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Stig Faltinsen

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Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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Stig Faltinsen†
Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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Abstract

Backward error analysis has proven to be very useful in stability analysis of numerical methods for ordinary differential equations. However the analysis has so far been undertaken in the Euclidean space or open subsets thereof. In this paper we study differential equations on manifolds. We prove a backward error analysis result for intrinsic numerical methods. Especially we are interested in Lie-group methods. The author proves elsewhere that if the Lie algebra is nilpotent a *global* stability analysis can be done in the Lie algebra. In the general case we must work on the nonlinear Lie group. In order to show that there is perturbed differential equation on the Lie group with a solution that is exponentially close to the numerical integrator after several steps, we prove a generalised version of Alekseev–Gröbner's theorem. A major motivation for this result is that it implies many stability properties of Lie-group methods.

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†Trinity Hall, University of Cambridge. Email: S.Faltinsen@damtp.cam.ac.uk

1 Introduction

Traditionally numerical methods integrate differential equations in the Euclidean space $\mathbb{R}^n$. Lately integrators that approximate equations on manifolds have been developed. The philosophy is that if the solution space is a manifold M, then the numerical approximation should stay on the same manifold. Motivated by problems in control theory, Crouch and Grossman formulated a class of such methods in [4]. In the last few years a lot of work has been put into Lie-group respecting methods [22, 17, 25, 33, 9]. Applications include problems in elasticity theory and in classical and quantum mechanics. The Lie group has in each case a physical significance. Bearing this in mind, imposing that the numerical method should stay on the Lie group becomes very natural. Likewise Leimkuhler and Patrick considered in [19] symplectic methods on Riemannian manifolds. Common to all of these methods is that they only exploit intrinsic features of the manifold and the differential equation. For example several Lie-group methods [17, 22, 9] approximate in the Lie algebra and advance the numerical solution on the Lie group using the exponential mapping. Hence the numerical approximation is automatically confined to the Lie group. In this paper we refer to these methods as *intrinsic*.

On the other hand, constraining the solution to stay on a submanifold of $\mathbb{R}^n$ has a long tradition in numerical analysis and is known as solving differential algebraic equations (DAE) [14]. One then thinks of the manifold as an open subset of $\mathbb{R}^n$: $M = \{y \in \mathbb{R}^n \ \ |\rho(y) = 0\} \subset \mathbb{R}^n$, where the Jacobian of the function ρ has full rank on M. An obvious question is then whether all problems can be formulated as a DAE. In other words can we always embed a manifold in the Euclidean space $\mathbb{R}^n$? If the manifold is compact this is possible, at least in theory, by Whitney's theorem. However for the vast category of non-compact manifolds this is not always the case. Moreover it is not always easy to construct an embedding, even though it exists for a given manifold. On the top of these considerations there are still other complications due to numerical aspects.

Hence when it comes to solving a differential equation on a manifold there is a natural dichotomy which very much depends on how the problem is formulated. One class of methods views the manifold as a constraint (DAE) while the other group of integrators sees the manifold as an intrinsic system. We do not avocate that one class is better then the other, we simply observe that it is a question of how the problem is posed. With this in mind we would like to study stability of intrinsic methods. To the best of our knowledge, there has been no work on the stability of these methods. By stability we mean that if the exact solution to the differential equation has a structural property, e.g. periodic orbit, stable hyperbolic fixed point or an attractor, then the method is stable if it shares this same property. This problem has already been investigated to great length in the theory of numerical methods approximating ordinary differential equations in the Euclidean space [30]. Unfortunately a Lie group is in general a nonlinear space, and the results do not follow immediately. One way of approaching the problem is by using backward error analysis.

In the Euclidean case backward error analysis has already been addressed by Neishtadt [23], Benettin and Giorgilli [2], Hairer and Lubich [13] and Reich [28]. Other papers on backward error analysis are Griffiths and Sanz-Serna [12], Sanz-Serna [29], Eirola [6] and Gonzalez, Higham and Stuart [11]. Moreover Reich has considered backward error analysis for differential equations on manifolds in the DAE setting. He assumes that the manifold is an open subset of $\mathbb{R}^n$, and shows elegantly how the standard backward error analysis can be extended to numerical methods for DAEs [27]. However intrinsic methods have not yet been treated in this manner.

The basic idea of backward error analysis can be described as follows. In section 3 we will see that to a differential equation on a manifold we can associate an equation on a Lie group by a theorem of Palais [26]. Consider therefore the differential equation

$$y'(t) = Y(t, y), \qquad y(t_0) = y_0, \tag{1.1}$$

where $Y(t, \cdot)$ is a vector field over G and G is a Lie group. We denote a numerical method that approximates the solution of equation (1.1) at time $t_0 + h$ by $\Psi_{h,t_0,Y}$. We refer to h as the step size, t_0 as the initial time and Y is the vector field we want to integrate. The question is then if there is a perturbed problem

$$\tilde{y}'(t) = \tilde{Y}(t, \tilde{y}), \qquad \tilde{y}(t_0) = y_0, \tag{1.2}$$

such that its solution coincides with $\Psi_{h,t_0,Y}$. If this was the case we would be able to monitor the behaviour of the numerical approximation exactly if we knew the solution of the perturbed problem (1.2). In general this is not possible, however, one is able to find a nearby problem whose solution at time $t_0 + h$ is exponentially close in the step-size parameter h to the numerical approximation $y_1 = \Psi_{h,t_0,Y}(y_0)$:

$$d(\tilde{y}(t_0 + h), y_1) = \mathcal{O}\left(e^{-\gamma/h}\right), \tag{1.3}$$

where $\gamma > 0$ is a constant and $d(\cdot, \cdot) : G \times G \to \mathbb{R}^+$ is a distance function on the Lie group.

Thereafter we extend the result to show that we retain exponential closeness also after n steps:

$$d(\tilde{y}(t_0 + nh), y_n) = \mathcal{O}\left(e^{-\gamma_*/h}\right), \tag{1.4}$$

where $nh < T$ and the range of T depends on the problem. Using this estimate we can take advantage of some of the classical results in backward error analysis. For example, suppose that equation (1.1) has an asymptotic stable periodic orbit, then we can show that the Lie-group numerical method also has a periodic orbit which is exponentially close to an asymptotic stable periodic orbit of the modified equation (1.2). This was proven in Euclidean case by Hairer and Lubich [13], and with the estimate (1.4) the result follows almost immediately in the Lie-group situation.

Several Lie-group methods exploit a locally equivalent equation in the Lie algebra to approximate (1.1). Since the Lie algebra is a linear space we would like to undertake the stability analysis there. However it is crucial to backward error analysis that the perturbed vector field in (1.2) is *global*. In [7] the author showed that the Lie algebra equation mentioned above is globally equivalent to (1.1) if and only if the Lie algebra is nilpotent. This result motivates a two-case study. In section 4 we study the nilpotent case where we can exploit the Lie algebra setting. The general setting is considered in section 5 where the analysis must be done on a nonlinear Lie group. In the latter case we must generalise the Alekseev–Gröbner theorem to Lie groups. The next section is devoted to some basic background material. Readers who are familiar with differential geometry and Lie groups can easily skip this section. In section 3 we study differential equations on manifolds. The remaining sections concern backward error analysis.

2 Basic background and setting

2.1 Geometric foundation

This is not a survey of the mathematical theory needed for this paper, merely a brief review meant to introduce requisite notation and basic concepts. We refer the reader to [32, 24, 1] for a more substantive exposition.

Let M be a smooth n-dimensional manifold with an atlas $\{(U_\alpha, \phi_\alpha)\}$. Typical examples of manifolds are the Euclidean space $\mathbb{R}^n$, the n-sphere S^n, and the set of all invertible $n \times n$ matrices $GL(n)$. The set of all tangent vectors at x is denoted by T_xM and the *tangent bundle* is $TM = \bigcup_{x \in M} T_xM$.

