On the construction of geometric integrators in the RKMK class

Kenth Engø*

Department of Informatics
University of Bergen
N-5020 Bergen
Norway

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Abstract

We consider the construction of geometric integrators in the class of RKMK methods. Any differential equation in the form of an infinitesimal generator on a homogeneous space is shown to be locally equivalent to a differential equation on the Lie algebra corresponding to the Lie group acting on the homogenous space. This way we obtain a distinction between the coordinate-free phrasing of the differential equation and the local coordinates used. In this paper we study methods based on arbitrary local coordinates on the Lie group manifold. By choosing the coordinates to be canonical coordinates of the first kind we obtain the original method of Munthe-Kaas [14]. Methods similar to the RKMK method are developed based on the different coordinatizations of the Lie group manifold, given by the Cayley transform, diagonal Padé approximants of the exponential map, canonical coordinates of the second kind, etc. Some numerical experiments are also given.

1 Introduction

In the past few years there has been a substantial development in the area of geometric integration of differential equations evolving on Lie groups and more generally homogeneous spaces. The present investigation was stimulated by a paper of Munthe-Kaas [14], where Runge-Kutta methods of arbitrary high order on homogeneous spaces are introduced. The main idea is to transform the differential equation evolving on the homogeneous space to an equivalent differential equation evolving on a Lie algebra. An appealing feature of Lie algebras is that they are vector spaces. Hence, a classical Runge-Kutta method

*Email: `Kenth.Engo@ii.uib.no`, WWW: `http://www.ii.uib.no/~kenth`

can be applied in approximately solving the transformed equation. Further, smoothness of the transformation map ensures the correct order of the numerical approximation on the homogenous space.

The exponetial map from the Lie algebra to the Lie group is of crucial importance in many of the geometric integration techniques developed. For a moment let us emphasize the manifold structure of Lie groups. Every smooth manifold is modeled by the use of smooth coordinate maps from an open subset of the manifold to some Banach space. For a Lie group this model space is the Lie algebra and the exponential map is called the canonical coordinates of the first kind. A point to make is that a manifold can have different types of coordinates. Another example of canonical coordinates are coordinates of the second kind. From general Lie theory it is known that every Lie group can be coordinatized by the canonical coordinates of the first and second kind [19]. Thus, to develop methods appropriate for *all* Lie groups, coordinatizations based on these two types of coordinates are among the natural choices.

For some Lie groups, however, there do exist coordinates other than the canonical coordinates of the first and second kind. An example is the Cayley transform. Cayley coordinatizations exist, for instance, for the matricial Lie groups $\mathrm{O}(n)$, $\mathrm{SO}(n)$, and $\mathrm{Sp}(n)$, the orthogonal, the special orthogonal, and the symplectic group, respectively. To develop integration techniques based on the Cayley transform would entail savings with respect to computational costs because of the lesser expense in computing the Cayley transform as compared to the exponential map. Introducing local geometric integration techniques, similar to the RKMK method, based on different coordinatizations of the Lie group is the main goal of this paper.

In [4], Celledoni and Iserles establishes the necessary conditions for a map ϕ analytic in a neighborhood around 0 of the Lie algebra, with $\phi(0) = 1$ and $\phi'(0) = 1$, to be a map from the Lie algebra to the Lie group in the case of the quadratic Lie groups. Diagonal Padé approximants of the exponential function are analytic functions that meet these conditions, and hence, are natural candidates as coordinates on the Lie group manifold. Thus, in the case of the quadratic Lie groups, geometric integration methods based on diagonal Padé approximants as coordinates should be considered.

There has also been done some work on developing software based on these new classes of integration techniques. It turns out that the new methods are well suited for the use of object oriented programming. All the geometric integrators are stated in a coordinate free language, that is; the methods are stated independently of the actual representation of the elements of the manifold. The algorithm is stated once and for all, in an abstract fashion, regardless of if the algorithm is to handle scalars, vectors, matrices, or even more abstract geometric objects. Traditionally, object orientation is used in all levels of the algorithm itself, but the new algorithms allow for the object orientation to be employed on the geometry instead. Developing mathematical software this way mimics the mathematics in a truly beautiful way, and the mathematics itself is the guiding star for how the software is developed. *DiffMan* is a MATLAB toolbox designed according to this philosophy, which implements many of the methods developed in this area of numerical ODE solvers. The interested reader is recommended to visit:

http://www.math.ntnu.no/num/diffman/

the home page of *DiffMan*.

