Lie algebra actions, an invaluable tool is to consider the action Λ by a *Lie group* G of which $\mathfrak{g}$ is the corresponding Lie algebra. In the present framework, we can think of a Lie group G as a submanifold of the set of $n \times n$ invertible matrices, such that the matrix product satisfies the group axioms. Examples are $\mathrm{SL}(n)$, the set of $n \times n$ matrices with unit determinant, and $\mathrm{SO}(n)$, the set of orthogonal $n \times n$ matrices with unit determinant. As usual the Lie algebra of a Lie group is the linear space of tangents at the identity matrix, furnished with the matrix commutator. It is for instance easy to verify that the Lie algebra of $\mathrm{SL}(n)$ is $\mathfrak{sl}(n)$, and that for $\mathrm{SO}(n)$ it is $\mathfrak{so}(n)$. We consider Lie group actions $\Lambda : G \times \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$, examples are $\Lambda(g, p) = g \cdot p$ and $\Lambda(g, p) = g \cdot p \cdot g^{-1}$. The above mentioned approach for finding a Lie algebra action is to consider local diffeomorphisms $\phi : \mathfrak{g} \to G$, such that for a given group action Λ, we obtain a Lie algebra action $\lambda(v, p) = \Lambda(\phi(v), p)$. In this setting, the above actions come out as the special case in which $\phi = \exp$. In looking for alternative maps $\phi : \mathfrak{g} \to G$, where $\mathfrak{g}$ is a subalgebra of $\mathfrak{gl}(n)$, it may seem natural to consider analytic maps, say $\phi(v) = \sum_{k=0}^{\infty} a_k v^k$. One here needs to require that $\phi(\mathfrak{g}) \subset G$, otherwise one cannot in general guarantee that the numerical approximation remains in the same orbit throughout the integration. There is a negative result in [6], essentially stating that the only analytic function that can be used if $\mathfrak{g} = \mathfrak{sl}(n)$, $n \geq 3$, is exp. However, for certain other Lie groups there are more possibilities. Letting v be an arbitrary matrix, we can consider the subalgebra of $\mathfrak{gl}(n)$ defined as

$$\mathfrak{g}_v = \{u \in \mathfrak{gl}(n) : v \cdot u + u^T \cdot v = 0\}.$$

We recognize as a special case, $\mathfrak{g}_I$ (I identity matrix) the set of skew-symmetric matrices previously denoted $\mathfrak{so}(n)$, but also the symplectic Lie algebra, $\mathfrak{g}_J$, can be obtained in this way. Here, $\mathfrak{g}_J \subset \mathfrak{gl}(2n)$ and

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \tag{4}$$

In the case that v is invertible, we can define the Lie group

$$G_v = \{y \in \mathbb{R}^{n \times n} : y^T v y = v\} \tag{5}$$

and its Lie algebra is $\mathfrak{g}_v$. It was proved by Celledoni and Iserles [1] that if ϕ is any analytic function satisfying $\phi(z) \cdot \phi(-z) = 1$, then $\phi(\mathfrak{g}_v) \subset G_v$. There is of course an abundance of such functions, but perhaps the most merited one in the literature on computational mechanics is the Cayley transform, or Padé(1,1), which we shall define as

$$\phi(z) = \frac{1 + \frac{z}{2}}{1 - \frac{z}{2}}.$$

This paper is devoted to construction of quadrature methods for quadratic Lie groups and focus the development on functions ϕ other than the exponential mapping. It should be mentioned that Diele et al. [3, 4] proposed integration methods based on the Cayley transform for the solution of unitary differential problems, and applied the methods to isospectral flows. Lewis and Simo [10] used the Cayley transform when analysing and integrating the dynamics given by the Euler equations on the group of spatial rotations, SO(3).

The rest of this paper is organised as follows. What remains of Section 1 will be used to briefly describe necessary background theory and define the notation we use. In Section 2, we describe the procedure and derive some numerical methods. Section 3 is devoted to some numerical simulations that illustrate the methods derived in Section 2. Finally, in Section 4 we present some concluding remarks.