A *vector field* F on M is a smooth section i.e. a function

$$F : M \to TM \text{ such that } x \mapsto F(x) \in T_xM$$

and $\pi \circ F = \mathrm{id}_M$ where π is the canonical projection from TM to M and id_M is the identity map on M. The set of vector fields on M is denoted by $\chi(M)$. If $\{x_i\}_{i=1}^n$ is a local basis on the chart U_α of M then $\left\{\frac{\partial}{\partial x_i} \equiv \partial_i\right\}_{i=1}^n$ is a basis of $\chi(U_\alpha)$. Hence any element $X \in \chi(U_\alpha)$ can be written as $X = \sum_{i=1}^n X^i\, \partial_i$. Furthermore $\left\{\frac{\partial}{\partial x_i}\Big|_x\right\}_{i=1}^n$ is a basis of T_xM. The dual space of TM is the *cotangent space* T^*M. The set of covector fields is denoted by $\chi^*(M)$.

Let M and N be two manifolds and consider a mapping $\phi : M \to N$. Corresponding to any such mapping there is an associated mapping between the tangent bundles which we denote by $\phi' = T\phi : TM \to TN$. For notational convenience we make an exception for curves. If $y : \mathbb{R} \to M$ then $y' : \mathbb{R} \to TM$ denotes the curve $y'(t) = Ty(t, 1)$ where $Ty : T\mathbb{R} \equiv \mathbb{R} \times \mathbb{R} \to TM$. Furthermore if Y is a vector field over M we define the *push forward* of Y to be

$$\phi_* Y\,(\phi(y)) = \frac{\partial \phi(y)}{\partial y} Y(y).$$

Let us write this out explicitly in local coordinates. Put $Y = \sum_{i=1}^{n} Y^i \frac{\partial}{\partial y_i}$, then

$$\phi_* Y\left(\phi(y)\right) = \sum_{i,j=1}^{n} Y^i \frac{\partial \phi^j(y)}{\partial y^i} \frac{\partial}{\partial \phi^j(y)}.$$

Note that the matrix $\left(\frac{\partial \phi^j(y)}{\partial y^i}\right)$ is nothing but the Jacobian of the map $\Phi : M \to M$. See [1] for further details.

2.2 Lie groups and Lie algebras

A *Lie group* G is a smooth manifold equipped with a group structure such that the mappings $(a, b) \mapsto a \cdot b$ and $a \mapsto a^{-1}$ are smooth. Let e be its identity element. We define the left and right multiplication on G

$$\begin{aligned} L_a(b) &= a \cdot b \quad \text{for } a, b \in G, \\ R_a(b) &= b \cdot a \quad \text{for } a, b \in G. \end{aligned}$$

Furthermore using the differential mapping we can define e.g. for the right multiplication

$$R'_y = T_e R_y : \mathfrak{g} \to T_y G. \tag{2.5}$$

The set $\mathfrak{g}$ is a *Lie algebra*: a vector space equipped with a bracket operation $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ which is linear, antisymmetric and satisfies the *Jacobi identity*:

$$[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0 \qquad \text{where } x, y, z \in \mathfrak{g}. \tag{2.6}$$

In the case where G is a matrix Lie group the bracket is simply the standard commutator, $[A, B] = AB - BA$ where $A, B \in \mathfrak{g}$. Geometrically the Lie algebra $\mathfrak{g}$ is isomorphic to the tangent space of the Lie group G at the identity element e. There exits a local diffeomorphism between $\mathfrak{g}$ and G called the *exponential map*

$$\exp : \mathfrak{g} \to G \qquad \text{such that} \qquad \exp(v) = \gamma_v(1), \tag{2.7}$$

where $\gamma_v(t)$ is an analytic curve in G such that $\gamma_v(0) = e$ and $\gamma'_v(0) = v$. In the case where G is a matrix group we have

$$\exp(tA) = \sum_{i=0}^{\infty} \frac{t^i}{i!} A^i.$$

The differential of the exponential mapping is important in our setting. It is given by

$$T\exp(u, v) = R'_{\exp u} \circ \mathrm{dexp}_u(v), \tag{2.8}$$

where $R'_{\exp u}$ is defined in (2.5) and $\mathrm{dexp}_u : \mathfrak{g} \to \mathfrak{g}$ is a linear map defined by

$$\mathrm{dexp}_u(v) = \frac{e^{\mathrm{ad}u} - 1}{\mathrm{ad}u}(v) = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}^k(u)(v),$$

where $\mathrm{ad}(u)(v) = [u, v]$ and we define iteratively $\mathrm{ad}^k(u)(v) = [u, \mathrm{ad}^{k-1}(u)(v)]$. The inverse of dexp_u is given by

$$\mathrm{dexp}_u^{-1}(v) = \frac{\mathrm{ad}u}{e^{\mathrm{ad}u} - 1}(v) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k(u)(v), \tag{2.9}$$

where B_k are the Bernoulli numbers [31]. The expansion above is the Taylor expansion about zero of the function $f(z) = z/(e^z - 1)$. Note that the expansion converges if only if $\|\mathrm{ad}u\| < 2\pi$.

Standard examples of matrix Lie groups include

1. *General linear group* $GL(n) = \{A \;\; n \times n \;\; \text{matrix} \mid \det A \neq 0\}$,
2. *Special linear group* $SL(n) = \{A \in GL(n) \mid \det A = 1\}$,
3. *Special orthogonal group* $SO(n) = \{A \in SL(n) \mid A^T A = I\}$.

It is easy to show that the corresponding Lie algebras are

1. $\mathfrak{gl}(n) = \{A \;\; n \times n \;\; \text{matrix}\}$,
2. $\mathfrak{sl}(n) = \{A \in \mathfrak{gl}(n) \mid \mathrm{tr} A = 0\}$,
3. $\mathfrak{so}(n) = \{A \in \mathfrak{sl}(n) \mid A = -A^T\}$.

Another example of a Lie group is $\mathrm{Diff}(M)$, the group of all diffeomorphisms on the manifold M. The Lie algebra is the set of all vector fields on M. We will be interested in Lie subgroups of $\mathrm{Diff}(M)$ later on.

In Section 3 we will need some definitions on Lie algebras. We define the series of derived algebras of $\mathfrak{g}$ by:

$$\mathfrak{g}^{(0)} = \mathfrak{g}, \; \dots \;, \mathfrak{g}^{(n+1)} = [\mathfrak{g}^{(n)}, \mathfrak{g}^{(n)}], \quad n = 0, 1, 2, \dots \tag{2.10}$$

A Lie algebra $\mathfrak{g}$ is called *solvable* if, for some positive integer n, $\mathfrak{g}^{(n)} = \{0\}$. Next consider the following series of ideals

$$\mathfrak{g}_{(0)} = \mathfrak{g}, \; \dots \; \mathfrak{g}_{(n+1)} = [\mathfrak{g}, \mathfrak{g}_{(n)}], \quad n = 0, 1, 2, \dots \tag{2.11}$$

We say that a Lie algebra $\mathfrak{g}$ is *nilpotent*, if there exist a positive integer n, such that $\mathfrak{g}_{(n)} = \{0\}$. Note that if we define the set $\mathrm{ad}^n \mathfrak{g} = \{\mathrm{ad}(X_1) \circ \mathrm{ad}(X_2) \circ \cdots \circ$

$\mathrm{ad}(X_n) \mid X_1, \ldots X_n \in \mathfrak{g} \}$, then $\mathfrak{g}$ nilpotent implies that $\mathrm{ad}^n \mathfrak{g} = 0$. Recall that a nilpotent algebra is solvable. A Lie algebra is said to be *semisimple* if it has no non-zero commutative ideals.

