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Numerical integration methods for the double-bracket flow☆

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Abstract

In this paper new methods up to order four based on the Magnus expansion are proposed for the numerical integration of the double-bracket equation. The Magnus series is constructed term-by-term by means of recurrences and a bound on the convergence domain is also provided. The new integrators preserve the most salient qualitative features of the flow and are computationally more efficient than other standard Lie-group solvers, such as the Runge–Kutta-Munthe-Kaas class of algorithms.

MSC: 65L05; 65L70

Keywords: Double-bracket equation; Magnus expansion; Lie-group solvers; Numerical integrators

1. Introduction

The double-bracket equation

$$Y' = [[Y,N],Y], \quad Y(0) = Y_0 \in \mathrm{Sym}(n) \tag{1}$$

was introduced in [6,10] to solve certain standard problems in applied mathematics, although similar equations also appear in the formulation of physical theories such as micromagnetics [16]. Here N and Y_0 are constant matrices in $\mathrm{Sym}(n)$, the set of $n\times n$ symmetric real matrices and $[A,B]=AB-BA$ represents the usual commutator.

The double-bracket equation possesses a number of features that make it worth of analysis. First, it is a particular example of an isospectral flow [11]

$$Y' = [A(t,Y),Y], \quad Y(0) = Y_0 \in \mathrm{Sym}(n), \tag{2}$$

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where $A \in \mathfrak{so}(n)$, the Lie algebra of $n \times n$ real skew-symmetric matrices. Then there exists a matrix function $Q(t)$ evolving in the Lie group SO(n) such that

$$Y(t) = Q(t)Y_0Q^{\mathrm{T}}(t) \tag{3}$$

and $Y(t)$ has the same eigenvalues as Y_0 for all $t > 0$.

Second, given the potential function

$$\psi(Y) = \|Y + N\|_{\mathrm{F}}, \tag{4}$$

where $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm and Y ranges across all symmetric matrices orthogonally similar to Y_0, then it is shown [10] that $\nabla\psi(Y) = [Y,[Y,N]]$ and thus (1) is precisely the gradient system $Y' = -\nabla\psi(Y)$. In this way, the double-bracket flow acts to minimize ψ: a fixed point $Y_\infty = \lim_{t\to\infty} Y(t)$ is a local minimizer of ψ [6].

The double-bracket flow can be used to diagonalize real symmetric matrices, and thus to find their eigenvalues: Brocket [6] showed that if N is a real diagonal matrix and both Y_0 and N have unrepeated eigenvalues, then $Y(t)$ tends exponentially to a diagonal matrix as $t \to +\infty$ and the eigenvalues are sorted accordingly to the diagonal entries of N. Other applications include sorting lists and solving certain linear programming problems [4].

Part of the flexibility and appeal of system (1) comes also from its dependence on the (arbitrary) matrix N. In fact, different choices of N correspond to special continuous realization processes. Thus, if $N = \mathrm{diag}(1,2,\ldots,n)$ and Y is tridiagonal, then (1) gives the Toda flow on tridiagonal matrices [4], whereas if it is chosen as the (nonconstant) matrix $N = \mathrm{diag}(Y)$, the corresponding flow may be regarded as a continuous analogue of the iterates generated by the Jacobi method of diagonalization [10].

While the double-bracket equation is relatively well understood from a theoretical point of view, there remains the question of efficiently computing their solutions. In [16] a numerical integration algorithm which produces an isospectral solution is proposed. The scheme is aimed primarily to evaluate the eigenvalues of Y_0 rather than to approximate the solution of (1) and has order one only.

On the other hand, several numerical methods, including families of Lie-group methods [12,21], have been designed during the last few years for Eq. (2) preserving under discretization its most important property, isospectrality [7]. In essence, the idea is to write the solution of (2) in the representation (3) and, instead of computing Y directly, in each step an orthogonal matrix Q_{k+1} is evaluated, so that $Y_{k+1} = Q_{k+1}Y_kQ_{k+1}^{\mathrm{T}}$. The matrix Q_{k+1} is chosen as the solution of the initial value problem

$$Q_{k+1}' = A(t, Q_{k+1}Y_kQ_{k+1}^{\mathrm{T}})Q_{k+1}, \quad Q_{k+1}(kh) = I$$

which is a particular example of a Lie-group flow: the solution evolves in the Lie group SO(n) for all t.

Recently, Iserles [11] has proposed to discretize Eq. (1) with a conveniently modified version of the Magnus series. As it is well known, for the linear matrix differential equation

$$Y' = A(t)Y, \quad Y(0) = Y_0 \tag{5}$$

the Magnus series provides the solution in the form

$$Y(t) = e^{\Omega(t)} Y_0, \tag{6}$$

where Ω is expanded as an infinite linear combination of multiple integrals over iterated commutators [14]

$$\begin{aligned}\Omega(t) = \Omega_1 + \Omega_2 + \Omega_3 + \cdots &= \int_0^t A_1 \, dt_1 + \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 \, [A_1, A_2] \\ &+ \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1,[A_2,A_3]] + [A_3,[A_2,A_1]]) + \cdots\end{aligned} \tag{7}$$

with $A_i \equiv A(t_i)$. The first analysis of the Magnus expansion as a numerical procedure for integrating (5) was given in [13], and subsequently several high efficient integration schemes up to eighth order have been obtained involving the minimum number of commutators [2,3].

In the approach developed in [11], the double-bracket flow is represented in the form $Y(t) = \exp(\Omega(t)) Y_0 \exp(-\Omega(t))$ and the Taylor expansion of Ω is constructed explicitly identifying individual expansion terms with certain rooted trees with bicolour leaves.

In this paper, by using techniques pioneered in [1], we construct Ω as an infinite series by recurrences and obtain a bound for the radius of convergence of the expansion. Then, by truncating appropriately the expansion we get approximate solutions up to order four with a much reduced number of commutators. These are used as numerical integration schemes for the double-bracket equation that preserve the main features of the exact solution and are computationally more efficient than another isospectral method for this particular problem.