1.1 Some Definitions and Notation

Let $\mathcal{M}$ be a smooth manifold and G a Lie group with corresponding Lie algebra $\mathfrak{g}$. As Munthe-Kaas [14] showed, we can now write any differential equation on $\mathcal{M}$ defined by

$$\dot{y} = F(t, y), \qquad y \in \mathcal{M}, \quad F(t, \cdot) \in \mathfrak{X}(\mathcal{M}) \tag{6}$$

in the form

$$\dot{y} = \big(\lambda_* f(t, y)\big)(y), \qquad f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g},$$

at least locally. $\mathfrak{X}(\mathcal{M})$ denotes the vector space of vector fields on $\mathcal{M}$, and is a Lie algebra when equipped with the Lie-Jacobi bracket (see e.g. [12, 15, 16]). The derivative map $\lambda_* : \mathfrak{g} \to \mathfrak{X}(\mathcal{M})$ is defined as

$$\lambda_*(v)(p) = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \lambda(sv, p).$$

For some fixed $p \in \mathcal{M}$ we define the map $\lambda_p : \mathfrak{g} \to \mathcal{M}$ by $\lambda_p(v) = \lambda(v, p)$, $v \in \mathfrak{g}$. Furthermore, the Lie algebra action λ is assumed to be of the form $\lambda(v, p) = \Lambda\big(\phi(v), p\big)$ with ϕ satisfying (3). The tangent mapping of ϕ at $u \in \mathfrak{g}$, identified with the differential $\mathrm{d}\phi_u : \mathfrak{g} \to \mathfrak{g}$, is assumed to be invertible for u in some neighborhood of 0. The differential of ϕ is related to the Jacobian, ϕ', through $\phi' = \mathrm{d}\phi \cdot \phi$. This setting is always possible; take for instance $\phi(u) = \exp(u)$ (see also [16]).

The following theorem, proved in [16], defines the basis for this paper.

Theorem 1.1. *Let the vector field $F \in \mathfrak{X}(\mathcal{M})$ in (6) be written in the form $F(t, y) = \big(\lambda_* f(t, y)\big)(y)$, where $f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$. Let $\mathfrak{g}$, λ and ϕ be as described above. Then the (locally defined) vector field*

$$\widetilde{f}(t, u) = \mathrm{d}\phi^{-1}\big(f(t, \lambda_p(u))\big)$$

satisfies $F \circ \lambda_p = \lambda_p' \circ \widetilde{f}$ (in some neighborhood of $p \in \mathcal{M}$).

Thus the solution of $\dot{y} = F(t, y)$ with $y(0) = p$ is given as $y(t) = \lambda_p\big(u(t)\big)$ where

$$u'(t) = \widetilde{f}\big(t, u(t)\big) \tag{7}$$

with initial value $u(0) = 0$.

Let, for the purpose of illustration, $\phi = \exp$, the matrix exponential, and assume that $a(t)$ in (1) belongs to $\mathfrak{sl}(n)$ for all $t \in [0, T]$. The algebra action is taken to be $\lambda(v, p) = \exp(v) \cdot p$. Equation (7) now takes the form (see also [14])

$$\dot{\sigma}(t) = \mathrm{dexp}^{-1}_{\sigma(t)}\big(a(t)\big), \qquad \sigma(0) = 0,$$

where dexp^{-1} is the inverse of the differential of the exponential mapping. If $y_0 \in \mathrm{SL}(n)$, then the solution of (1) evolves on $\mathrm{SL}(n)$, and if $y_0 \in \mathbb{R}^n$ then it evolves in the orbit $\mathcal{O}_{y_0}$ generated by the Lie algebra action.