The paper is organized as follows. Section 2 reviews all the necessary theory about actions and equivariant maps between homogeneous spaces. In Section 3 we consider the infinitesimal description of actions, relatedness of vector fields and develop the main theorem from which we infer the numerical algorithms. Section 4 presents different numerical algorithms based on different coordinates and some numerical examples. Finally, some concluding remarks.

2 Actions on manifolds and equivariant maps

We assume the reader to be familiar with the basic concepts of manifold, Lie group and Lie algebra. Two good references on this material - among a wealth of others - are Section 4.1 of [1] and Chapter 9 in [13]. Throughout this paper we will tacitly assume that every manifold is a differentiable manifold.

Actions of Lie groups on manifolds are of crucial importance to us. The action of the Lie group G is the tool for moving around on the manifold $\mathcal{M}$. We start with the standard definition of a Lie group action on a manifold.

Definition 2.1 (Lie group action)
*Let $\mathcal{M}$ be a manifold and let G be a Lie group. A **(left) action** of a Lie group G on $\mathcal{M}$ is a smooth mapping $\Phi : G \times \mathcal{M} \to \mathcal{M}$ such that:*

i) $\Phi(e,x) = x$ *for all* $x \in \mathcal{M}$*; and*

ii) $\Phi(g, \Phi(h,x)) = \Phi(gh,x)$ *for all* $g,h \in G$ *and* $x \in \mathcal{M}$.

For every $g \in G$ let $\Phi_g : \mathcal{M} \to \mathcal{M}$ denote the smooth map given by $x \mapsto \Phi(g,x)$, and for every $m \in \mathcal{M}$ let $\Phi_m : G \to \mathcal{M}$ denote the smooth map $g \mapsto \Phi(g,m)$. This notation might cause some confusion at first. Remember that the map is defined by the properties of the subindex element, so keep in mind the type of this element. With this notation Definition 2.1 is equivalent to the following definition:

Definition 2.2 (Lie group action – alternative definition)
*Let $\mathcal{M}$, G and Φ be as in Definition 2.1. A **(left) action** of G on $\mathcal{M}$ is a map Φ such that $g \mapsto \Phi_g$ is a group homomorphism of G into Diff($\mathcal{M}$). Diff($\mathcal{M}$) being the group of diffeomorphisms of $\mathcal{M}$. In other words;*

i) $\Phi_e = Id_{\mathcal{M}}$*; and*

ii) $\Phi_{gh} = \Phi_g \circ \Phi_h$ *for all* $g,h \in G$.

Further, one can classify actions on manifolds as **transitive**, if for every pair $x,y \in \mathcal{M}$ there exists at least one element $g \in G$ such that $\Phi_g(x) = y$.

Definition 2.3 (Homogeneous space)
A manifold with a transitive Lie group action is called a ***homogeneous space****. That is; the triple* $(\mathcal{M}, G, \Phi)$ *constitutes the homogeneous space.*

In this paper we will exclusively consider ordinary differential equations evolving on homogeneous spaces. Considering only this type of domain should by no means be considered as a restriction, as most domains used in mathematical modeling are included in the category of homogeneous spaces.

We now turn our attention to a particular class of smooth maps between homogeneous spaces.

Definition 2.4 (Equivariant map)
Let $\mathcal{M}$ *and* $\mathcal{N}$ *be manifolds and let* G *be a Lie group which acts on* $\mathcal{M}$ *by* $\Phi_g : \mathcal{M} \to \mathcal{M}$ *and on* $\mathcal{N}$ *by* $\Psi_g : \mathcal{N} \to \mathcal{N}$*. A smooth map* $f : \mathcal{M} \to \mathcal{N}$ *is called* ***equivariant*** *with respect to these actions if, for all* $g \in G$*,*

$$f \circ \Phi_g = \Psi_g \circ f, \tag{1}$$

that is, the following diagram commutes:

$$\begin{tikzcd} \mathcal{M} \arrow[r, "f"] & \mathcal{N} \\ \mathcal{M} \arrow[u, "\Phi_g"] \arrow[r, "f"'] & \mathcal{N} \arrow[u, "\Psi_g"'] \end{tikzcd}$$

Loosely speaking, the effects of the two actions on $\mathcal{M}$ and $\mathcal{N}$ are related through the equivariant map. To study the action of G on $\mathcal{N}$ we can instead study the action of G on $\mathcal{M}$. As we will see, the concept of an equivariant map is very important in the development of numerical algorithms. The idea is to choose the manifold $\mathcal{M}$ to be a vector space which supports the classical Runge-Kutta method. Instead of studying the action of G on some non-linear homogeneous space $\mathcal{N}$, we find an appropriate equivariant map that 'transforms' us to an equivalent action of G on our vector space.