Finally we need a distance function on the Lie group: $d(\cdot, \cdot) : G \times G \to \mathbb{R}^+$. This function should of course satisfy the the standard metric axioms (positivity, symmetry and the triangle inequality). Furthermore we want a metric that is compatible with the topology of the Lie group. There is a very natural way to do this. It is a standard result from differential geometry, see for example [24]. The left multiplication on G induces a map on the cotangent space at a point x, $T^*G\big|_x$, which we will denote L_a^*. We say that a one form ω is *left invariant* if $L_a^*\,\omega = \omega$. For every Lie group there exists a set of left-invariant one-forms $\omega^1, \ldots, \omega^n$, where $n = \dim G$, spanning the cotangent space at each point of G. Define a left invariant Riemannian metric

$$g = \sum_{i,j} g_{i,j} \omega^i \otimes \omega^j$$

where $g_{i,j}$ is an arbitrary symmetric, positive definite $n \times n$ matrix and $\otimes$ is the tensor product. One way of defining such an inner product is by using the *Killing form* defined by

$$K(A, B) = \mathrm{tr}\ \mathrm{ad}A\ \mathrm{ad}B.$$

If the Lie algebra is semisimple, it is well known that the Killing form is non-degenerate. Furthermore if the Lie algebra is compact, the Killing form is either positive or negative definite. It is not difficult to show that in the case of the compact and semisimple Lie algebra $\mathfrak{so}(n)$, we get $K(A, B) = -(n-2)\mathrm{tr}A^T B$. So we can define inner product to be $g(A, B) = \mathrm{tr}A^T B$ where $A, B \in \mathfrak{so}(n)$.

Given a smooth curve on G parametrised by $\gamma : [0, 1] \to G$, we define the length functional

$$l(\gamma) = \int_0^1 \left[g(\gamma'(t), \gamma'(t))\right]^{1/2} dt.$$

The distance between $h \in G$ and $k \in G$ is then defined as

$$d(h, k) = \inf\{l(\gamma) | \gamma(0) = h, \gamma(1) = k\}.$$

The curve γ that minimises the length functional is a *geodesic*. Hence we call the distance function d the *geodesic metric*. Let us again take an example. Let $h, k \in SO(n)$ then $d(h, k) = \left(\sum_{j=1}^n \eta_j^2\right)^{1/2}$ where $\{e^{i\eta_j}\}_{j=1}^n$ are the eigenvalues of $h^T k$.

For every Lie group G we say that d is *left invariant* if

$$\forall \;\; g, h, k \in G \quad d(kg, kh) = d(g, h).$$

We would like d to also be *right invariant*, and hence *bi-invariant*. But this is not always possible and we must relax it to *almost right invariant*, i.e. there exists a function $\rho : G \to \mathbb{R}$ such that $\forall \;\; g, h, k \in G$

$$d(gk, hk) \leq \rho(k) d(g, h)$$

and $\rho(k)$ is finite. In what follows we will denote

$$\rho_{\max} = \max_{k \in G} \rho(k).$$

The Birkhoff–Kakutani theorem [3, 18] states that every Lie group admits a left invariant, almost right invariant metric. Moreover it is well known that nilpotent Lie groups, compact Lie groups, and direct products thereof all admit bi-invariant metrics [21].

We have now completed the introduction of the basic concepts which we require in this work.

3 Differential equations and global solutions

Let M be an analytic manifold and X a vector field on M. The flow of the vector field X after a time t will be denoted $\exp(tX)$. We say that the vector field X is *complete* if $\exp(tX)$ is defined for all $t \geq 0$. In this paper we will consider the following differential equation on a manifold M:

$$\hat{y}'(t) = \hat{Y}(t, \hat{y}) = \sum_{i=1}^{m} \alpha_i(t, \hat{y}) \hat{Y}_i(\hat{y}), \qquad \hat{y}(t_0) = y_0, \tag{3.12}$$

where $\alpha_i(t, \hat{y})$ are scalar functions. The vector fields $\hat{Y}_i$ and $\hat{Y}_j$ do not necessarily commute for different i and j. The set of vector fields $\{\hat{Y}_i\}_{i=1}^m$ generate a Lie algebra through successive commutators. We denote this Lie algebra by $\hat{\mathfrak{g}}$.

By Lie's second fundamental theorem the one-parameter groups $\exp(t\hat{Y}_i)$ generated by $\hat{Y}_i$ for t sufficiently small, define a local group structure on M. But if the vector fields are defined on the whole of M, we would like to know if there is a group structure for all values of t. Hence under which conditions does there exist a global group of transformation G acting on M? Palais' globalisation theorem answers this question in [26]. Assume that the vector fields $\hat{Y}_i$ are complete and that the Lie algebra $\hat{\mathfrak{g}}$ is finite dimensional then there exist a Lie group G with a Lie algebra $\mathfrak{g}$, which is isomorphic to $\hat{\mathfrak{g}}$, that acts on M in the following way. We know that to $\hat{X} \in \hat{\mathfrak{g}}$ there corresponds a global one-parameter group $\exp(t\hat{X})$. So we define the Lie group action $\Lambda : G \times M \to M$ of $\exp(tX)$ where $X \in \mathfrak{g}$ corresponds to $\hat{X}$, on a point $p \in M$ by

$$\Lambda(\exp(tX), p) = \exp(t\hat{X})(p).$$

Moreover we can associate to (3.12) an equation on G:

$$y'(t) = Y(t,y) = \sum_{i=1}^{m} \alpha_i(t,y) Y_i(y), \qquad y(t_0) = e, \tag{3.13}$$

where e is the identity element in G and Y_i is the element corresponding to $\hat{Y}_i$. The solution to (3.12) is simply given by

$$\hat{y}(t) = \Lambda(y(t), y_0).$$

When we present this well-known material is this way it becomes clear that it is the original differential equation (3.12) which defines the Lie algebra and the Lie group associated to it. Reciprocally one could also say that given a Lie algebra $\mathfrak{g}$ and a Lie group actions Λ of G on a manifold M we obtain a vector field on M by

$$\hat{Y} = \left.\frac{d}{dt}\Lambda(\exp(tY), p)\right|_{t=0},$$

where $Y \in \mathfrak{g}$ and $p \in M$. This yields a differential equation on M.

Let us illustrate this circle of ideas with some examples. The standard differential equation in Euclidean space $\mathbb{R}^n$, $y'(t) = A(t,y)$, corresponds to the Lie group action $\Lambda(\exp(X), p) = X + p$. But we could also consider the full equation (3.12) with non-commuting vector fields. Note that in the case of the linear space $M = \mathbb{R}^n$, the Lie group G is nonlinear. An other example is the matrix equation

$$y'(t) = A(t,y)y(t), \qquad y(t_0) = y_0 \in G. \tag{3.14}$$

We can write $A(t,y) = \sum_{i=1}^{d} \alpha_i(t,y) E_i$ where $\{E_i\}_{i=1}^{d}$ is a basis of a Lie algebra $\mathfrak{g}$. In this case the manifold $M = G$ and $\hat{Y}_i(\hat{y}) = Y_i(y) = E_i y$. The single rigid body has as configuration space $SO(3)$ and its equation of motion can be naturally formulated as (3.14).

Having established the connection with Palais' theorem, we realize that we can think of the configuration space of the differential equation (3.12) as a Lie group G. Often G is a nonlinear space, while the Lie algebra is a linear space. Numerically this would be a nice feature to exploit. A proposition which is due to Hausdorff is thus very interesting. In what follows we will for notational convenience not distinguish between $\mathfrak{g}$ and $\hat{\mathfrak{g}}$, and only write $\mathfrak{g}$.

Proposition 1 *Let $t = t_0 + \tau$ then the solution to equation (3.12) is given, for sufficiently small τ, as*

$$\hat{y}(t) = \Lambda(\exp(u(t)), y_0)$$

where $u(t) \in \mathfrak{g}$ satisfies the differential equation

$$u'(t) = U(t,u) = \mathrm{dexp}_u^{-1}\left(\sum_{i=1}^{m} \alpha_i(t, \exp(u(t))) Y_i(e)\right), \qquad u(t_0) = 0, \tag{3.15}$$

where dexp_u^{-1} is defined by (2.9).

The proof of this result can be found for example in [22]. Note that the equivalence is valid only for sufficiently small τ. Several numerical methods [17, 22, 9] exploit the Lie algebra equation (3.15). For example the method of Munthe-Kaas uses a Runge–Kutta scheme to approximate the solution of (3.15) and then advance the solution on the manifold M by

$$y_{n+1} = \Lambda(\exp(u_n), y_n),$$

where y_n and u_n are the numerical approximations of respectively equations (3.12) and (3.15).