2 Quadrature Methods

To the end of this paper we let G denote a Lie group of the form (5) and $\mathfrak{g}$ its Lie algebra. Let $\lambda : \mathfrak{g} \times \mathcal{M} \to \mathcal{M}$ be the Lie algebra action $\lambda(v,p) = \phi(v) \cdot p$, where $\phi : \mathfrak{g} \to G$. Letting $\phi(v) = \exp(v)$ gives

$$\lambda_*(v)(p) = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \exp(sv) \cdot p = v \cdot p,$$

whereas $\phi(v) = \mathrm{cay}(v)$ gives

$$\lambda_*(v)(p) = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} (\mathrm{I} - \tfrac{sv}{2})^{-1}(\mathrm{I} + \tfrac{sv}{2}) \cdot p = v \cdot p,$$

hence both of these choices of ϕ satisfy the requirement (3) and can be used to write differential equations in the general form

$$\dot{y} = f(t,y) \cdot y, \qquad f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}, \quad y \in \mathcal{M}.$$

Let $\phi(v) = \mathrm{cay}(v)$. Simple calculations verify that, for a fixed $p \in \mathcal{M}$,

$$\widetilde{f}(t,u) = (\mathrm{I} - \tfrac{u}{2}) f\big(t, \mathrm{cay}(u) \cdot p\big)(\mathrm{I} + \tfrac{u}{2}).$$

We want to integrate problem (1). The differential equation to be solved on $\mathfrak{g}$ now reads

$$\sigma' = (\mathrm{I} - \tfrac{\sigma}{2}) a(t) (\mathrm{I} + \tfrac{\sigma}{2}), \qquad \sigma(0) = 0,$$

and we integrate from $t_0 = 0$ to $t_{\text{end}} = h$. An implicit Runge-Kutta method with s stages applied to this system yields the Picard iteration

$$\sigma_i^{[k+1]} = h \sum_{j=1}^{s} \widetilde{a}_{ij} \left\{ a_j - \tfrac{1}{2}\big[\sigma_j^{[k]}, a_j\big] - \tfrac{1}{4}\sigma_j^{[k]} a_j \sigma_j^{[k]} \right\}, \qquad i = 1,\dots,s, \qquad k = 0,1,2,\dots, \tag{8}$$

with $\sigma_i^{[0]} = 0$, where $\widetilde{a}$ denotes the Butcher matrix. Again, $[\cdot,\cdot]$ is the matrix commutator. The approximation to $\sigma(h)$ is then given as $\widehat{\sigma} = h \sum_{i=1}^{s} b_i K_i$, where

$$K_i = a_i - \tfrac{1}{2}\big[\sigma_i^{[\ell]}, a_i\big] - \tfrac{1}{4}\sigma_i^{[\ell]} a_i \sigma_i^{[\ell]}, \qquad i = 1,\dots,s, \qquad \ell > 0. \tag{9}$$

If we choose a symmetric Runge-Kutta method, we know that the expansion of $\widehat{\sigma}$ contains only odd powers of h, or, alternatively, the error $\sigma(h) - \widehat{\sigma}$ has an expansion in even powers of h. To obtain an approximation of order $p \leq q$, where q is the order of the Runge-Kutta scheme, it hence suffices to let $\ell = q - 1$ when q is odd and $\ell = q - 2$ when q is even.

Iserles and Nørsett [8] analysed quadrature problems on general matrix Lie groups. They devised very efficient numerical methods based on analysis involving certain rooted trees and multivariate quadrature. The analysis has been extended in [7, 9]. It is possible to proceed along the same line for the methods based on the Cayley transform or other functions $\phi : \mathfrak{g} \to G$ satisfying $\phi(z) \cdot \phi(-z) = 1$, but in this paper we only present some schemes and perform simulations to verify some of the methods' properties.