2. The Magnus expansion for the double-bracket equation

2.1. Exponential representation

The point of departure is to consider representation (3) for $Y(t)$ and write the orthogonal matrix $Q(t)$ as $Q(t) = \exp(\Omega(t))$, with Ω skew-symmetric. Then

$$Y(t) = e^{\Omega(t)} Y_0 e^{-\Omega(t)} = e^{\mathrm{ad}_\Omega} Y_0, \quad t \geqslant 0, \tag{8}$$

where $e^{\mathrm{ad}_\Omega} = \sum_{m=0}^{\infty} (1/m!) \mathrm{ad}_\Omega^m$ and ad_Ω is the adjoint operator in the Lie algebra [19]: $\mathrm{ad}_\Omega^0 A = A$, $\mathrm{ad}_\Omega^m A = [\Omega, \mathrm{ad}_\Omega^{m-1} A]$. Differentiating (8) leads to

$$Y' = \frac{d}{dt}(e^{\Omega(t)}) Y_0 e^{-\Omega(t)} + e^{\Omega(t)} Y_0 \frac{d}{dt}(e^{-\Omega(t)}),$$

but [20]

$$\frac{d}{dt}(e^{B(t)}) = d\exp_{B(t)}(B'(t)) e^{B(t)} \equiv \frac{e^{\mathrm{ad}_{B(t)}} - I}{\mathrm{ad}_{B(t)}} B'(t) e^{B(t)},$$

so that

$$Y' = [d\exp_\Omega(\Omega'), Y] = [[Y, N], Y]$$

for all Y. This is satisfied if

$$d\exp_{\Omega} \Omega' = [Y, N].$$

By inverting the $d\exp$ operator we arrive finally at the corresponding 'dexpinv equation' for the double-bracket flow [11]

$$\Omega' = d\exp_{\Omega}^{-1}[\mathrm{e}^{\mathrm{ad}_{\Omega}} Y_0, N], \quad \Omega(0) = 0$$

or, equivalently,

$$\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^k [\mathrm{e}^{\mathrm{ad}_{\Omega}} Y_0, N], \quad \Omega(0) = 0, \tag{9}$$

where B_k is the kth Bernoulli number. Thus, instead of solving (1), one has to solve nonlinear Eq. (9) in the Lie algebra $\mathfrak{so}(n)$.

2.2. Recurrence for the Magnus series

To clarify the discussion we introduce a parameter $\varepsilon > 0$ multiplying N, so that Eq. (1) reads

$$Y' = [[Y, \varepsilon N], Y]$$

and accordingly

$$Y = \mathrm{e}^{\Omega(\varepsilon,t)} Y_0 \mathrm{e}^{-\Omega(\varepsilon,t)}, \tag{10}$$

where now

$$\frac{\partial \Omega}{\partial t} = d\exp_{\Omega}^{-1}([\mathrm{e}^{\mathrm{ad}_{\Omega}} Y_0, \varepsilon N]), \quad \Omega(\varepsilon, 0) = 0. \tag{11}$$

We seek to expand $\Omega(\varepsilon, t)$ in (10) as an infinite series in ε

$$\Omega(\varepsilon, t) = \sum_{n=1}^{\infty} \varepsilon^n \Omega_n(t), \tag{12}$$

which is called, by analogy with the linear case, the Magnus series for this particular problem. Our purpose is to determine the terms Ω_n by a recursion procedure.

Theorem 1. *The coefficients $\Omega_n(t)$ in expansion (12) are determined by the recursion formula*

$$\Omega_1(t) = t[Y_0, N]$$

$$\Omega_n(t) = \left[\sum_{j=1}^{n-1} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=n-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \int_0^t \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}} Y_0 \,\mathrm{d}\tau, N \right]$$

$$+\sum_{j=1}^{n-1}\frac{B_j}{j!}\sum_{\substack{k_1+\cdots+k_j=n-1\\ k_1\geqslant 1,\ldots,k_j\geqslant 1}}\int_0^t \mathrm{ad}_{\Omega_{k_1}}\cdots\mathrm{ad}_{\Omega_{k_j}}([Y_0,N])\,\mathrm{d}\tau$$

$$+\sum_{j=2}^{n-1}\int_0^t \mathrm{d}\tau\left(\sum_{l=1}^{j-1}\frac{B_l}{l!}\sum_{\substack{k_1+\cdots+k_l=j-1\\ k_1\geqslant 1,\ldots,k_l\geqslant 1}}\mathrm{ad}_{\Omega_{k_1}}\cdots\mathrm{ad}_{\Omega_{k_l}}\right)$$

$$\left(\left[\sum_{p=1}^{n-j}\frac{1}{p!}\sum_{\substack{k_1+\cdots+k_p=n-j\\ k_1\geqslant 1,\ldots,k_p\geqslant 1}}\mathrm{ad}_{\Omega_{k_1}}\cdots\mathrm{ad}_{\Omega_{k_p}}Y_0,N\right]\right),\qquad n\geqslant 2 \tag{13}$$

Proof. If we denote by $\mathcal{O}(\varepsilon^k)$ any function of the form $\varepsilon\mapsto\varepsilon^k f(\varepsilon)$, where f is analytic around $\varepsilon=0$, it is clear that

$$\frac{\partial\Omega}{\partial t}(\varepsilon,t)=\sum_{j=1}^{n}\varepsilon^j\Omega_j'(t)+\mathcal{O}(\varepsilon^{n+1})$$

and

$$\mathrm{ad}_{\Omega(\varepsilon,t)}=\varepsilon\,\mathrm{ad}_{\Omega_1}+\varepsilon^2\,\mathrm{ad}_{\Omega_2}+\cdots+\varepsilon^{n-1}\,\mathrm{ad}_{\Omega_{n-1}}+\mathcal{O}(\varepsilon^n).$$

In general,

$$\mathrm{ad}^j_{\Omega(\varepsilon,t)}=\sum_{l=j}^{n-1}\varepsilon^l\sum_{\substack{k_1+\cdots+k_j=l\\ k_1\geqslant 1,\ldots,k_j\geqslant 1}}\mathrm{ad}_{\Omega_{k_1}}\mathrm{ad}_{\Omega_{k_2}}\cdots\mathrm{ad}_{\Omega_{k_j}}+\mathcal{O}(\varepsilon^n).$$

On the other hand,

$$\begin{aligned}
d\exp_\Omega^{-1}([\mathrm{e}^{\mathrm{ad}_\Omega}Y_0,\varepsilon N])&=\varepsilon[\mathrm{e}^{\mathrm{ad}_\Omega}Y_0,N]+\varepsilon\sum_{j=1}^{n-1}\frac{B_j}{j!}\mathrm{ad}^j_\Omega([\mathrm{e}^{\mathrm{ad}_\Omega}Y_0,N])+\mathcal{O}(\varepsilon^{n+1})\\
&=\varepsilon[Y_0,N]+\varepsilon\left[\sum_{j=1}^{n-1}\frac{1}{j!}\mathrm{ad}^j_\Omega Y_0,N\right]+\varepsilon\sum_{j=1}^{n-1}\frac{B_j}{j!}\mathrm{ad}^j_\Omega([Y_0,N])\\
&\quad+\varepsilon\sum_{j=1}^{n-2}\frac{B_j}{j!}\mathrm{ad}^j_\Omega\left(\left[\sum_{k=1}^{n-2}\frac{1}{k!}\mathrm{ad}^k_\Omega Y_0,N\right]\right)+\mathcal{O}(\varepsilon^{n+1})\\
&\equiv\varepsilon[Y_0,N]+\mathscr{A}+\mathscr{B}+\mathscr{C}+\mathcal{O}(\varepsilon^{n+1}).
\end{aligned}$$