As the fist step to accomplish this we establish the equivariance of Φ_p for $p \in \mathcal{M}$. Remember that Φ_p is a map from G to $\mathcal{M}$. Thus, any action on a homogeneous space can be equally well studied as an action of the Lie group on itself. Define L_g to be the **left** translation map on G, that is $L_g(h) = gh$, $\forall h \in G$.

Lemma 2.5 (Equivariance of Φ_p)
Given a left action $\Phi : G \to \mathit{Diff}(\mathcal{M})$ *of* G *on* $\mathcal{M}$*. Then for all* $p \in \mathcal{M}$ *the smooth map* $\Phi_p : G \to \mathcal{M}$ *is equivariant with respect to the action* L_g *of* G *on itself, and the action* Φ_g *of* G *on* $\mathcal{M}$*,* $g \in G$*:*

$$\Phi_p \circ L_g = \Phi_g \circ \Phi_p$$

That is; the following diagram commutes:

$$\begin{tikzcd} G \arrow[r, "\Phi_p"] & \mathcal{M} \\ G \arrow[u, "L_g"] \arrow[r, "\Phi_p"'] & \mathcal{M} \arrow[u, "\Phi_g"'] \end{tikzcd}$$

The proof of this is a mere consequence of the definition of an action, see Definition 2.2. In the case of a ***right*** *action, L_g must be substituted with R_g, the right translation map on G.*

To be able to apply classical Runge-Kutta methods, the domain space ought to be a vector space. The Lie algebra of a Lie group is a vector space with the additional structure of a commutator. Hence, the Lie algebra of the Lie group acting on the homogeneous space is the natural choice of space for our Runge-Kutta method.

Let $f : \mathfrak{g} \to G$ be a local coordinate map on G, hence f is smooth and invertible. Our goal is to find an action of G on $\mathfrak{g}$ such that f will be an equivariant map with respect to this action of G on $\mathfrak{g}$ and the left action of G on itself.

Lemma 2.6 (The action $\mathrm{B} : G \to \mathbf{Diff}(\mathfrak{g})$)
For $g \in G$ denote the left action of G on itself by L. B defined as

$$\mathrm{B}_g = f^{-1} \circ L_g \circ f \tag{2}$$

with respect to the coordinate map $f : \mathfrak{g} \to G$, is a local action of G on $\mathfrak{g}$ by construction.

In the case where f is the exponential map, B is nothing else than the well-known Baker-Campbell-Hausdorff (BCH) formula. For $x, y \in \mathfrak{g}$, $\mathrm{BCH}(x, y)$ is defined to be $\exp(\mathrm{BCH}(x, y)) = \exp(x)exp(y)$. What we get is $B_g(u) = \log(g \cdot \exp(u))$, which implies $\exp(\mathrm{BCH}(\log(g), u)) = g \cdot \exp(u)$.

Since the composition of two equivariant maps is an equivariant map, we can construct an equivariant map from $\mathfrak{g}$ to $\mathcal{M}$ with respect to the actions B on $\mathfrak{g}$ and Φ on $\mathcal{M}$. Just choose the composition $\Phi_p \circ f : \mathfrak{g} \to \mathcal{M}$ and the following diagram commutes:

$$\begin{tikzcd} \mathfrak{g} \arrow[r, "f"] & G \arrow[r, "\Phi_p"] & \mathcal{M} \\ \mathfrak{g} \arrow[u, "\mathrm{B}_g"] \arrow[r, "f"'] & G \arrow[u, "L_g"'] \arrow[r, "\Phi_p"'] & \mathcal{M} \arrow[u, "\Phi_g"'] \end{tikzcd} \tag{3}$$

The commutative diagram (3) sums up all the important concepts introduced in this section. We have constructed an action of the Lie group G on the Lie algebra $\mathfrak{g}$ and an equivariant map $\Phi_p \circ f$ from $\mathfrak{g}$ to $\mathcal{M}$. We are now in a position were studying the action of B on $\mathfrak{g}$ is equivalent to study the action Φ on $\mathcal{M}$.

3 Infinitesimal description of actions and relatedness

We now turn to the infinitesimal description of actions and equivariant maps. Let us first define an infinitesimal generator of an action:

Definition 3.1 (Infinitesimal generator)
Suppose $\Phi : G \to \mathit{Diff}(\mathcal{M})$ defined by $g \mapsto \Phi_g$ is an action of the Lie group G with Lie algebra $\mathfrak{g}$ on the manifold $\mathcal{M}$. The ***infinitesimal generator*** *of the action corresponding to $\xi \in \mathfrak{g}$ is*

$$\xi_{\mathcal{M}}(x) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Phi_{\exp(t\xi)}(x), \quad \forall x \in \mathcal{M}. \tag{4}$$

The infinitesimal generator is a vector field on $\mathcal{M}$.