Example 2.1. *Consider the Gauss-Legendre weights of order 4:*

$$c_1 = \tfrac{1}{2} - \tfrac{\sqrt{3}}{6}, \qquad c_2 = \tfrac{1}{2} + \tfrac{\sqrt{3}}{6}.$$

Let a_i^n be the function a evaluated at the abscissae values, $a_i^n = a(t_n + c_i h)$, $i = 1,2$, and define

$$a_1^n = w_1^n - \alpha h w_2^n \qquad \textit{and} \qquad a_2^n = w_1^n + \alpha h w_2^n,$$

with $\alpha = \frac{\sqrt{3}}{6}$. *The resulting fourth order quadrature method based on the Cayley transform is then given by*

$$\begin{aligned} \sigma_4^n &= hw_1^n - \tfrac{1}{12}h^3[w_1^n, w_2^n] - \tfrac{1}{12}h^3(w_1^n)^3 \\ y_{n+1} &= \operatorname{cay}(\sigma_4^n)y_n. \end{aligned} \tag{10}$$

Alternatively, expressed in terms of a_i^n,

$$\begin{aligned} \sigma_4^n &= \tfrac{1}{2}h(a_1^n + a_2^n) - \tfrac{1}{4\sqrt{3}}h^2[a_1^n, a_2^n] - \tfrac{1}{96}h^3(a_1^n + a_2^n)^3 \\ y_{n+1} &= \operatorname{cay}(\sigma_4^n)y_n. \end{aligned}$$

Example 2.2. *Consider the Gauss-Legendre weights of order* 6*:*

$$c_1 = \tfrac{1}{2} - \alpha, \qquad c_2 = \tfrac{1}{2}, \qquad c_3 = \tfrac{1}{2} + \alpha,$$

with $\alpha = \frac{\sqrt{15}}{10}$, *and let* $a_i^n = a(t_n + c_i h)$, $i = 1, \dots, 3$, *be the function* a *evaluated at the abscissae values. Let* w_1^n, w_2^n *and* w_3^n *be defined as follows:*

$$a_1^n = w_1^n - \alpha h w_2^n + (\alpha h)^2 w_3^n, \qquad a_2^n = w_1^n \qquad \textit{and} \qquad a_3^n = w_1^n + \alpha h w_2^n + (\alpha h)^2 w_3^n.$$

The resulting sixth order quadrature method based on the Cayley transform is then given by

$$\begin{aligned} \sigma_6^n &= hw_1 + \tfrac{1}{12}h^3(w_3 - [w_1, w_2] - w_1^3) \\ &\quad + h^5\Big(\tfrac{1}{240}([w_2, w_3] - [w_2, [w_1, w_2]] - w_1^2 w_3 - w_3 w_1^2 + [w_1 w_2 w_1, w_1]) \\ &\qquad - \tfrac{1}{80}w_1 w_3 w_1 + \tfrac{1}{120}([w_1^3, w_2] + w_1^5)\Big) \\ y_{n+1} &= \operatorname{cay}(\sigma_6^n)y_n. \end{aligned}$$

In the quadrature methods above, terms like w^k, $w^k z^\ell + z^\ell w^k$ and $w^k z^\ell w^k$ appear, and it may not be immediately clear that σ belongs to $\mathfrak{g}_v$. However, due to the special form of the elements in $\mathfrak{g}_v$, all of these elements do belong to the specific Lie algebras that we consider here for certain values of k and ℓ. To see this, let $w, z \in \mathfrak{g}_v$ and recall that an element $u \in \mathfrak{g}_v$ satisfies the relation $v \cdot u + u^T \cdot v = 0$. We have that

$$v \cdot w^k = (v \cdot w) \cdot w^{k-1} = -w^T \cdot (v \cdot w) \cdot w^{k-2} = \dots = (-1)^{k-1}(w^T)^{k-1} \cdot (v \cdot w) = (-1)^k (w^k)^T \cdot v,$$

and hence $w^k \in \mathfrak{g}_v$ when k is odd. In the same way, it is straightforward to show that $w^k z^\ell + z^\ell w^k \in \mathfrak{g}_v$ when $k + \ell$ is odd and that $w^k z^\ell w^k \in \mathfrak{g}_v$ whenever ℓ is odd.