Now we analyse each term in this expression. First of all

$$\mathscr{A} = \varepsilon \left[\sum_{j=1}^{n-1} \frac{1}{j!} \mathrm{ad}_\Omega^j\, Y_0, N \right] = \varepsilon \left[\sum_{j=1}^{n-1} \frac{1}{j!} \sum_{l=j}^{n-1} \varepsilon^l \sum_{\substack{k_1+\cdots+k_j=l \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}}\, Y_0, N \right]$$

$$+\mathcal{O}(\varepsilon^{n+1}) = \left[\sum_{l=2}^{n} \varepsilon^l \sum_{j=1}^{l-1} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}}\, Y_0, N \right] + \mathcal{O}(\varepsilon^{n+1}).$$

By following a similar procedure we get

$$\mathscr{B} = \varepsilon \sum_{j=1}^{n-1} \frac{B_j}{j!} \mathrm{ad}_\Omega^j([Y_0, N]) = \sum_{l=2}^{n} \varepsilon^l \sum_{j=1}^{l-1} \frac{B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}}\, ([Y_0, N]) + \mathcal{O}(\varepsilon^{n+1}).$$

Finally, a straightforward calculation shows that

$$\mathscr{C} = \varepsilon \sum_{j=1}^{n-2} \frac{B_j}{j!} \mathrm{ad}_\Omega^j \left(\left[\sum_{l=1}^{n-2} \frac{1}{l!} \mathrm{ad}_\Omega^l\, Y_0, N \right] \right) = \sum_{s=2}^{n-1} \varepsilon^s \sum_{j=1}^{s-1} \frac{B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=s-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}}$$

$$\left(\sum_{l=1}^{n-2} \varepsilon^l \left[\sum_{p=1}^{l} \frac{1}{p!} \sum_{\substack{k_1+\cdots+k_p=l \\ k_1 \geqslant 1,\ldots,k_p \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_p}}\, Y_0, N \right] \right) + \mathcal{O}(\varepsilon^{n+1})$$

$$= \sum_{j=3}^{n} \varepsilon^j \sum_{l=2}^{j-1} \left(\sum_{m=1}^{l-1} \frac{B_m}{m!} \sum_{\substack{k_1+\cdots+k_m=l-1 \\ k_1 \geqslant 1,\ldots,k_m \geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_m}} \right)$$

$$\left(\left[\sum_{p=1}^{j-l} \frac{1}{p!} \sum_{\substack{r_1+\cdots+r_p=j-l \\ r_1 \geqslant 1,\ldots,r_p \geqslant 1}} \mathrm{ad}_{\Omega_{r_1}} \cdots \mathrm{ad}_{\Omega_{r_p}}\, Y_0, N \right] \right) + \mathcal{O}(\varepsilon^{n+1}).$$

If we substitute these expressions for $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ in (11) and identify the coefficients of ε^l on both sides we get

$$\Omega_1'(t) = [Y_0, N],$$

$$\Omega_2'(t) = [\mathrm{ad}_{\Omega_1} Y_0, N] + B_1 \mathrm{ad}_{\Omega_1}([Y_0, N])$$

and, for $l \geqslant 3$,

$$\Omega_l'(t) = \left[\sum_{j=1}^{l-1} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1\geqslant 1,\ldots,k_j\geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}} Y_0, N \right]$$

$$+ \sum_{j=1}^{l-1} \frac{B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1\geqslant 1,\ldots,k_j\geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_j}} ([Y_0, N])$$

$$+ \sum_{j=2}^{l-1} \left(\sum_{s=1}^{j-1} \frac{B_s}{s!} \sum_{\substack{k_1+\cdots+k_s=j-1 \\ k_1\geqslant 1,\ldots,k_s\geqslant 1}} \mathrm{ad}_{\Omega_{k_1}} \cdots \mathrm{ad}_{\Omega_{k_s}} \right)$$

$$\left(\left[\sum_{p=1}^{l-j} \frac{1}{p!} \sum_{\substack{r_1+\cdots+r_p=l-j \\ r_1\geqslant 1,\ldots,r_p\geqslant 1}} \mathrm{ad}_{\Omega_{r_1}} \cdots \mathrm{ad}_{\Omega_{r_p}} Y_0, N \right] \right).$$

The initial condition $\Omega(\varepsilon, 0) = \sum_{l\geqslant 1} \varepsilon^l \, \Omega_l(0) = 0$ for all $\varepsilon > 0$ implies $\Omega_l(0) = 0$. This proves the theorem. □

2.3. Convergence of the Magnus series

Our next objective is to examine the convergence of the Magnus series $\sum_{i\geqslant 1} \Omega_i$. To this end we choose a norm in $\mathfrak{so}(n)$ and a number $\mu > 0$ such that

$$\|[X, Y]\| \leqslant 2\mu \, \|X\| \, \|Y\| \tag{14}$$

for all X, Y in $\mathfrak{so}(n)$. Here μ incorporates any additional information one has on the norm. Of course, for a norm in $\mathfrak{so}(n)$ satisfying $\|XY\| \leqslant \|X\| \, \|Y\|$ inequality (14) holds with $\mu = 1$. The advantage of considering (14) rests in the fact that for some norms μ is actually less than 1. For instance, if $\|\cdot\|$ is the Frobenius norm then $\mu = \frac{1}{\sqrt{2}}$ [11].

To proceed, let us consider the series

$$v(\varepsilon, t) = \sum_{j=1}^{\infty} \varepsilon^j \|\Omega_j(t)\|. \tag{15}$$

Lemma 2. *With a norm in $\mathfrak{so}(n)$ satisfying (14) then*

$$v(\varepsilon, t) \leqslant \frac{1}{\mu} G^{-1}(2\mu^2 \varepsilon t \|N\| \|Y_0\|), \quad 0 \leqslant t \leqslant t_c \tag{16}$$

holds, where

$$G(\tau)=\int_0^{\tau}\frac{\mathrm{e}^{-2x}}{2+x(1-\cot x)}\,\mathrm{d}x \tag{17}$$

and $t_c=\sup\{t\geqslant 0: 2\mu^2\varepsilon t\|N\|\|Y_0\|<G(\pi)\equiv\xi=0.34438794\ldots\}$.