When we want to study the stability of equation (3.12) and likewise the stability of numerical methods, it is tempting to consider the Lie algebra equation (3.15). The Lie algebra is as mentioned above, a linear space so the analysis becomes simpler. But a backward error analysis result relies on the perturbed vector field being global. This leads us to the following question on globality.

> (Q): When can the solution to equation (3.12) be globally represented as $y(t) = \exp(u(t))y_0$ where $u(t)$ solves (3.15) for all $t \geq t_0$?

The essence of question (Q) is asking when is the exponential mapping regular? The differential of the exponential mapping is given by (2.8), so to obtain regularity the mapping dexp_u must be an isomorphism. Recall that while dexp_u is valid on the entire Lie algebra, its inverse dexp_u^{-1}, may have singularities. We must therefore study the validity of the mapping dexp_u^{-1}. Note that the Magnus expansion [20], its numerical version [17], the RKMK numerical schemes [22] and the BCH formula [31] all rely on the expansion of dexp_u^{-1} given in (3.16) below. We prove the following result in [7].

Theorem 1 *Let $\mathfrak{g}$ be a Lie algebra over $\mathbb{R}$ or $\mathbb{C}$. The expansion*

$$\mathrm{dexp}_u^{-1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k(u) \tag{3.16}$$

is global, i.e. valid for all $u \in \mathfrak{g}$ if and only if $\mathfrak{g}$ is nilpotent.

Corollaries of Theorem 1 are that the Magnus expansion and the Baker–Campbell–Hausdorff formula is valid globally if and only if $\mathfrak{g}$ is nilpotent. In [7] we also give several examples to illustrate this point. Moreover we answer question (Q) in its full generality. It turns out that a specified subset of real solvable Lie algebras is the largest class of admissible Lie algebras.

Theorem 1 implies that in the nilpotent case $\mathfrak{g}$ is globally isomorphic to G. Hence we can undertake stability analysis in $\mathfrak{g}$ just as well as on G. Note that nilpotent Lie algebras often appear in problems in control theory and stochastic differential equations [10]. Theorem 1 gives rise to yet another intriguing question from numerical point of view. Experiments show that for example the Magnus expansion seems to behave well globally even for non-nilpotent groups. A way to explain this phenomenon, is that when we solve (3.15) numerically using the RKMK method [22] or the Magnus expansion [17] we truncate the mapping dexp^{-1}. Hence we impose $\mathrm{ad}^n \mathfrak{g} = 0$ for some $n \geq 0$. Mathematically we are the working in a nilpotent Lie algebra. This theme is treated in [7]. When concerned with stability analysis, we want to compare the exact solution with the numerical approximation. Theorem 1 then implies that global stability analysis can be undertaken in the Lie algebra $\mathfrak{g}$ if and only if $\mathfrak{g}$ is nilpotent. If this is not the case we must do the analysis on G. In what follows we will therefore first consider the nilpotent case and then the general situation.

4 Backward error analysis via the Lie algebra: the nilpotent case

Let G be a nilpotent Lie group. In this section we will exploit the global correspondence between the Lie group G and its Lie algebra $\mathfrak{g}$ provided by Theorem 1. If we define $\lambda_p(u) = \Lambda(\exp(u), p)$ we have the following commutative diagram:

$$\begin{array}{ccc} T\mathfrak{g} & \xrightarrow{\lambda_p'} & TM \\ {\scriptstyle U}\uparrow & & \uparrow{\scriptstyle \hat{Y}} \\ \mathfrak{g} & \xrightarrow{\lambda_p} & M \end{array} \tag{4.17}$$

The proof of the commutativity $\lambda_p' \circ U = \hat{Y} \circ \lambda_p$ can be found in [22].

Throughout the remainder of this paper we must make some assumptions.

Assumption 1 *We assume that the vector fields in equation (3.12) are real analytic, and moreover that there exist positive real numbers K, R and $t_{\max}$ such that*

$$\|\hat{Y}(t, \hat{y})\|_{T_{\hat{y}}M} \leq K, \qquad \forall\, \hat{y} \in B(y_0, R), \qquad \forall\, t \in [t_0, t_{\max}], \tag{4.18}$$

where $B(y_0, R) = \{y \in M \mid d(y, y_0) \leq R\}$.

Note that we will consider the case when the Palais theorem applies, otherwise a global Lie group analysis approach is meaningless. The Assumption 1 implies bounds on the Lie group equation (3.13). With the same constants as above we have

$$\|Y(t, y)\|_{T_yG} \leq K, \qquad \forall\, y \in B(e, R), \qquad \forall\, t \in [t_0, t_{\max}],$$

where $B(e, R) = \{\hat{y} \in G \mid d(y, e) \leq R\}$.

Our intention is to study the Lie algebra problem (3.15) which, by Theorem 1, is equivalent to the original equation. Linearity of $\mathfrak{g}$ makes this change of focus interesting. However, to be able to work in the Lie algebra we need a bound on the vector field in equation (3.15).

Lemma 1 *For equation (3.12), Assumption 1 implies that there exist positive real numbers* $K_\mathfrak{g}, R_\mathfrak{g}$ *and* $t_{\mathfrak{g},\max}$ *such that*

$$\|U(t,u)\|_\mathfrak{g} \leq K_\mathfrak{g}, \qquad \forall\, u \in B(u_0, R_\mathfrak{g}), \qquad \forall\, t \in [t_0, t_{\mathfrak{g},\max}]. \tag{4.19}$$

Moreover if $\mathfrak{g}$ *is nilpotent then* $R_\mathfrak{g} = R$ *and* $t_{\mathfrak{g},\max} = t_{\max}$.

Proof Consider

$$\begin{aligned} \|U(t,u)\| &= \left\| \mathrm{dexp}_u^{-1}\big(\sum_{i=1}^{m} \alpha_i(t, \exp(u(t))) Y_i(e)\big) \right\| \\ &\leq \left\| \mathrm{dexp}_u^{-1} \right\| \left\| \sum_{i=1}^{m} \alpha_i(t, \exp(u(t))) Y_i(e) \right\|. \end{aligned}$$

By the continuity of the function $u \to \mathrm{dexp}_u^{-1}$ and since $\mathrm{dexp}_0^{-1} = \mathrm{id}$, for every $\epsilon > 0$ there exists a number $R_\mathfrak{g} > 0$ such that for all u such that $\|u\|_\mathfrak{g} \leq R_\mathfrak{g}$ it is true that $\|\mathrm{dexp}_u^{-1}\| \leq 1 + \epsilon$. Moreover we have

$$\begin{aligned} \left\| \sum_{i=1}^{m} \alpha_i(t, \exp(u(t))) Y_i(e) \right\| &\leq \rho_{\max} \left\| T_e R_y \left(\sum_{i=1}^{m} \alpha_i(t, \exp(u(t))) Y_i(e) \right) \right\| \\ &= \rho_{\max} \left\| Y(t, \exp(u(t))) \right\|. \end{aligned}$$

Note that if G is compact or nilpotent the inequality above becomes an equality and $\rho_{\max} = 1$. $\square$

To avoid confusion with the exponential mapping we will denote the exact flow of a vector field Y after a time t by $\Phi_{t,t_0,Y}$. A numerical integrator approximating the flow of Y will be denoted by $\Psi_{h,t_0,Y}$ where h is the step size. Note that the Lie group methods in [22, 17, 9] can be written as

$$y_{n+1} = \Psi_{h,t_n,Y}(y_n) = \exp\left(\Psi_{h,t_n,U}(0)\right) y_n, \tag{4.20}$$

if Y and U are the vector fields in equations (3.12) and (3.15) respectively. The relation $\Phi_{t,t_0,Y}(y_0) = \exp\left(\Phi_{h,t_0,U}(0)\right) y_0$ holds obviously in the exact case as well. We assume that the numerical integrator has an order $p \geq 1$.