What the infinitesimal generator describes is the direction of the motion on the manifold, subject to the action of the Lie group element $\exp(t\xi)$. This is the tangent of the flow and the direction of where to proceed. The next Lemma answers what the flow of an infinitesimal generator is.

Lemma 3.2 (Flow of infinitesimal generator)
Suppose $\Phi : G \to \mathit{Diff}(\mathcal{M})$ is an action of the Lie group G on the manifold $\mathcal{M}$ with infinitesimal generator $\xi_{\mathcal{M}}$. Then $\Phi_{\exp(t\xi)} : \mathcal{M} \to \mathcal{M}$ is the flow of $\xi_{\mathcal{M}}$. A flow is an $\mathbb{R}$-action on $\mathcal{M}$.

Proof: We simply take the time derivative of the flow and apply a simple trick:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Phi_{\exp(t\xi)}(m) &= \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=t} \Phi_{\exp(s\xi)}(m) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \Phi_{\exp((s+t)\xi)}(m) && (5) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} \Phi_{\exp(s\xi)} \circ \Phi_{\exp(t\xi)}(m) && (6) \\
&= \xi_{\mathcal{M}} \circ \Phi_{\exp(t\xi)}(m)
\end{aligned}$$

The equality of (5) and (6) is justified by noticing that $[t\xi, s\xi] = 0$ and remembering that Φ is an action. This completes the proof.

Referring to Definition 2.2, an action of a Lie group G on a manifold $\mathcal{M}$ can be regarded as a homomorphism from G to $\mathrm{Diff}(\mathcal{M})$. Similarly, we can define a Lie algebra action.

Definition 3.3 (Lie algebra action)
A ***Lie algebra action*** *of $\mathfrak{g}$ on $\mathcal{M}$ is a map $\lambda : \mathfrak{g} \mapsto \mathfrak{X}(\mathcal{M})$ such that $\xi \mapsto \xi_{\mathcal{M}}$ is a Lie algebra homomorphism of $\mathfrak{g}$ into $\mathfrak{X}(\mathcal{M})$. $\mathfrak{X}(\mathcal{M})$ is the left Lie algebra*

of Diff($\mathcal{M}$) with the negative Lie-Jacobi bracket as Lie algebra bracket. The Lie-Jacobi bracket is given as:

$$Z^i = [X, Y]^i = \sum_j X^j \frac{\partial Y^i}{\partial x^j} - Y^j \frac{\partial X^i}{\partial x^j},$$

where X, Y, Z are vector fields over $\mathcal{M}$.

Both a Lie group action and a Lie algebra action can be viewed as homomorphisms, and the latter can be interpreted as the tangent lift of the former. The precise requirements to establish this connection are given by a theorem of Palais (See [1] page 270, or [18]).

Theorem 3.4 (Palais)
Let G be a simply connected Lie group, $\mathcal{M}$ a compact manifold, and $\phi : \mathfrak{g} \to \mathfrak{X}(\mathcal{M})$ a Lie algebra homomorphism. Then there exists a unique action $\Phi : G \to$ Diff($\mathcal{M}$) such that $\mathrm{T}\Phi = \phi$.

Thus, in the case of a simply connected Lie group we have an bijection between the Lie group actions on a compact manifold $\mathcal{M}$ and the Lie algebra actions on $\mathcal{M}$. In cases where the group is not simply connected consider instead the action of the universal covering group which is always simply connected. In our numerical calculations we are always working locally, hence we can always find a local domain on the manifold being compact.

Next, we turn our attention to vector fields.

Definition 3.5 (Relatedness of vector fields)
Let $\phi : \mathcal{M} \to \mathcal{N}$ be a smooth map between manifolds. The vector fields $X \in \mathfrak{X}(\mathcal{M})$ and $Y \in \mathfrak{X}(\mathcal{N})$ are called ϕ-related, denoted $X \sim_\phi Y$, if $\mathrm{T}\phi \circ X = Y \circ \phi$. The definition means that the following diagram commutes:

$$\begin{array}{ccc} \mathrm{T}\mathcal{M} & \xrightarrow{\mathrm{T}\phi} & \mathrm{T}\mathcal{N} \\ {\scriptstyle X}\uparrow & & \uparrow{\scriptstyle Y} \\ \mathcal{M} & \xrightarrow[\phi]{} & \mathcal{N} \end{array}$$

In the case of ϕ being a diffeomorphism, $X \sim_\phi Y$ is equivalent to saying that X is the pull-back of Y.