Proof. For a norm satisfying (14), repeated application of the triangle inequality to (13) leads for $l\geqslant 2$ to

$$\begin{aligned}\|\Omega_l(t)\| \leqslant{} & 2\mu\|N\|\|Y_0\|\sum_{j=1}^{l-1}(2\mu)^j\frac{1}{j!}\sum_{\substack{k_1+\cdots+k_j=l-1\\ k_1\geqslant 1,\ldots,k_j\geqslant 1}}\int_0^t\|\Omega_{k_1}\|\cdots\|\Omega_{k_j}\|\,\mathrm{d}\tau\\ &+2\mu\|N\|\|Y_0\|\sum_{j=1}^{l-1}(2\mu)^j\frac{|B_j|}{j!}\sum_{\substack{k_1+\cdots+k_j=l-1\\ k_1\geqslant 1,\ldots,k_j\geqslant 1}}\int_0^t\|\Omega_{k_1}\|\cdots\|\Omega_{k_j}\|\,\mathrm{d}\tau\\ &+2\mu\|N\|\|Y_0\|\sum_{j=2}^{l-1}\sum_{s=1}^{j-1}(2\mu)^s\frac{|B_s|}{s!}\sum_{\substack{k_1+\cdots+k_s=j-1\\ k_1\geqslant 1,\ldots,k_s\geqslant 1}}\int_0^t\|\Omega_{k_1}\|\cdots\|\Omega_{k_s}\|\\ &\cdot\left(\sum_{p=1}^{l-j}(2\mu)^p\frac{1}{p!}\sum_{\substack{r_1+\cdots+r_p=l-j\\ r_1\geqslant 1,\ldots,r_p\geqslant 1}}\|\Omega_{r_1}\|\cdots\|\Omega_{r_p}\|\right)\mathrm{d}\tau. \end{aligned}\tag{18}$$

For a given positive integer N, let us introduce the truncated series $v_N(\varepsilon,t)=\sum_{l=1}^{N}\varepsilon^l\|\Omega_l(t)\|$. Then it is easy to show that

$$(v_N(\varepsilon,t))^p=\sum_{l=p}^{pN}\varepsilon^l\sum_{\substack{k_1+\cdots+k_p=l\\ k_1\geqslant 1,\ldots,k_p\geqslant 1}}\|\Omega_{k_1}\|\cdots\|\Omega_{k_p}\|, \tag{19}$$

where p is any positive integer. From inequality (18) we have

$$\sum_{l=2}^{N}\varepsilon^l\|\Omega_l(t)\|\leqslant 2\mu\varepsilon\|N\|\|Y_0\|(U_1+U_2+U_3). \tag{20}$$

Here

$$U_1\equiv\sum_{l=2}^{N}\sum_{j=1}^{l-1}(2\mu)^j\frac{1}{j!}\sum_{\substack{k_1+\cdots+k_j=l-1\\ k_1\geqslant 1,\ldots,k_j\geqslant 1}}\varepsilon^{l-1}\int_0^t\|\Omega_{k_1}\|\cdots\|\Omega_{k_j}\|\,\mathrm{d}\tau$$

$$\leqslant \sum_{j=1}^{N-1} (2\mu)^j \frac{1}{j!} \sum_{l=j+1}^{N} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \varepsilon^{l-1} \int_0^t \|\Omega_{k_1}\| \cdots \|\Omega_{k_j}\| \, \mathrm{d}\tau$$

$$= \sum_{j=1}^{N-1} (2\mu)^j \frac{1}{j!} \sum_{l=j}^{N-1} \varepsilon^l \sum_{\substack{k_1+\cdots+k_j=l \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \int_0^t \|\Omega_{k_1}\| \cdots \|\Omega_{k_j}\| \, \mathrm{d}\tau$$

$$\leqslant \sum_{j=1}^{N-1} (2\mu)^j \frac{1}{j!} \int_0^t (v_N(\varepsilon, s))^j \, \mathrm{d}s, \tag{21}$$

where the last inequality follows readily from (19). Analogously,

$$U_2 \equiv \sum_{l=2}^{N} \sum_{j=1}^{l-1} (2\mu)^j \frac{|B_j|}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1 \geqslant 1,\ldots,k_j \geqslant 1}} \varepsilon^{l-1} \int_0^t \|\Omega_{k_1}\| \cdots \|\Omega_{k_j}\| \, \mathrm{d}s$$

$$\leqslant \sum_{j=1}^{N-1} (2\mu)^j \frac{|B_j|}{j!} \int_0^t (v_N(\varepsilon, s))^j \, \mathrm{d}s. \tag{22}$$

Finally,

$$U_3 \equiv \sum_{l=3}^{N} \varepsilon^{l-1} \sum_{j=2}^{l-1} \left(\sum_{s=1}^{j-1} (2\mu)^s \frac{|B_s|}{s!} \sum_{\substack{k_1+\cdots+k_s=j-1 \\ k_1 \geqslant 1,\ldots,k_s \geqslant 1}} \int_0^t \mathrm{d}\tau \, \|\Omega_{k_1}\| \cdots \|\Omega_{k_s}\| \right)$$

$$\left(\sum_{p=1}^{l-j} (2\mu)^p \frac{1}{p!} \sum_{\substack{r_1+\cdots+r_p=l-j \\ r_1 \geqslant 1,\ldots,r_p \geqslant 1}} \|\Omega_{r_1}\| \cdots \|\Omega_{r_p}\| \right)$$

$$= \int_0^t \mathrm{d}\tau \sum_{j=2}^{N-1} \sum_{l=j}^{N-1} \varepsilon^l \left(\sum_{s=1}^{j-1} (2\mu)^s \frac{|B_s|}{s!} \sum_{\substack{k_1+\cdots+k_s=j-1 \\ k_1 \geqslant 1,\ldots,k_s \geqslant 1}} \|\Omega_{k_1}\| \cdots \|\Omega_{k_s}\| \right)$$

$$\left(\sum_{p=1}^{l+1-j} (2\mu)^p \frac{1}{p!} \sum_{\substack{r_1+\cdots+r_p=l+1-j \\ r_1 \geqslant 1,\ldots,r_p \geqslant 1}} \|\Omega_{r_1}\| \cdots \|\Omega_{r_p}\| \right).$$