Assumption 2 *The numerical method is consistent to order* p*, i.e.*

$$d\left(\Phi_{h,t_0,Y}(y_0), \Psi_{h,t_0,Y}(y_0)\right) = \mathcal{O}\big(h^{p+1}\big). \tag{4.21}$$

By (4.20) and Proposition 1, Assumption 2 implies that

$$\|\Phi_{h,t_0,U}(u_0) - \Psi_{h,t_0,U}(u_0)\| = \mathcal{O}\big(h^{p+1}\big).$$

We can now exploit the backward error analysis of [13, 28] on equation (3.15). Hence there exist a perturbed global vector field $\tilde{U}(t,\cdot)$ on the Lie algebra such that its flow is exponentially close to the numerical approximation after one step and after several steps. To be able to relate these and similar results to corresponding statements on the manifold M, we need a technical lemma.

Lemma 2 *Let $X, Y \in \mathfrak{g}$ be sufficiently close to 0 and $\epsilon = X - Y$. Then $d(\exp X, \exp Y) = \operatorname{dexp}_X \epsilon + \mathcal{O}\left(\|\epsilon\|^2\right)$. Hence*

$$d(\exp X, \exp Y) \leq C\|X - Y\|,$$

and $C \to 1$ as $X \to 0$ or $Y \to 0$.

Proof By the Baker–Campbell–Hausdorff formula [31] we can write

$$\Gamma(t) = e^{tX} e^{t(-X+\epsilon)} = e^{\gamma(t)}, \tag{4.22}$$

for X and Y sufficiently close to 0. If we differentiate we get

$$\begin{aligned}
\Gamma'(t) &= X \exp(tX) \exp(t(-X+\epsilon)) + \exp(tX)(-X+\epsilon) \exp(t(-X+\epsilon)) \\
&= \operatorname{dexp}_{\gamma(t)}(\gamma'(t)) \exp(\gamma(t)).
\end{aligned}$$

Hence $e^{tX}\epsilon e^{-tX} = \operatorname{dexp}_{\gamma(t)}(\gamma'(t))$. So $\gamma'(t) = \operatorname{dexp}^{-1}_{\gamma(t)} e^{tX}\epsilon e^{-tX}$, and therefore

$$\gamma(t) = \int_0^t e^{\xi X}\epsilon e^{-\xi X} d\xi + \mathcal{O}\left(\|\epsilon\|^2\right).$$

The adjoint operator is defined by $\operatorname{Ad}_{\exp(u)} v = \exp(u) v \exp(-u)$ where $u, v \in \mathfrak{g}$. In what follows we exploit the well known formula that $\operatorname{Ad}_{\exp(u)} = \exp(\operatorname{ad} u)$ [31]. Therefore

$$\begin{aligned}
\int_0^t e^{\xi X}\epsilon e^{-\xi X} d\xi &= \int_0^t e^{\operatorname{ad}\xi X}\epsilon d\xi = \int_0^t \sum_{k=0}^{\infty} \frac{1}{k!} \operatorname{ad}^k(\xi X)\epsilon d\xi \\
&= \int_0^t \sum_{k=0}^{\infty} \frac{1}{k!} \xi^k \operatorname{ad}^k(X)\epsilon d\xi \\
&= \sum_{k=0}^{\infty} \frac{1}{(k+1)!} t^{k+1} \operatorname{ad}^k(X)\epsilon = \operatorname{dexp}_{tX} t\epsilon.
\end{aligned}$$

Let $t = 1$ and the first part follows since

$$d(\exp X, \exp Y) = d(\exp X \exp(-Y), e) = \|\gamma(1)\|$$

for X and Y sufficiently close to $0 \in \mathfrak{g}$. Similarly we get

$$d(\exp X, \exp Y) = \operatorname{dexp}_Y(-\epsilon) + \mathcal{O}\left(\|\epsilon\|^2\right).$$

Hence $C = \|\mathrm{dexp}_X\| + \mathcal{O}(\|\epsilon\|) = \|\mathrm{dexp}_Y\| + \mathcal{O}(\|\epsilon\|)$ so as $X \to 0$, $\mathrm{dexp}_X \to \mathrm{id}$ and from (4.22) it follows that $C \to 1$. $\square$

Note that if the Lie algebra is nilpotent then the Baker–Campbell–Hausdorff formula is globally convergent [7]. However we will only need the lemma when ϵ is small. The ideas of this section can be formally stated as a theorem.

Theorem 2 *Assume that we solve equation (3.12) with a Lie-group numerical method. Let $Y(t,\cdot)$ be a global vector field on the manifold M. Let the Lie algebra corresponding to equation (3.12) be nilpotent. Subject to Assumptions 1 and 2 there is a global vector field $\tilde{Y}(t,\cdot)$ on M with solution $\tilde{y}(t)$ such that*

$$\begin{aligned} d(\tilde{y}(t_0+h), y_1) &= \mathcal{O}\left(e^{-\gamma_1/h}\right), \\ d(\tilde{y}(t_0+nh), y_n) &= \mathcal{O}\left(e^{-\gamma_2/h}\right), \end{aligned}$$

where γ_1 and γ_2 are positive constants such that $\gamma_2 \leq \gamma_1$ and $nh < T$.

Note that the time interval of length T depends on the problem. Estimates of T can be found in [13] and also Theorem 5 in this paper. *Proof* The main idea is to exploit the Lie-algebra equation (3.15). By Theorem 1 and Proposition 1 equations (3.12) and (3.15) are globally equivalent if the Lie algebra is nilpotent. Moreover the Lie-group numerical integrator can either step several times in the Lie algebra or return to the manifold at every step. Let us illustrate this by some diagrams. To do

$$\begin{array}{ccc} u_0 \in \mathfrak{g} & \xrightarrow{\Psi_{h,t_0,U}} & u_1 \in \mathfrak{g} \\ \uparrow & & \downarrow \mathrm{exp} \\ y_0 \in M & \xrightarrow{\Psi_{h,t_0,Y}} & y_1 \in M \end{array} \quad \text{and then} \quad \begin{array}{ccc} u_1 \in \mathfrak{g} & \xrightarrow{\Psi_{h,t_0+h,U}} & u_2 \in \mathfrak{g} \\ \uparrow & & \downarrow \mathrm{exp} \\ y_1 \in M & \xrightarrow{\Psi_{h,t_0+h,Y}} & y_2 \in M \end{array}$$

is the same as just taking two steps in the Lie algebra:

$$\begin{array}{ccc} u_0 \in \mathfrak{g} & \xrightarrow{\Psi_{h,t_0+h,U} \circ \Psi_{h,t_0,U}} & u_{21} \in \mathfrak{g} \\ \uparrow & & \downarrow \mathrm{exp} \\ y_0 \in M & \xrightarrow{\Psi_{h,t_0+h,Y} \circ \Psi_{h,t_0,Y}} & y_2 \in M \end{array} \tag{4.23}$$

We obtain $u_{21} = \mathcal{B}(u_2, u_1)$ where $\mathcal{B}$ is the Baker–Campbell–Hausdorff formula [31]. In general we can define $u_{n\ldots 1} = \mathcal{B}(u_n, \mathcal{B}(\ldots, u_1))$. Note that a corollary to Theorem 1 ensures that the BCH formula is well defined globally since $\mathfrak{g}$ is nilpotent [7]. We therefore study the Lie group method operating as in the diagram (4.23). By Assumption 1 and Lemma 1 we have a bounded real analytic vector field U in $\mathfrak{g}$. Since $\mathfrak{g}$ is a linear space we can apply the backward error analysis results of [13, 28]. We obtain a global perturbed vector field $\tilde{U}$ with solution curves which are exponentially close to the numerical integrator in the Lie algebra. Related to $\tilde{U}$ there is a global vector field on the manifold M given by

$$\tilde{Y}(t,y) = \tilde{Y}(t,\Lambda(\exp(u),y_0)) = \operatorname{dexp}_u \tilde{U}(t,u).$$