3 Numerical Experiments

Let us by **MC4** and **MC6** denote the fourth and sixth order quadrature methods based on the Cayley transform from Examples 2.1 and 2.2. We compare these methods to the fourth and sixth order Magnus methods presented in [9]:

MG4: order 4:

$$\begin{aligned} \widehat{\sigma}_4^n &= \tfrac{1}{2}h(a_1^n + a_2^n) + \tfrac{\sqrt{3}}{12}h^2[a_2^n, a_1^n] \\ y_{n+1} &= \exp(\widehat{\sigma}_4^n)y_n \end{aligned}$$

MG6: order 6:

$$\begin{aligned}\widehat{\sigma}_6^n &= \tfrac{1}{18}h(5a_1^n + 8a_2^n + 5a_3^n) - \tfrac{\sqrt{15}}{108}h^2(2a_{1,2}^n + a_{1,3}^n + 2a_{2,3}^n) \\ &\quad + \tfrac{1}{432}h^3(a_{1,3,1,2}^n + a_{1,3,2,3}^n) + \tfrac{\sqrt{15}}{2160}h^4 a_{1,3,1,3}^n \\ y_{n+1} &= \exp(\widehat{\sigma}_6^n)y_n,\end{aligned}$$

where

$$\begin{aligned}a_{1,2}^n &= [a_1^n, a_2^n], & a_{1,3}^n &= [a_1^n, a_3^n], & a_{2,3}^n &= [a_2^n, a_3^n], \\ a_{1,3,1,2}^n &= [a_1^n - 5a_3^n, a_{1,2}^n], & a_{1,3,2,3} &= [5a_1^n - a_3^n, a_{2,3}^n], & a_{1,3,1,3}^n &= [a_1^n, [a_3^n, a_{1,3}^n]].\end{aligned}$$

All simulations have been performed using MATLAB. The exponential mapping is computed using `expm` and the flops counting has been done using the `flops` function.

The theoretical cost of the methods is as follows. **MC4** uses four matrix multiplications as well as linear combinations to compute σ_4^n, **MC6** uses eighteen matrix multiplications and a number of linear combinations to compute σ_6^n, while **MG4** and **MG6** need two and fourteen matrix multiplications as well as linear combinations to compute $\widehat{\sigma}_4^n$ and $\widehat{\sigma}_6^n$, respectively. These numbers would favor the original Magnus series methods. However, while **MG4** and **MG6** use the matrix exponential, **MC4** and **MC6** are based on the Cayley transform. The cost of computing the matrix exponential depends on the particular matrix being exponentiated (e.g. the norm of the matrix), but numerical simulations indicate that the MATLAB implementation uses between $20n^3$ and $30n^3$ flops, where n is the dimension of the matrix. On the other hand, computing $(\mathrm{I}-u)^{-1}(\mathrm{I}+u)$ can be done using e.g. Gaussian elimination with a cost of about $\frac{8}{3}n^3$ flops. Since a matrix multiplication naively costs $2n^3$ flops, this shows that the new methods compute a step with less work than the original Magnus series methods. The simulations will show the efficiency of the codes, measured as global error versus total number of flops used.

In addition to the Magnus type and quadrature integrators, we have added simulations performed by **MKC4**, which is the fourth order Munthe-Kaas method [14] based on the classical, explicit **RK4** method, implemented using the Cayley transform. The implementation does not take advantage of the fact that we are solving Lie type problems.

Problem 1. As a first example we solve the **Orthogonal problem** presented in [7]. It is a Lie type problem, defined by the skew-symmetric matrix $a(t) \in \mathfrak{so}(n)$, whose upper triangular entries are

$$(-1)^{i+j}\frac{i}{j+1}t^{j-i}, \qquad 1 \le i < j \le n. \tag{11}$$

As initial values we take the $n \times n$ identity matrix, and we integrate from $t_0 = 0$ to $t_{\text{end}} = 0.5$ with constant stepsize $h = 0.02$. We have chosen $n = 30$.