In addition one has

$$\sum_{l=j}^{N-1} \varepsilon^l \sum_{p=1}^{l+1-j} (2\mu)^p \frac{1}{p!} \sum_{\substack{r_1+\cdots+r_p=l+1-j \\ r_1\geqslant 1,\ldots,r_p\geqslant 1}} \|\Omega_{r_1}\| \cdots \|\Omega_{r_p}\|$$

$$=\varepsilon^{j-1} \sum_{p=1}^{N-j} (2\mu)^p \frac{1}{p!} \sum_{l=p+j-1}^{N-1} \varepsilon^{l-(j-1)} \sum_{\substack{r_1+\cdots+r_p=l-(j-1) \\ r_1\geqslant 1,\ldots,r_p\geqslant 1}} \|\Omega_{r_1}\| \cdots \|\Omega_{r_p}\|$$

$$=\varepsilon^{j-1} \sum_{p=1}^{N-j} (2\mu)^p \frac{1}{p!} \sum_{l=p}^{N-j} \varepsilon^l \sum_{\substack{r_1+\cdots+r_p=l \\ r_1\geqslant 1,\ldots,r_p\geqslant 1}} \|\Omega_{r_1}\| \cdots \|\Omega_{r_p}\| \leqslant \varepsilon^{j-1} \sum_{p=1}^{N-j} (2\mu)^p \frac{1}{p!} v_N^p,$$

so that

$$U_3 \leqslant \int_0^t \mathrm{d}\tau \sum_{s=1}^{N-2} (2\mu)^s \frac{|B_s|}{s!} \sum_{j=s+1}^{N-1} \varepsilon^{j-1} \sum_{\substack{k_1+\cdots+k_s=j-1 \\ k_1\geqslant 1,\ldots,k_s\geqslant 1}} \|\Omega_{k_1}\| \cdots \|\Omega_{k_s}\|$$

$$\cdot \left(\sum_{p=1}^{N-j} \frac{(2\mu)^p}{p!} v_N^p \right) \leqslant \int_0^t \mathrm{d}\tau \left(\sum_{s=1}^{N-2} (2\mu)^s \frac{|B_s|}{s!} v_N^s \right) \left(\sum_{p=1}^{N} (2\mu)^p \frac{1}{p!} v_N^p \right).$$

In this way

$$v_N(\varepsilon,t) \leqslant 2\mu\|N\|\|Y_0\|\varepsilon(t+U_1+U_2+U_3)$$

$$\leqslant 2\mu\|N\|\|Y_0\|\varepsilon \left(\int_0^t \sum_{j=0}^{N-1} (2\mu)^j \frac{1}{j!} v_N^j \,\mathrm{d}s + \int_0^t \sum_{j=1}^{N} (2\mu)^j \frac{|B_j|}{j!} v_N^j \,\mathrm{d}s \right.$$

$$\left. + \int_0^t \mathrm{d}s \left(\sum_{j=1}^{N} (2\mu)^j \frac{|B_j|}{j!} v_N^j \right) \left(\sum_{p=1}^{N} (2\mu)^p \frac{1}{p!} v_N^p \right) \right)$$

$$\leqslant 2\mu\|N\|\|Y_0\|\varepsilon \left(\int_0^t \mathrm{d}s \sum_{j=0}^{N} (2\mu)^j \frac{1}{j!} v_N^j \right.$$

$$\left. + \int_0^t \mathrm{d}s \left(\sum_{j=1}^{N} (2\mu)^j \frac{|B_j|}{j!} v_N^j \right) \left(\sum_{p=0}^{N} (2\mu)^p \frac{1}{p!} v_N^p \right) \right)$$

$$= 2\mu\|N\|\|Y_0\|\varepsilon \int_0^t \mathrm{d}s \left(\sum_{j=0}^{N} (2\mu)^j \frac{|B_j|}{j!} v_N^j \right) \left(\sum_{p=0}^{N} (2\mu)^p \frac{1}{p!} v_N^p \right).$$

Taking the limit $N \to \infty$ in this expression we have

$$v(\varepsilon,t) \leqslant 2\mu\|N\|\|Y_0\|\varepsilon \int_0^t g(\mu v(\varepsilon,s))\mathrm{e}^{2\mu v(\varepsilon,s)}\,\mathrm{d}s \tag{23}$$

since

$$\sum_{j=0}^{\infty} \frac{|B_j|}{j!}(2x)^j = 2 + x(1-\cot x) \equiv g(x). \tag{24}$$

Now the proof is completed by applying a result obtained in [15] for linear Eq. (5) and the discussion in [18].

Let us introduce the function $F(\varepsilon,t) \equiv 2\mu\|N\|\|Y_0\|\varepsilon \int_0^t g(\mu v(\varepsilon,s))\mathrm{e}^{2\mu v(\varepsilon,s)}\,\mathrm{d}s$. Then

$$\frac{\partial F}{\partial t} = 2\mu\|N\|\|Y_0\|\varepsilon g(\mu v(\varepsilon,t))\mathrm{e}^{2\mu v(\varepsilon,t)} \leqslant 2\mu\|N\|\|Y_0\|\varepsilon g(\mu F(\varepsilon,t))\,\mathrm{e}^{2\mu F(\varepsilon,t)},$$

since g is a nondecreasing function in the domain $[0,\pi)$. Thus we have

$$\frac{\partial F}{\partial t}\,\frac{1}{g(\mu F)\mathrm{e}^{2\mu F}} \leqslant 2\mu\|N\|\|Y_0\|\varepsilon$$

because g is positive on the real axis. By integrating this inequality we get

$$\frac{1}{\mu}\int_0^{\mu F(\varepsilon,t)} \frac{1}{g(x)\mathrm{e}^{2x}}\,\mathrm{d}x \leqslant 2\mu\|N\|\|Y_0\|\varepsilon t$$

or

$$G(\mu F(\varepsilon,t)) \leqslant 2\mu^2\|N\|\|Y_0\|\varepsilon t,$$

where $G(t) \equiv \int_0^t (\mathrm{e}^{-2x}/g(x))\,\mathrm{d}x$. Now $G(t)$ is continuous in t for t in $[0,\pi]$ and continuously differentiable and nondecreasing in $[0,\pi)$. The inverse function $t = G^{-1}(y)$ exists in a neighbourhood of any t for which $G'(t)$ is nonzero, so the limiting value of t for which the inverse function G^{-1} exists must be one such that $G'(t) = 0$. The value of t nearest zero is precisely $t = \pi$ and the corresponding value of y is $G(\pi)$. In consequence,

$$v(\varepsilon,t) \leqslant F(\varepsilon,t) \leqslant \frac{1}{\mu}\,G^{-1}(2\mu^2\|N\|\|Y_0\|\varepsilon t)$$

for t such that $2\mu^2\|N\|\|Y_0\|\varepsilon t$ belongs to the domain of G^{-1}, i.e.,

$$2\mu^2\|N\|\|Y_0\|\varepsilon t < G(\pi) = \int_0^{\pi} \frac{1}{g(x)\mathrm{e}^{2x}}\,\mathrm{d}x \equiv \xi = 0.34438794\ldots \qquad \square$$