Let $\tilde{y}(t)$ be the integral curve of the vector field $\tilde{Y}(t,\cdot)$. Then we get by Lemma 2

$$d(\tilde{y}(t_0+h),y_1) \leq C \left\| \Phi_{h,t_0,\tilde{U}}(u_0) - \Psi_{h,t_0,U}(u_0) \right\| = \mathcal{O}\left(e^{-\gamma_1/h}\right),$$

where γ_1 is a positive constant. Moreover we have

$$y_n = \exp(u_n)\exp(u_{n-1})\cdots\exp(u_1)y_0 = \exp(u_{n\ldots 1})y_0,$$

but $u_{n\ldots 1} = \Psi_{h,t_0+(n-1)h,U} \circ \cdots \circ \Psi_{h,t_0,U}(u_0)$ so

$$\begin{aligned} d(\tilde{y}(t_0+nh),y_n) &= d\left(\exp(\Phi_{nh,t_0,\tilde{U}}(u_0)), u_{n\ldots 1}\right) \\ &\leq C \left\| \Phi_{nh,t_0,\tilde{U}}(u_0) - u_{n\ldots 1} \right\| = \mathcal{O}\left(e^{-\gamma_2/h}\right), \end{aligned}$$

where γ_2 is a positive constant. □

Note 1 *The assumption on the globality of the vector field Y is not necessary. The more precise statement is that the perturbed vector field $\tilde{Y}$ can be extended to the same domain as Y.*

In the case where the Lie algebra $\mathfrak{g}$ is nilpotent, all stability analysis can be done in the Lie algebra. The crucial ingredient is Theorem 1 which tells us that the Lie algebra and the Lie group are analytic diffeomorphic as manifolds when $\mathfrak{g}$ is nilpotent. We find the simplicity of this approach appealing. Moreover it is a natural way to study the Lie group methods in [17, 22, 9] since they all exploit the Lie algebra and equation (3.15) when approximating equation (3.12).

On the other hand Theorem 1 tells us that nilpotency of the Lie algebra $\mathfrak{g}$ is also the limit of this approach. When the Lie algebra is for example semisimple we must operate directly on the nonlinear space G. Moreover for the numerical methods considered in [16, 4, 25] it is natural to do the backward error analysis on the Lie group.

5 Backward error analysis on the Lie group: the general case

5.1 Exponential closeness after one step

Several Lie-group integrators do not exploit the Lie algebra explicitly. The Crouch–Grossman methods [4, 25] and the Fer expansion [16, 33] are examples of such approximation schemes. In this section we will see how one can do backward error analysis directly on the Lie group.

Throughout this section we will consider the equation (3.12) with the vector field $\hat{Y}$ over M. The Palais theorem then tells us that there is the equivalent equation (3.13) with the vector field Y over the Lie group G. For notational convenience we will write Y for both Y and $\hat{Y}$.

Optimally we seek a global perturbed vector field $\tilde{Y}$ on G such that its flow, $\Phi_{t,t_0,\tilde{Y}}$, coincides with the numerical integrator $\Psi_{h,t_0,Y}$, i.e.

$$y_1 = \Psi_{h,t_0,Y}(y_0) = \Phi_{t,t_0,\tilde{Y}}(y_0) = \tilde{y}(t_0 + h).$$

This is not always possible, but we can find a perturbed vector field $\tilde{Y}$ whose solutions are very close to the numerical integrator.

By analyticity there exist Taylor expansions of the exact and the numerical flows in terms of the time parameter h,

$$\begin{aligned}
\Phi_{h,t_0,Y}(y_0) &= \sum_{k=0}^{\infty} \frac{h^k}{k!} \frac{\partial^k \Phi_{t,t_0,Y}(y_0)}{\partial t^k}\bigg|_{t=t_0}, \\
\Psi_{h,t_0,Y}(u_0) &= \sum_{k=0}^{\infty} \frac{h^k}{k!} \frac{\partial^k \Psi_{t,t_0,Y}(y_0)}{\partial t^k}\bigg|_{t=t_0},
\end{aligned}$$

We can now define an iteration of vector fields on the Lie group. The same iteration has been defined in the Euclidean case by Reich [28]. For notational convenience we write only the dependence on time, i.e. $Y_i(t) \equiv Y_i(y(t), t)$.

$$\begin{aligned}
Y_0(t_0 + h) &= Y(t_0 + h), \\
Y_{i+1}(t_0 + h) &= Y_i(t_0 + h) + \triangle_{i+1}(t_0 + h), \qquad (5.24) \\
\triangle_{i+1}(t_0 + h) &= \frac{h^{p+i+1}}{(p+i+1)!} \left[\frac{\partial^{p+i+1} \Psi_{t,t_0,Y}(y_0)}{\partial t^{p+i+1}} - \frac{\partial^{p+i+1} \Phi_{t,t_0,Y_i}(y_0)}{\partial t^{p+i+1}} \right]\Bigg|_{t=t_0}.
\end{aligned}$$

The iteration is defined for all h sufficiently small. However the iteration does not necessarily converge, so we seek an iterate with index i_* so that we get a best possible approximation of the numerical flow. We let the initial value of the iteration be the vector field Y. This is a natural choice since the numerical method is of order p. Furthermore we note that by construction we get

$$d\left(\Phi_{h,t_0,Y_i}(y_0), \Psi_{h,t_0,Y}(y_0)\right) = \mathcal{O}\left(h^{p+i+1}\right). \qquad (5.25)$$

We can now adapt the proof in Reich [28] to prove the following statement about flows on the Lie group G. Numerical values of the constants a and b can be found in [28].

Theorem 3 *Under Assumptions 1 and 2 there exists an index i_* such that*

$$d\left(\Phi_{h,t_0,Y_{i_*}}(y_0), \Psi_{h,t_0,Y}(y_0)\right) \le aMhe^{-p}e^{-\frac{\gamma}{h}},$$

where $\gamma \le \frac{R}{bM}$, $M \ge K$, h is the step size, $p \ge 1$ is the order of the method, a and b are constants.

Proof This result was proved by Reich in [28] in the Euclidean case (Theorem 2). The Lemma 1 in [28] follows from the definition of the distance function. The main proof follows from the triangle inequality for the distance function and linearity of the tangent space of G at $y(t)$, $T_{y(t)}G$. $\square$

Our prime interest is to prove that there exists a perturbed solution that stays exponentially close to the numerical approximation after n steps. Obviously such a result will rely on Theorem 3. In the Euclidean case one way of proving this is to use the Alekseev–Gröbner theorem. To the best of our knowledge such a theorem is not available to us in a manifold setting, and has to be proved first. The Alekseev–Gröbner theorem is the nonlinear version of the variation of constants formula.

5.2 The Alekseev–Gröbner theorem on manifolds

We recall the Alekseev–Gröbner theorem on Euclidean space. It can be found for example in [14, 15]. As before we denote the flow of a vector field by $\Phi_{\tau,t_0,Y}$, and assume that the push forward of this flow exists. Hence $\partial\Phi_{\tau,t_0,Y}/\partial y_0$ is continuous.

Proposition 2 *Let y and z be the solutions of*

$$\begin{aligned} y'(t) &= Y(t,y), & y(t_0) = y_0, \\ z'(t) &= Y(t,z) + B(t,z), & z(t_0) = y_0. \end{aligned}$$

Suppose that $\partial\Phi_{t,t_0,Y}/\partial y_0$ is continuous, then

$$z(t) = y(t) + \int_{t_0}^{t} \frac{\partial\Phi_{t,s,Y}(z(s))}{\partial y_0} B(s, z(s))ds.$$

Our intention is to extend Alekseev–Gröbner's theorem to manifolds. We saw in Section 3 that equation (3.12) could be associated to a Lie algebra $\mathfrak{g}$ and that we could consider the equation (3.13) on the Lie group G. We will now consider a perturbed differential equation

$$z'(t) = Y(t,z) + B(t,z), \qquad z(t_0) = y_0.$$

We assume that the Lie algebra associated with this equation is the same Lie algebra $\mathfrak{g}$.