Figure 1 depicts the 2-norm of the global error, the distance from the manifold (computed as $\|y_i y_i^T - y_0 y_0^T\|$), global error versus stepsize as well as the efficiency, computed as global error versus number of flops. The efficiency shown by **MC4** is better than the one by **MG4**, while **MC6** and **MG6** are almost equal on this test problem.

Problem 2. As a second example we solve the third problem presented in [9]. The solution evolves on SO(4) and the problem is defined by the function

$$a(t) = \begin{bmatrix} 0 & t\sin\frac{\pi t}{4} & 0 & 0 \\ -t\sin\frac{\pi t}{4} & 0 & t\sin\frac{\pi t}{2} & 0 \\ 0 & -t\sin\frac{\pi t}{2} & 0 & t\sin\frac{3\pi t}{4} \\ 0 & 0 & -t\sin\frac{3\pi t}{4} & 0 \end{bmatrix} \in \mathfrak{so}(4). \tag{12}$$

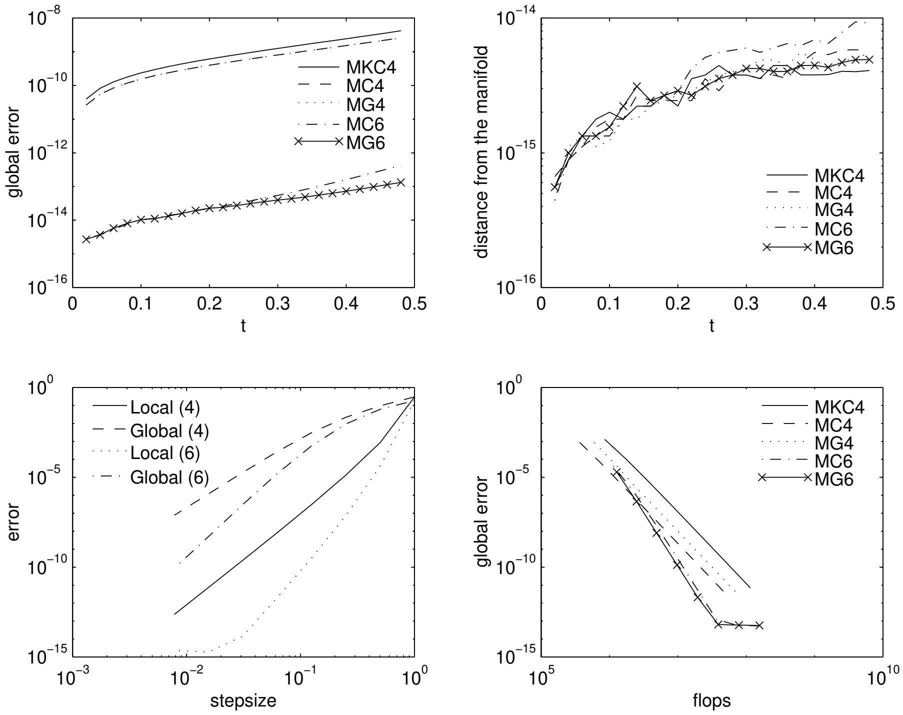

Figure 1: Solution of the orthogonal problem defined by (11). The upper figures show global error versus time and the deviation from the configuration space of the problem, respectively. The lower left figure verifies the claimed order (asymptotic global/local order 4/5 and 6/7, respectively) while the lower right figure shows the efficiency of the integrators.

We integrate from $t_0 = 0$ to $t_{\text{end}} = 20$ with constant stepsize $h = 0.1$ and the identity matrix as initial value.

Again we see that **MC4** performs better than **MG4**, while **MC6** and **MG6** are indistinguishable. For accuracies less than 10^{-6}, **MC4** would be the method of choice.