If we take $\varepsilon = 1$ in (16) then

$$v(\varepsilon = 1,t) = \sum_{n=1}^{\infty} \|\Omega_n(t)\| < \frac{1}{\mu}\,G^{-1}(\xi) = \frac{\pi}{\mu}$$

for $0 \leqslant t < t_c$. In other words, the Magnus series $\sum_{n \geqslant 1} \Omega_n(t)$ is absolutely convergent for $0 \leqslant t < t_c$. We have then proved the following

Theorem 3. *The double-bracket equation* (1) *admits a solution*

$$Y(t) = e^{\Omega(t)} Y_0 e^{-\Omega(t)},$$

where the series $\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t)$ *given by recurrence* (13) *is absolutely convergent for every value of* t *satisfying*

$$0 \leqslant t \leqslant t_c = \frac{1}{\mu^2 \xi \|N\| \|Y_0\|}$$

with

$$\frac{1}{\xi} = \frac{1}{2} \int_0^{\pi} \frac{e^{-2x}}{2 + x(1 - \cot x)} \, dx = \frac{1}{5.8074...}.$$

2.4. Structure of the Ω series

The recurrences given in Theorem 1 can be easily programmed in a symbolic computation package, thus providing, in principle, any order of the expansion. In particular, the first terms of the Magnus series for the double-bracket flow read

$$\begin{aligned}
\Omega_1(t) &= t[Y_0, N], \\
\Omega_2(t) &= \tfrac{1}{2} t^2 [Y_0, N, Y_0, N], \\
\Omega_3(t) &= t^3 (-\tfrac{5}{36} [Y_0, Y_0, N, N, Y_0, N] + \tfrac{1}{3} [Y_0, N, Y_0, N, Y_0, N] - \tfrac{1}{36} [N, N, Y_0, Y_0, Y_0, N]), \\
\Omega_4(t) &= t^4 (\tfrac{1}{36} [Y_0, N, Y_0, Y_0, N, N, Y_0, N] - \tfrac{1}{12} [Y_0, N, Y_0, N, Y_0, N, Y_0, N] \\
&\quad + \tfrac{1}{72} [Y_0, N, N, N, Y_0, Y_0, Y_0, N] - \tfrac{5}{36} [N, Y_0, Y_0, Y_0, N, N, Y_0, N] \\
&\quad + \tfrac{1}{3} [N, Y_0, Y_0, N, Y_0, N, Y_0, N] + \tfrac{1}{72} [N, Y_0, N, N, Y_0, Y_0, Y_0, N] \\
&\quad - \tfrac{7}{24} [N, N, Y_0, N, Y_0, Y_0, Y_0, N] + \tfrac{1}{6} [N, N, N, Y_0, Y_0, Y_0, Y_0, N]),
\end{aligned} \tag{25}$$

where $[A, B, \ldots, Y, Z]$ stands for the nested commutator $[A, [B, \ldots, [Y, Z]]]$.

At this point, it is useful to determine the number of independent terms appearing in Ω_m for all $m \geqslant 1$. In fact, an upper bound on this number can be obtained by noting that (i) Ω belongs to the free Lie algebra generated by $\{Y_0, N\}$ and (ii) there are exactly m occurrences of Y_0 and N in each Ω_m. If we arbitrarily assign a unit grade to each generator, then the problem is determining the dimension of the linear space $\mathfrak{S}_{2m}$ spanned by all $2m$-grade terms with m occurrences of Y_0 and N. This is given in [5,11]

$$\chi_m = \dim \mathfrak{S}_{2m} = \frac{1}{2m} \sum_{d|m} \mu(d) \binom{2m/d}{m/d}. \tag{26}$$

Here $\mu(d)$ is the Möbius function and the sum is extended over all $d \in \mathbb{N}$ which are divisors of the integer m [5]. The first 10 values of χ_m are

$$1, 1, 3, 8, 25, 75, 245, 800, 2700, 9225.$$

Observe that, at least up to $m = 4$, χ_m provides the actual number of terms in Ω_m.

3. Numerical integrators based on the Magnus expansion

The procedure to implement the Magnus expansion as a numerical integration algorithm for the double-bracket flow involves three steps. First, the Ω series must be truncated at the appropriate order. Second, some strategy to reduce to a minimum the total number of commutators is required. Third, one must evaluate the exponential map from the Lie algebra $\mathfrak{so}(n)$ to the Lie group $\mathrm{SO}(n)$.

Concerning the first aspect, it is clear that for achieving an mth-order integration method only terms up to Ω_m have to be considered. With respect to the third step, several approximation schemes to the matrix exponential have been designed such that the outcome lies in the correct Lie group and differs from the exact mapping in a way that is consistent with the order of the underlying integration method [8,9,12].

In view of the number of commutators already present in (25) and the explosive growth of the dimension χ_m with m it does not make much sense, in principle, consider integration methods of order higher than four. In addition, it should be noticed that in general the actual number of commutators appearing in Ω_m is much higher than χ_m. For instance, in Table 1 we show the dimension and the number NC_χ of commutators involved in the truncated series $\Omega^{[m]} \equiv \sum_{i=1}^{m} \Omega_i$ up to $m = 4$ according to (25). If, as is usually the case, $2n^3$ operations are needed for evaluating one commutator, n being the dimension of the matrices involved, then it is evident that reducing to a minimum the number of commutators is a key point in order to build efficient numerical schemes.

In fact, it turns out to be more advantageous to work directly with the recurrence (13) rather than with the explicit expression (25) for two reasons. First, the number of commutators involved in (13) is significantly lower: for a given $m \geqslant 2$, one can prove that there are exactly $\rho_m \equiv m^2 - 2m + 3$

Table 1
Dimension and number of commutators in the truncated series $\Omega^{[m]}$

$\Omega^{[m]} \equiv \sum_{i=1}^{m} \Omega_i$	$\sum_{i=1}^{m} \chi_i$	NC_χ	$\sum_{i=1}^{m} \rho_i$	NC_ρ
$\Omega^{[1]}$	1	1	1	1
$\Omega^{[2]}$	2	3	4	3
$\Omega^{[3]}$	5	12	10	7
$\Omega^{[4]}$	13	26	21	11
$\Omega^{[5]}$	38		39	
$\Omega^{[6]}$	113		66	
$\Omega^{[7]}$	358		104	
$\Omega^{[8]}$	1158		155	

NC_χ stands for the number of commutators appearing in (25), whereas NC_ρ is the number of commutators appearing after optimization.