Where is the numerics in all of this abstract theory? The guiding principle is the following simple observation. Let $\Phi_{\exp(t\xi)}$ and $\Psi_{\exp(t\xi)}$ be two flows on $\mathcal{M}$ and $\mathcal{N}$, respectively, generated by the element $\xi \in \mathfrak{g}$ and the action Φ on $\mathcal{M}$ and Ψ on $\mathcal{N}$ of the Lie group G. Recall that a flow can be regarded as an action of $\mathbb{R}$ on the manifold. Our goal is to solve for a flow on a simpler manifold $\mathcal{M}$ so that the effect is the same as if one solved for the flow on $\mathcal{N}$. 'Simpler' means in our context that the manifold is a vector space.

We now consider the infinitesimal consequences of equivariance. Suppose that the map $\phi : \mathcal{M} \to \mathcal{N}$ is equivariant with respect to the two flows $\Phi_{\exp(t\xi)}$

and $\Psi_{\exp(t\xi)}$. The next theorem states that if ϕ is an equivariant map, the infinitesimal generators of the actions with respect to the same element $\xi \in \mathfrak{g}$ are ϕ-related vector fields.

Theorem 3.6
Let $\phi : \mathcal{M} \to \mathcal{N}$ be a smooth map between manifolds. Further, let $\Phi_{\exp(t\xi)}$ and $\Psi_{\exp(t\xi)}$ be the flows of the infinitesimal generators $\xi_{\mathcal{M}}$ and $\xi_{\mathcal{N}}$. Then ϕ is an equivariant map with respect to the flows $\Phi_{\exp(t\xi)}$ and $\Psi_{\exp(t\xi)}$, that is; $\phi \circ \Phi_{\exp(t\xi)} = \Psi_{\exp(t\xi)} \circ \phi$, iff $\xi_{\mathcal{M}}$ and $\xi_{\mathcal{N}}$ are ϕ-related, that is; $\xi_{\mathcal{M}} \sim_{\phi} \xi_{\mathcal{N}}$.

Proof: (From [2]). Take the time derivative of the relation $\phi \circ \Phi_{\exp(t\xi)}(m) = \Psi_{\exp(t\xi)} \circ \phi(m)$, $m \in \mathcal{M}$, and use the flow/vector field property to get

$$\begin{aligned}
\mathrm{T}\phi \circ \frac{\mathrm{d}}{\mathrm{d}t}\Phi_{\exp(t\xi)}(m) &= \frac{\mathrm{d}}{\mathrm{d}t}\Psi_{\exp(t\xi)} \circ \phi(m) \\
\mathrm{T}\phi \circ \xi_{\mathcal{M}} \circ \Phi_{\exp(t\xi)}(m) &= \xi_{\mathcal{N}} \circ \Psi_{\exp(t\xi)} \circ \phi(m) \\
&= \xi_{\mathcal{N}} \circ \phi \circ \Phi_{\exp(t\xi)}(m) \\
\Rightarrow \quad \mathrm{T}\phi \circ \xi_{\mathcal{M}} &= \xi_{\mathcal{N}} \circ \phi
\end{aligned}$$

Starting with this relation, let $c(t) = \Phi_{\exp(t\xi)}(m)$ denote the integral curve of $\xi_{\mathcal{M}}$ through $m \in \mathcal{M}$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}(\phi \circ c)(t) = \mathrm{T}\phi \circ \frac{\mathrm{d}c(t)}{\mathrm{d}t} = \mathrm{T}\phi \circ \xi_{\mathcal{M}} \circ c(t) = \xi_{\mathcal{N}} \circ \phi \circ c(t). \tag{7}$$

This says that $\phi \circ c$ is the integral curve of $\xi_{\mathcal{N}}$ through the point $\phi(c(0)) = \phi(m)$. By uniqueness of integral curves, we get $\phi \circ \Phi_{\exp(t\xi)}(m) = \phi \circ c(t) = \Psi_{\exp(t\xi)}(\phi(m))$. This completes the proof.