Problem 3. Our final example is a problem evolving on the symplectic group Sp(4). It was first presented in [7]. The matrix function

$$g(t) = \begin{bmatrix} 1 & -1 & t & 1 \\ 2 & 2 & 1 & -t \\ -2t & -1 & -1 & -2 \\ -1 & 1 & 1 & -2 \end{bmatrix} \in \mathfrak{sp}(4) \tag{13}$$

defines the problem. We integrate from $t_0 = 0$ to $t_{\text{end}} = 20$ with the identity matrix as initial condition and constant stepsize $h = 0.1$.

The results from the simulations are similar to the ones obtained from Problems 1 and 2. **MC4** seems to perform slightly better than **MG4** while in this case **MG6** performs better than **MC6**. The distance from the symplectic group is computed as $\|y^T Jy - J\|_2$, where J is as in (4).

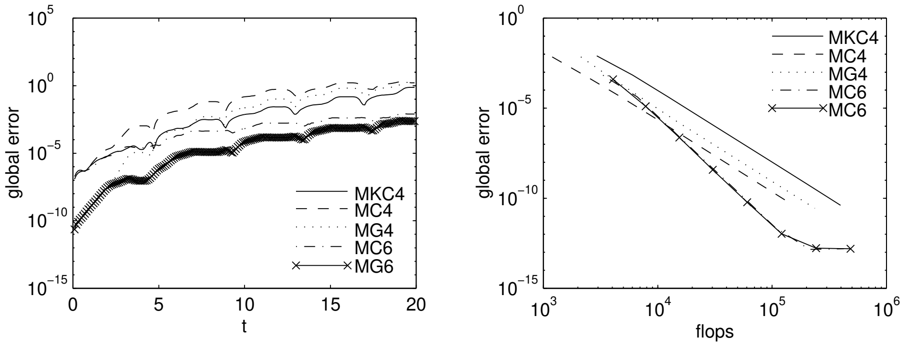

Figure 2: Solution of the orthogonal problem defined by (12). The left figure shows the global error of the approximations during the time-stepping while the right figure shows the efficiency of the codes.

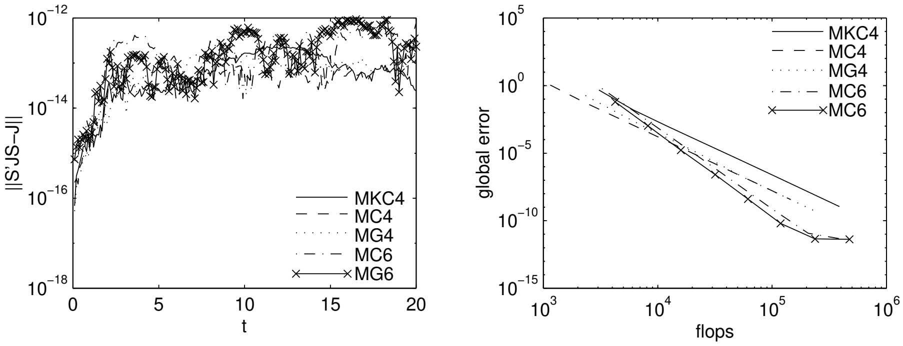

Figure 3: Solution of the symplectic problem defined by (13). The left figure shows the deviation from the configuration space of the problem while the right figure shows the efficiency of the codes.

4 Concluding Remarks

We have considered quadrature methods for integration of Lie type problems on quadratic Lie groups. The idea is similar to the one presented by Iserles and Nørsett [8], but we use the fact that there exist other mappings between a quadratic Lie algebra and the corresponding Lie group than the exponential mapping. We have constructed quadrature type methods based on the Cayley transform. These methods are especially tailored solution of Lie type problems. It should be noted, however, that the use of Cayley transform and Padé approximants are connected to integration on quadratic Lie groups and could therefore be applied in the settings of Munthe-Kaas for general, not only Lie type, problems. This was done in [3, 4].

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