commutators not previously available in Ω_m. For comparison with χ_m, the first 10 values of ρ_m are

$$1, 3, 6, 11, 18, 27, 38, 51, 66, 83,$$

so that the construction of integration methods of order higher than four is more feasible with this approach. Second, these numbers can be reduced even further by generalizing the optimization procedure designed in [3] for Lie-group methods based on the Magnus expansion for linear differential equations. For instance, a detailed analysis of recurrence (13) allows to obtain expressions for $\Omega^{[m]}$ involving a number of commutators NC_ρ less than NC_χ for $m > 2$. These numbers are also collected in Table 1. In particular, one has the following expressions for $\Omega^{[m]}$ up to $m = 4$:

- *Order* 1: $\Omega^{[1]}(h) = hd_1 \quad \text{with } d_1 = [Y_0, N]. \qquad (27)$

- *Order* 2:
$$\begin{aligned} d_2 &= [Y_0, d_1] \\ d_3 &= [N, d_2] \\ \Omega^{[2]}(h) &= hd_1 + \tfrac{1}{2} h^2 d_3. \end{aligned} \qquad (28)$$

- *Order* 3:
$$\begin{aligned} d_4 &= [Y_0, d_3], \\ d_5 &= [d_1, d_2], \\ d_6 &= [N, d_4 + d_5], \\ \Omega^{[3]}(h) &= hd_1 + \tfrac{1}{2} h^2 d_3 + \tfrac{1}{6} h^3 (d_6 - \tfrac{1}{2}[d_1, d_3]). \end{aligned} \qquad (29)$$

- *Order* 4:
$$\begin{aligned} & d_7 = [Y_0, d_6], \quad d_8 = [d_2, d_3], \\ & d_9 = [d_1, d_4 + d_5], \quad d_{10} = [N, d_7 - 2d_8 + d_9], \\ & d_{11} = [d_1, d_3 + \tfrac{1}{2} hd_6], \\ & \Omega^{[4]}(h) = hd_1 + \tfrac{1}{2} h^2 d_3 + \tfrac{1}{6} h^3 d_6 + \tfrac{1}{24} h^4 d_{10} - \tfrac{1}{12} h^3 d_{11}. \end{aligned} \qquad (30)$$

The resulting mth-order algorithms ($m \leqslant 4$) based on the Magnus expansion read

$$Y(t_k + h) = \mathrm{e}^{\Omega^{[m]}(h)}\, Y(t_k)\, \mathrm{e}^{-\Omega^{[m]}(h)}, \qquad (31)$$

where Y_0 has to be replaced by $Y(t_k)$ in the corresponding expression of $\Omega^{[m]}(h)$, $m = 1, 2, 3, 4$, and involve 1, 3, 7 and 11 commutators, respectively. This represents a meaningful saving with respect to the naive implementation (25).

4. Numerical examples

Next, we illustrate some of the properties of the fourth-order integration method (30)–(31) based on the Magnus expansion for the double-bracket flow (M4). Our purpose, rather than providing a complete analysis of M4 as a numerical integrator, is just to show how it behaves in practice

Table 2
Computational cost of different fourth-order methods for the double-bracket flow

Method	NC	P	Ex
M4	11	24	1
RKMK4	6	20	4
RK4	8	16	0

P also includes the matrix–matrix products coming from the commutators.

in comparison with other well-known fourth-order schemes. In particular, we consider the classical Runge–Kutta method (RK4) with Butcher tableau

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \tag{32}$$

and the Runge–Kutta–Munthe-Kaas integrator (RKMK4) also based on the tableau (32) with the algorithm proposed in [17]. The computational cost of the methods may be estimated by considering the total number of commutators (or matrix–matrix products) and matrix exponentials involved. These numbers are collected in Table 2. Here NC stands for the number of commutators, Ex is the number of matrix exponentials and P indicates the total number of matrix–matrix products (including commutators).

It should be noticed that in (31) only the matrix exponential $Q = \exp(\Omega^{[m]})$ has to be computed because $\exp(-\Omega^{[m]}) = Q^{\mathrm{T}}$ by construction. In general, each action $\mathrm{e}^{U} Y(t_k)\mathrm{e}^{-U}$ in M4 and RKMK4 requires the calculation of one matrix exponential and two matrix–matrix products.

As we can observe, the computational cost of RK4 is smaller than the corresponding to M4 and RKMK4, although these preserve the Lie group structure of the flow by construction. On the other hand, since M4 requires less matrix exponentials than RKMK4, one expects that for a sufficiently high dimension n the new Lie group method M4 will be more efficient than RKMK4.

Example 1. As a first illustration we consider a random initial condition $Y_0 \in \mathrm{Sym}\,(n = 10)$ with eigenvalues $1, 2, \dots, 10$ and the matrix $N = \mathrm{diag}(1, 2, \dots, 10)$. As we mentioned in the introduction, in that case the flow tends to a diagonal matrix. We check numerically how the Lyapunov function $\psi(Y)$ (4) is minimized along the evolution with M4 by determining ψ_∞ and then $\mathrm{Lf} \equiv \psi(Y) - \psi_\infty$ as a function of time with $h = 0.03$. We also compute

$$S(t) \equiv \sum_{j \neq l} |y_{jl}|^2,$$

the sum of the squares of the off-diagonal elements of the matrix $Y(t_k)$. These two functions are depicted in Fig. 1, where, for comparison, we also present the results achieved by the second-order

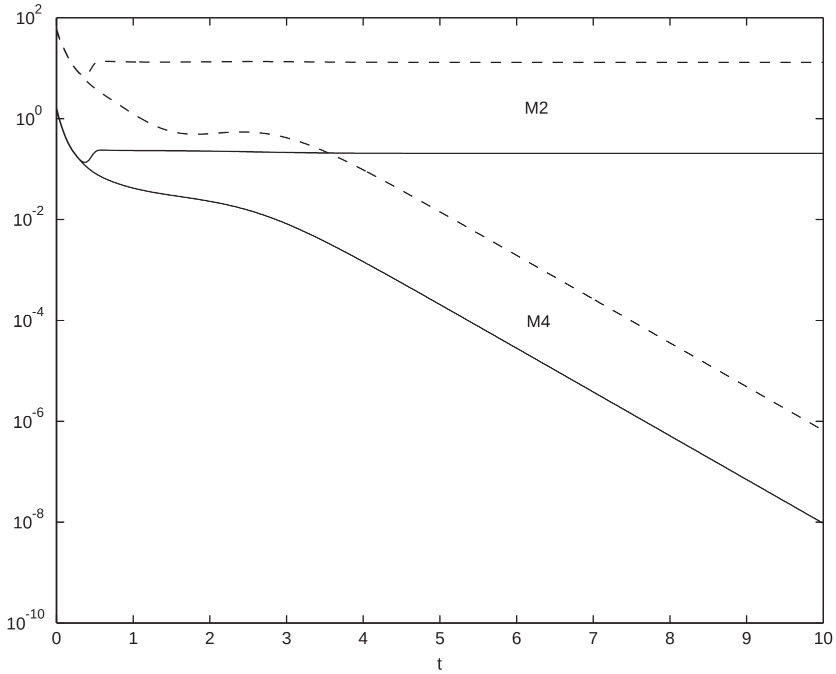

Fig. 1. Convergence of the numerical solution of Example 1 to a diagonal matrix. Solid curves correspond to Lf $\equiv \psi(Y) - \psi_\infty$ and dashed lines stand for $S(t)$, both computed with methods M2 and M4.

method M2 based on Magnus expansion (28). We observe, in particular, that the numerical solution obtained with M4 converges to a diagonal matrix (even when h is much larger than the convergence time $t_c \simeq 8.94 \cdot 10^{-4}$), whereas M2 requires a smaller step size to recover the correct asymptotic behaviour. In this case the use of the higher order numerical method M4 allows to consider large time steps while preserving the qualitative features of the system.