In the case of the equivariant map $\Phi_p \circ f : \mathfrak{g} \to \mathcal{M}$, we have the following commutative diagram relating the flows on the manifold $\mathcal{M}$ and the Lie algebra $\mathfrak{g}$:

$$\begin{tikzcd}
\mathfrak{g} \arrow[r, "f"] & G \arrow[r, "\Phi_p"] & \mathcal{M} \\
\mathfrak{g} \arrow[r, "f"'] \arrow[u, "\mathrm{B}_{\exp(t\xi)}"] & G \arrow[r, "\Phi_p"'] \arrow[u, "L_{\exp(t\xi)}"'] & \mathcal{M} \arrow[u, "\Phi_{\exp(t\xi)}"']
\end{tikzcd}$$

From Theorem 3.6 we know that the infinitesimal generators of the flows $\mathrm{B}_{\exp(t\xi)}$ and $\Phi_{\exp(t\xi)}$ on $\mathfrak{g}$ and $\mathcal{M}$ are $\Phi_p \circ f$-related. That is;

$$\xi_{\mathcal{M}} \circ \Phi_p \circ f = \mathrm{T}\Phi_p \circ \mathrm{T}f \circ \xi_{\mathfrak{g}}. \tag{8}$$

It is implicit, and an assumption that we know that the differential equation evolving on the manifold $\mathcal{M}$ can be written as an infinitesimal generator of the action. Having established equation (8), the next question is: What is $\xi_{\mathfrak{g}}$?

Theorem 3.7
Let $f : \mathfrak{g} \to G$ be a coordinate map on G and $\Phi_p \circ f$ equivariant with respect to the flows $\mathrm{B}_{\exp(t\xi)}$ and $\Phi_{\exp(t\xi)}$. The infinitesimal generator of B *satisfying equation (8), is $\xi_{\mathfrak{g}}(u) = \mathrm{df}_u^{-1}(\xi)$. $\mathrm{df} : \mathfrak{g} \to \mathfrak{g}$ is the trivialization of $\mathrm{T}f$ defined as $\mathrm{df}_u = TR_{f(u)^{-1}} \circ \mathrm{T}f_u$.*

Proof: Since every Lie group action Φ on a manifold $\mathcal{M}$ by equivariance of Φ_p is equivalent to an action of G on itself, we only need to consider infinitesimal generators over $\mathfrak{g}$ and G. T denotes the tangent lift of a mapping between manifolds to a mapping between tangent bundles. Denote by d the part of such a lifted mapping that maps $\mathfrak{g}$ to $\mathfrak{g}$. Hence f takes $u \mapsto f(u)$ and the lift is $\mathrm{T}f_u : \mathrm{T}\mathfrak{g}_u \to \mathrm{T}G_{f(u)}$. $\mathrm{T}\mathfrak{g}_u \approx \mathfrak{g}$ and $\mathrm{T}G_{f(u)}$ can be identified with $\mathfrak{g}$ through a translation $\mathrm{T}R$, R being the right translation map on G. Because of this, $\mathrm{T}f_u$ can be represented by a map $\mathrm{df}_u : \mathfrak{g} \to \mathfrak{g}$, that is:

$$\mathrm{T}f_u = \mathrm{T}R_{f(u)} \circ \mathrm{df}_u\,.$$

According to Theorem 3.6 and $f \circ \mathrm{B}_{\exp(t\xi)} = L_{\exp(t\xi)} \circ f$ the following equality must be satisfied:

$$\begin{aligned} \mathrm{T}f_u \circ \xi_{\mathfrak{g}}(u) = \xi_G \circ f(u) = \mathrm{T}R_{f(u)}(\xi) \\ \mathrm{T}R_{f(u)} \circ \mathrm{df}_u \circ \xi_{\mathfrak{g}}(u) = \mathrm{T}R_{f(u)}(\xi) \end{aligned} \tag{9}$$

Choosing $\xi_{\mathfrak{g}}(u) = \mathrm{df}_u^{-1}(\xi)$ in (9) completes the proof.

The following commutative diagram sums up what we have accomplished:

$$\begin{array}{ccccc} \mathrm{T}\mathfrak{g} & \xrightarrow{\mathrm{T}f} & \mathrm{T}G & \xrightarrow{\mathrm{T}\Phi_p} & \mathrm{T}\mathcal{M} \\ {\scriptstyle \mathrm{df}_u^{-1}(\xi)}\uparrow & & \uparrow{\scriptstyle \mathrm{T}R_p(\xi)} & & \uparrow{\scriptstyle \xi_{\mathcal{M}}(p)} \\ \mathfrak{g} & \xrightarrow[f]{} & G & \xrightarrow[\Phi_p]{} & \mathcal{M} \end{array} \tag{10}$$

As a concluding remark of this section we emphasize the two-fold role of the Lie algebra $\mathfrak{g}$. Given a differential equation on $\mathcal{M}$ we want to solve an equivalent differential equation on $\mathfrak{g}$. This is because $\mathfrak{g}$ has the structure of a vector space. To do this we construct an equivariant map from $\mathfrak{g}$ to $\mathcal{M}$. On the other hand, $\mathfrak{g}$ is also the Lie algebra of the Lie group that acts on the manifold $\mathcal{M}$. Because of this we also find elements $\xi \in \mathfrak{g}$ as parameters in the infinitesimal generators.