Theorem 4 *Let y and z be the solutions of*

$$\begin{aligned} y'(t) &= Y(t,y), & y(t_0) &= y_0, \\ z'(t) &= Y(t,z) + B(t,z), & z(t_0) &= y_0. \end{aligned}$$

Suppose that $\partial\Phi_{t,t_0,Y}/\partial y_0$ is continuous, then

$$d(y(t), z(t)) = \int_{t_0}^{t} \left\| \frac{\partial \Phi_{t,s,Y}(z(s))}{\partial y_0} B(s, z(s)) \right\| ds.$$

Proof One way of constructing a curve between $y(t)$ and $z(t)$ is $\gamma(s) = \Phi_{t,s,Y}(z(s))$. Clearly $\gamma(t_0) = y(t)$ and $\gamma(t) = z(t)$. Consider next

$$\begin{aligned} \gamma'(s) &= \frac{\partial \Phi_{t,s,Y}(z(s))}{\partial s} + \frac{\partial \Phi_{t,s,Y}(z(s))}{\partial y_0} z'(s), \\ &= -\frac{\partial \Phi_{t,s,Y}(z(s))}{\partial y_0} Y(t, z(s)) + \frac{\partial \Phi_{t,s,Y}(z(s))}{\partial y_0} z'(s), \\ &= \frac{\partial \Phi_{t,s,Y}(z(s))}{\partial y_0} B(t, z(s)), \end{aligned}$$

where the second line follows from Theorem 14.4 in [14]. Note that in geometrical terms this is push forward of a vector field on $z(s)$ to a vector field on $\gamma(s)$. The derivative obeys the identity $\gamma'(s) = (\Phi_{t,s,Y}(z(s))_* B)(\gamma(s))$. Both equations correspond to the same Lie algebra $\mathfrak{g}$. Hence $\Phi_{t,s,Y}(z(s)) \in G$ and $B \in \mathfrak{g}$ and therefore $\Phi_{t,s,Y}(z(s))_* B \in \mathfrak{g}$. In other words $\gamma(s)$ is a geodesic on G and by the definition of the distance function we get equality. $\square$

It should be mentioned that the extension to a situation where y and z have different initial values is not difficult, but since the proof is of no further enlightenment it has been omitted.

5.3 Exponential closeness after several steps

From Theorem 3 we know that there is a solution $\tilde{y}$ to the perturbed equation (1.2),

$$\tilde{y}'(t) = \tilde{Y}(\tilde{y}, t) = Y(\tilde{y}, t) + h^p B(\tilde{y}, t), \tag{5.26}$$

where B is the backward error vector field or the perturbation to the exact equation. We must make some further assumptions on the vector fields in equations (1.1) and (1.2). The assumptions are similar to the ones made in the classical case by Hairer and Lubich in [13]. We say that a vector field $B \in T_yG$ is Lipschitz if

$$\|T_y R_{y^{-1}} B(y,t) - T_z R_{z^{-1}} B(z,t)\|_{\mathfrak{g}} \leq C_1\, d(y,z).$$

For notational convenience and clarity of exposition we write $\Phi = \Phi_{t,s,Y}$ when there is no danger of confusion. Define

$$\chi(t, y(s)) = T_{\Phi(y(s))} R_{\Phi(y(s))^{-1}} \frac{\partial \Phi(y(s))}{\partial y_0} T_e R_{y(s)}.$$

Note that this is essentially push forward along the flow of the vector field Y. By translations we have made it into an endomorphism of the Lie algebra $\mathfrak{g}$. We will denote the space of endomorphisms of $\mathfrak{g}$ by $\mathrm{End}\mathfrak{g}$. It is a linear space.

Assumption 3 *Both the numerical solution y_n and the exact solution of equation 3.13 for a sufficiently long time t are contained in a compact set $K \subset G$. Let U be an open neighbourhood of K. We assume that the vector field B is Lipschitz with constant C_1, and bounded for all $y \in U$ with constant C_2. Moreover, for all $y \in U$*

$$\begin{aligned} &\|\chi(t, y(s))\|_{\mathrm{End}\mathfrak{g}} \le C_3\, e^{\mu(t-s)} \quad \text{and} \\ &\|\chi(t, y(s)) - \chi(t, z(s))\|_{\mathrm{End}\mathfrak{g}} \le C_3\, e^{\mu(t-s)} d(y(s), z(s)). \end{aligned}$$

The main reason we need these assumptions is that they imply a time-dependent Lipschitz condition for the vector field B pushed forward by the flow of Y.

Theorem 5 *Under Assumption 1, 2 and 3 there is a time interval of length*

$$T = \begin{cases} \infty & \mu < 0 \\ \mathcal{O}\big(h^{-(p+1)}\big) & \mu = 0 \\ \mathcal{O}\big(h^{-1}\big) & \mu > 0, \end{cases}$$

such that the numerical solution and the solution of the perturbed equation (1.2) remain exponentially close

$$d(y_n, \tilde{y}(nh)) = \mathcal{O}\left(e^{-\gamma^*/2h}\right) \qquad \text{for} \quad nh < T,$$

where $\gamma^* = \min\{\gamma(y_0) | y_0 \in K\}$ and γ is given in Theorem 3.

Proof See the appendix □

Using Theorem 5 we can prove a whole series of results on qualitative behaviour of Lie-group methods. It is at this point that one realizes the importance of using intrinsic tools of Lie groups to prove the estimates in this paper. Without this we could not have immediately asserted that for example a periodic orbit really stays on the manifold G. We will now include an example of the type of statements that can be proven. The Euclidean-space version of this statement and its proof can be found in Hairer and Lubich [13].

Corollary 1 *Assume that the differential equation (1.1) has an asymptotic stable periodic orbit. Subject to Assumptions 1, 2 and 3 and for sufficiently small step sizes, the numerical method has an asymptotic stable invariant closed curve which is exponentially close to the periodic orbit of the perturbed differential equation (1.2).*

Proof The proof follows directly from the estimate in Theorem 5 and the classical proof in [13]. □

6 Concluding remarks

This paper, together with the work in [8], constitutes our starting point for research on exact and numerical stability on Lie groups. We have proven that the exponential closeness result known from the classical backward error analysis theory also applies in a Lie-group setting. Theorem 1 made it natural to study the nilpotent case separately. Global analysis was then done in the Lie algebra. In the general case we needed to prove a version of Alekseev–Gröbner's theorem on manifolds. Corollary 1 is an example of the type of stability results that follow from the backward error analysis in this paper. As a matter of fact only minor considerations are now needed to extend the results in [13] and [11] to a manifold setting.

Finally we believe that the Alekseev–Gröbner result can also be used to extend ideas of stability from the Euclidean setting in [14, 15]. This will be the subject of future research.

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A Proof of Theorem 5

We need two technical lemmas.

Lemma 3 *Under Assumption 3 we get*

$$\|T_{\Phi(y)}R_{\Phi(y)^{-1}}\Phi_*B(y(s)) - T_{\Phi(z)}R_{\Phi(z)^{-1}}\Phi_*B(z(s))\|_{\mathfrak{g}} \leq C_4\, e^{\mu(t-s)}\, d(y(s), z(s)).$$

Proof By definition We have

$$\Phi_*B(y(s),t) = \frac{\partial\Phi(y(s))}{\partial y_0}B(y(s),t) = \frac{\partial\Phi(y(s))}{\partial y_0}T_eR_y\left(T_yR_y^{-1}B(y(s),t)\right).$$

Hence

$$\begin{aligned}
T_{\Phi(y)}R_{\Phi(y)^{-1}}\Phi_*B(y(s)) - T_{\Phi(z)}R_{\Phi(z)^{-1}}\Phi_*B(z(s)) = \\
= \chi(t,y(s))\left[T_yR_y^{-1}B(y(s),t)\right] - \chi(t,z(s))\left[T_zR_z^{-1}B(z(s),t)\right] \\
= \left[\chi(t,y(s)) - \chi(t,z(s))\right]T_yR_y^{-1}B(y(s),t) + \\
+\chi(t,z(s))\left[T_yR_y^{-1}B(y(s),t) - T_zR_z^{-1}B(z(s),t)\right].
\end{aligned}$$