Next, for this same problem, initial condition and step size we calculate the difference between the diagonal elements of the numerical solution $Y(t_f = 10)$ and the eigenvalues of Y_0 with M2, M4, RKMK4 and RK4. The logarithm of the corresponding results are collected in Table 3.

As we can see, the Lie-group solvers M4 and RKMK4 applied to the double-bracket equation provide an excellent approximation to the eigenvalues of a symmetric real matrix just by computing numerically the flow for a sufficiently large time. The different asymptotic behaviour of the solution provided by M2 manifests in discrepancies in two eigenvalues of $Y(t_f)$.

Example 2. Next, we analyse the efficiency of the fourth-order algorithms M4, RKMK4 and RK4 when both N and Y_0 are taken as random symmetric matrices of dimension $n = 10, 20, 40$. The integration is carried out in the interval $t \in [0, 6]$ for several values of h and the error is determined at the final time $t_f = 6$ by computing the Frobenius norm of the difference between approximate and the exact solution matrices. We represent this error as a function of the computational effort measured both in CPU time and in terms of the number of flops required. The computation is

Table 3
Logarithm of the difference between diagonal elements of $Y(t = 10)$ and eigenvalues of Y_0 computed with M2 and different fourth-order methods for the double-bracket flow

M2	M4	RKMK4	RK4
−0.0989	−8.3425	−8.3459	−2.8482
−8.9343	−8.4574	−8.4620	−2.6065
−8.9351	−8.9772	−8.9768	−3.0952
−6.4336	−6.4836	−6.4841	−2.8445
−6.4337	−6.4838	−6.4843	−2.3482
−10.6260	−10.6771	−10.6751	−2.5853
−9.9582	−9.8991	−9.8966	−2.6390
−9.2894	−9.2862	−9.2851	−4.0992
−9.2770	−9.4513	−9.4521	−2.1639
−0.0989	−9.7350	−9.7322	−2.3158

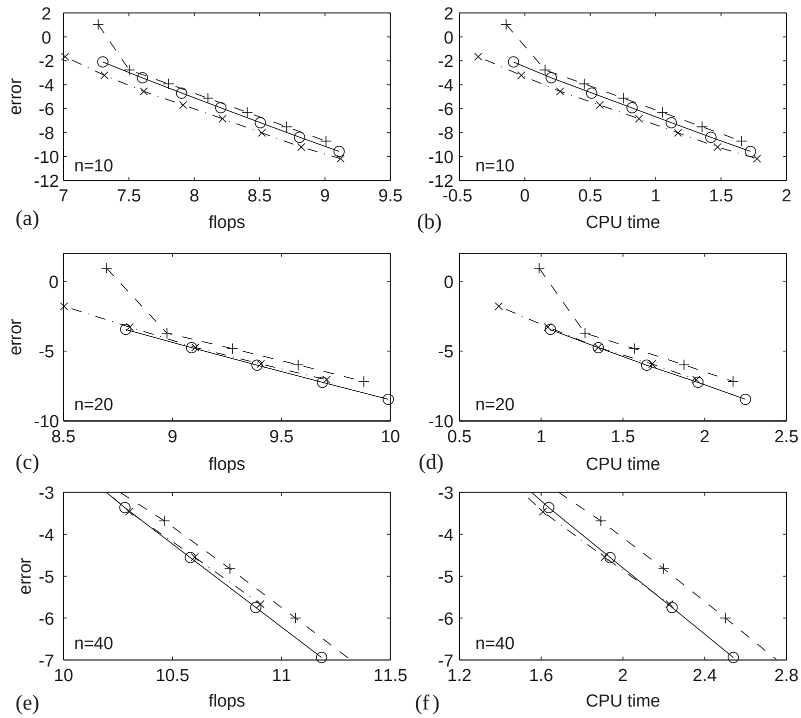

Fig. 2. Error in norm as a function of the number of flops (plots (a), (c) and (e)) and the CPU time (plots (b), (d) and (f)) obtained with the fourth-order integrators M4 (solid lines with circles), RKMK4 (dashed lines with +) and RK4 (dash-dotted lines with ×).

done in Matlab and the commands `expm` and `flops` are employed to evaluate the matrix exponentials and the number of flops, respectively. The corresponding efficiency curves are plotted in Fig. 2.

Several comments are in order. First, the graph clearly exhibits the order of consistency of the algorithms. Second, for this example the new scheme M4 has apparently more favourable stability properties than RKMK4. We can, at present, give no satisfying theoretical explanation for this observed phenomenon. Third, M4 is more efficient than RKMK4, in agreement with the theoretical estimate of Table 2. What is more remarkable, the efficiency of M4 is slightly higher than that of RK4 for $n=20,40$, even when the computational cost of the latter is lower (in particular it does not require the evaluation of matrix exponentials). At this point we should mention that the computation of one matrix exponential (to machine precision) in Matlab typically requires $\approx 25-30n^3$ flops, but it is also possible to use some of the special methods of computation designed in [8,9,12] which require significantly less floating point operations, so that in principle the efficiency of M4 can be further improved. In fact, we have also computed the matrix exponentials with the $[4,4]$ Padé approximant, and the efficiency obtained with M4 is superior for this example. Nevertheless, since the cost of evaluating matrix exponentials increases with the dimension n, there is no substantial improvement when moving from $n=20$ to $n=40$ with respect to RK4. We should have in mind, however, that RK4 does not provide a correct qualitative description of the system with the values of h considered. Fourth, some of the time steps h considered in Fig. 2 are larger than the convergence time t_c of the Magnus series. Thus we should contemplate t_c as a (nonnecessarily optimal) bound where the convergence of the expansion is guaranteed. Alternatively, t_c could also be used for devising a step size control in the algorithm.

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