4 Applications of the theory

We want to numerically solve differential equations evolving on a homogeneous space $\mathcal{M}$. Our strategy is to transform the vector field on $\mathcal{M}$ to an equivalent vector field on the Lie algebra $\mathfrak{g}$. The reason for choosing the Lie algebra is because this manifold is a vector space, and for instance Runge-Kutta methods can be used to solve for the differential equation on $\mathfrak{g}$. The solution on $\mathcal{M}$ is then advanced through the equivariant map.

4.1 Algorithmic overview

Formalizing the situation, we want to solve the differential equation

$$y' = F(y), \qquad y_0 = \Phi_{y_0} \circ f(0) \in \mathcal{M}$$

where F is assumed to be written as the infinitesimal generator

$$F(y) = \xi_{\mathcal{M}}(y) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Phi(\exp(t \cdot \xi(s,y)), y)$$

for some $\xi : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$ that describes the differential equation.

What we obtained in the previous section is the following commutative diagram (a compressed version of (10)):

$$\begin{tikzcd}
\mathrm{T}\mathfrak{g} \arrow[r, "\mathrm{T}\Phi_y \circ \mathrm{T}f"] & \mathrm{T}\mathcal{M} \\
\mathfrak{g} \arrow[u, "\mathrm{df}_u^{-1}(\xi(s,y))"] \arrow[r, "\Phi_y \circ f"'] & \mathcal{M} \arrow[u, "F(y)=\xi_{\mathcal{M}}(y)"']
\end{tikzcd}$$

Observe that once the map ξ describing the differential equation on $\mathcal{M}$ has been found, the transformation to an equivalent system on $\mathfrak{g}$ is simply done by choosing as parameter input to the vector field df_u^{-1}, the output of the function ξ. Hence, we are able to solve all those differential equations evolving on the homogeneous space $\mathcal{M}$ that can be described as an infinitesimal generator with respect to the action Φ of G on $\mathcal{M}$ for some map ξ into the Lie algebra. A general time-dependent differential equation in this family is described by a map $\xi : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$. Assuming that differential equations on $\mathcal{M}$ can be written as an infinitesimal generator is by no means a limitation. All Lie type equations fit into this framework, as well as isospectral flows, rigid frames, and of course all classical equations evolving on $\mathbb{R}^n$. For more details on this, see [16].

The following algorithm incorporates all the above ideas.

Algorithm 4.1
Assume that the vector field F over the homogeneous space $\mathcal{M}$ can be written as an infinitesimal generator of the action Φ of the Lie group G on the manifold $\mathcal{M}$. That is; $F(y) = \xi_{\mathcal{M}}(y)$ for some map $\xi : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$ which describes the differential equation. The following is a q'th order Runge-Kutta based numerical method for the solution $y(t) \in \mathcal{M}$:

- *Choose the initial point $u_0 = 0$ in $\mathfrak{g}$. For any initial point $y_0 \in \mathcal{M}$ we have $y_0 = \Phi_{y_0} \circ f(u_0)$.*

- *Solve $u' = \mathrm{df}_u^{-1}(\xi(s,y))$, $u(0) = u_0$ by taking one step with any q'th order Runge-Kutta method. Denote the solution by u_1.*

- *Advance the solution on $\mathcal{M}$ from y_0 to y_1 by the equivariant map $\Phi_{y_0} \circ f$. That is; $y_1 = \Phi_{y_0} \circ f(u_1)$.*

This is a q'th order method on $\mathcal{M}$ since $\Phi_y \circ f$ is smooth, and a q'th order modification on $\mathfrak{g}$ will result in a corresponding modification on $\mathcal{M}$ with at least order q.

4.2 Different coordinate implementations

We will now see how the function $\mathrm{df}_u^{-1}(\xi(s,y))$ manifests itself for different choices of the local coordinate map f.

4.2.1 Canonical coordinates of the first kind

Choosing $f = \exp : \mathfrak{g} \to G$ in Algorithm 4.1 we obtain the original method of Munthe-Kaas [14]. Since every Lie group can be coordinatized by the exponential map there is no restriction on the applicability of the method. In the case of the exponential map, the vector field on $\mathfrak{g}$, dexp_u^{-1}, is represented by the infinite sum

$$\mathrm{dexp}_u^{-1}(v) = v - \frac{1}{2}[u,v] + \sum_{k=2}^{\infty} \frac{B_k}{k!} \overbrace{[u,[u,[\cdots,[}^{k} u,v]\cdots]]]. \tag{11}$$

$[\cdot,\cdot]$ denotes the commutator in the Lie algebra $\mathfrak{g}$, and B_k is the kth Bernoulli number. In an implementation of the RKMK method this infinite sum must be truncated. For a q'th order classical Runge-Kutta method we introduce the following q'th order truncation of (11):

$$\mathrm{dexpinv}(u,v,q) = \sum_{k=0}^{q-1} \frac{B_k}{k!} \overbrace{[u,[u,[\cdots,[}^{k} u,v]\cdots]]].$$

This truncated version of dexp_u^{-1} is used as the vector field on $\mathfrak{g}$.