Taking norms on both sides, using Assumption 3 and setting $C_4 = C_3(C_1 + C_2)$ we deduce the statement of the lemma. □

Lemma 4 *Let $y(t)$ and $z(t)$ be solutions to the differential equation (1.1) with initial values y_0 and z_0 respectively. Under Assumption 3 we obtain the following bound*

$$d(y,z) \leq \hat{C}_3 e^{\mu(t-t_0)} d(y_0,z_0),$$

where

$$\hat{C}_3 = \begin{cases} C_3, & \textit{if } G \textit{ is compact,} \\ C_3\cdot\rho_{\max}, & \textit{if } G \textit{ is non-compact.}\end{cases}$$

Proof Let us construct a curve between $y(t)$ and $z(t)$. Define

$$\gamma(s) = \Phi_{t,t_0,Y}(i(s)),$$

where $i(s) = \exp\left(s\log(z_0y_0^{-1})\right)y_0$ and $s\in[0,1]$. The derivative of the curve is

$$\gamma'(s) = \frac{\partial\Phi}{\partial y_0}i'(s),$$

and $i'(s) = T_eR_{i(s)}\log(z_0y_0^{-1})$. Therefore by the definition of the distance function

$$\begin{aligned}
d(y(t),z(t)) &\leq \int_0^1 \|\gamma'(s)\|ds \\
&\leq \int_0^1 \left\|\frac{\partial\Phi}{\partial y_0}T_eR_{i(s)}\log(z_0y_0^{-1})\right\|ds, \\
&\leq \left(\int_0^1\left\|\frac{\partial\Phi}{\partial y_0}T_eR_{i(s)}\right\|ds\right)d(y_0,z_0), \\
&\leq \hat{C}_3e^{\mu(t-t_0)}d(y_0,z_0),
\end{aligned}$$

where the last line follows from Assumption 3. $\square$

The proof of Theorem 5 now follows.

Proof Our intention is to stay as close as possible to the proof in the Euclidean case given in [13]. We need to show how the solution to the perturbed equation propagates initial values. Let $y(t)$ and $z(t)$ be solutions to the exact equation 1.1 with initial values y_0 and z_0 respectively. Let $\tilde{y}(t)$ and $\tilde{z}(t)$ be solutions to the perturbed equation 1.2 with the same initial conditions. Then

$$\begin{aligned} d(\tilde{y}(t),\tilde{z}(t)) &= d(e,\tilde{y}^{-1}(t)\tilde{z}(t)) \\ &\leq d(e,y^{-1}z)+d(y^{-1}z,\tilde{y}^{-1}(t)\tilde{z}(t)) \\ &\leq d(y,z)+d(y^{-1}z,\tilde{y}^{-1}\tilde{z}). \end{aligned}$$

To get a bound on the distance between $y^{-1}z$ and $\tilde{y}^{-1}\tilde{z}$ we do as before and construct a curve. Consider

$$\gamma(s)=(\Phi(\tilde{y}(s)))^{-1}\ \Phi(\tilde{z}(s)).$$

Note that $\gamma(0)=y^{-1}z$ and $\gamma(t)=\tilde{y}^{-1}\tilde{z}$. Furthermore we recall that

$$\left(w^{-1}\right)'=-w^{-1}\,(w)'\,w^{-1}.$$

We now deduce from the proof of Theorem 4 that

$$\begin{aligned} \frac{d}{ds}\gamma(s) &= -\Phi(\tilde{y}(s))^{-1}\ \frac{\partial\Phi(\tilde{y}(s))}{\partial y_0}h^pB(t,\tilde{y}(s))\ \Phi(\tilde{y}(s))^{-1}\Phi(\tilde{z}(s)) \\ &\qquad +\Phi(\tilde{y}(s))^{-1}\ \frac{\partial\Phi(\tilde{z}(s))}{\partial y_0}h^pB(t,\tilde{z}(s)) \\ &= h^p\Phi(\tilde{y}(s))^{-1}\left[\Phi_*B\left(\Phi(\tilde{y}(s))\right)\ \Phi(\tilde{y}(s))^{-1}-\right. \\ &\qquad \left.\Phi_*B\left(\Phi(\tilde{z}(s))\right)\ \Phi(\tilde{z}(s))^{-1}\right]\ \Phi(\tilde{z}(s)). \end{aligned}$$

The above argument can be extended to general Lie groups (as opposed to matrix Lie groups), yielding:

$$\frac{d}{ds}\gamma(s)=h^pT_e\left(L_{\Phi(\tilde{y})^{-1}}\circ R_{\Phi(\tilde{z})}\right)\left[T_{\Phi(\tilde{y})}R_{\Phi(\tilde{y})^{-1}}\Phi_*B(\tilde{y}(s))-T_{\Phi(\tilde{z})}R_{\Phi(\tilde{z})^{-1}}\Phi_*B(\tilde{z}(s))\right].$$

We then get

$$\|\gamma'(s)\|_{T_{\Phi(\tilde{y})^{-1}\Phi(\tilde{z})}G}\leq h^p\rho_{\max}\|T_{\Phi(\tilde{y})}R_{\Phi(\tilde{y})^{-1}}\Phi_*B(\tilde{y}(s))-T_{\Phi(\tilde{z})}R_{\Phi(\tilde{z})^{-1}}\Phi_*B(\tilde{z}(s))\|_{\mathfrak{g}}.$$

If G is compact we have equality and $\rho_{\max}=1$ because of the bi-invariance. So define

$$\hat{C}_4=\begin{cases} C_4, & \text{if } G \text{ is compact,} \\ C_4\cdot\rho_{\max}, & \text{if } G \text{ is non-compact.} \end{cases}$$

From Lemma 3 we then obtain

$$d(y^{-1}z,\tilde{y}^{-1}\tilde{z})\leq h^p\int_0^t\hat{C}_4\ e^{\mu(t-s)}\ d(\tilde{y}(s),\tilde{z}(s))ds,$$

and from Lemma 4 we have

$$d(y,z) \le \hat{C}_3 \; e^{\mu t} \; d(y_0,z_0).$$

Gronwall's Lemma, see [30], then gives

$$d(\tilde{y}(t),\tilde{z}(t)) \le \hat{C}_3 \; e^{(\mu+\hat{C}_4 h^p)t} \; d(y_0,z_0).$$

Having obtained this bound we can proceed,

$$\begin{aligned}
d(y_n,\tilde{y}(nh)) &\le \sum_{k=1}^{n} d\left(\Phi_{t_n-t_{k-1},\tilde{Y}}(y_{k-1}),\Phi_{t_n-t_k,\tilde{Y}}(y_k)\right)\\
&= \sum_{k=1}^{n} d\left(\Phi_{t_n-t_k,\tilde{Y}}(\Phi_{t_k-t_{k-1},\tilde{Y}}(y_{k-1})),\Phi_{t_n-t_k,\tilde{Y}}(y_k)\right)\\
&\le \sum_{k=1}^{n} \hat{C}_3 \; e^{(\mu+\hat{C}_4 h^p)(t_n-t_k)} \; d\left(\Phi_{t_k-t_{k-1},\tilde{Y}}(y_{k-1}),y_k\right)\\
&\le \sum_{k=1}^{n} \hat{C}_3 \; e^{(\mu+\hat{C}_4 h^p)(t_n-t_k)} C_5 e^{-\gamma^*/h}\\
&= \hat{C}_3 C_5 e^{-\gamma^*/h}\left(\frac{1-e^{(\mu+\hat{C}_4 h^p)nh}}{1-e^{(\mu+\hat{C}_4 h^p)h}}\right),
\end{aligned}$$

where the second last line follows from Theorem 3 with

$$d\left(\Phi_{t_k-t_{k-1},\tilde{Y}}(y_{k-1}),y_k\right) \le C_5^k \cdot e^{-\gamma_k/h},$$

and

$$C_5 = \max_{1\le k\le n} C_5^k \qquad\qquad \gamma^* = \min_{1\le k\le n} \gamma_k.$$

The result follows. □

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