Channell and Scovel reformulate the Ge-Marsden Lie-Poisson integration algorithm by coordinatizing the Lie group through the exponential map [5]. Their approach is very similar to ours, albeit not as general. They also find the first terms in the expansion (11) for dexp^{-1}.

4.2.2 Canonical coordinates of the second kind

Let $\{x_1, \dots, x_n\}$ denote a basis of the n-dimensional Lie algebra $\mathfrak{g}$. Every element in the Lie algebra can be written as a linear combination of elements in this basis. Let the n-tuple of real numbers $\xi = (\xi_1, \dots, \xi_n)$ represent the element $(\xi_1 x_1 + \cdots + \xi_n x_n)$ of the Lie algebra. Canonical coordinates of the second kind are then defined as the following map depending on the basis of the Lie algebra:

$$\phi : \xi = (\xi_1, \dots, \xi_n) \mapsto \exp(\xi_1 x_1)\exp(\xi_2 x_2)\cdots\exp(\xi_n x_n) \tag{12}$$

A straight forward calculation will produce the desired differential of this mapping, namely $\mathrm{d}\phi$:

$$\mathrm{d}\phi_u(v) = \sum_{k=1}^{n} \mathrm{Ad}_{\prod_{i=1}^{k-1}\exp(u_i x_i)} v_k x_k \tag{13}$$

Inverting to find $\mathrm{d}\phi^{-1}$ is not a trivial task, and has very recently been studied by Owren and Marthinsen in [17].

Wei and Norman, in [20, 21], studied the global properties of canonical coordinates of the second kind. Their main theorem states that the coordinates of the second kind are global whenever the Lie algebra $\mathfrak{g}$ is of finite dimension and solvable.

4.2.3 Cayley coordinates of the first kind

The Cayley transform, $\mathrm{cay} : \mathfrak{g} \to G$ is defined as:

$$\mathrm{cay}(u) = \frac{1+\frac{u}{2}}{1-\frac{u}{2}}$$

As mentioned in the introduction, the Cayley transform exists for several of the matricial Lie groups. The appealing feature of this map is the lesser expense in computing it, as compared to the exponential map. Thus using a method based on the Cayley transform should be an appealing option whenever possible.

By a simple calculation the corresponding vector field on the Lie algebra dcay_u^{-1} is calculated to be

$$\mathrm{dcay}_u^{-1}(v) = v - \frac{1}{2}[u,v] - \frac{1}{4}u\cdot v\cdot u, \tag{14}$$

where $[\cdot,\cdot]$ denotes the matrix commutator and '$\cdot$' denotes matrix multiplication. Notice the resemblance of this expression to that of dexp_u^{-1} in (11). The first two terms are identical. The Cayley transform is the first diagonal Padé approximant to the exponential, and it is therefore natural that dcay_u^{-1} behaves in a similar manner to dexp_u^{-1}. dcay_u^{-1} is also exactly computable, since no truncation of the series is necessary.

The Cayley transform has been used in the numerical solution of unitary differential systems and isospectral flows, see the work of Diele et.al. [6, 7] and Zanna [23]. There is also an interesting application of the Cayley transform in the energy-momentum method in the solution of Hamiltonian systems on Lie groups, see Lewis and Simo [11].

4.2.4 Cayley coordinates of the second kind

Conforming with the use of the term 'canonical coordinates of the second kind' as synonymous to products of exponentials, we choose to name products of Cayley transforms as 'Cayley coordinates of the second kind'.

Similarly to the situation in Subsection 4.2.2, we have a Lie algebra with basis $\{x_1, \ldots, x_n\}$ and the n-tuple of real numbers $\xi = (\xi_1, \ldots, \xi_n)$ represents an element of the Lie algebra. Cayley coordinates of the second kind are then defined as the following product of Cayley transforms, depending on the basis:

$$\phi : \xi = (\xi_1, \ldots, \xi_n) \mapsto \operatorname{cay}(\xi_1 x_1) \operatorname{cay}(\xi_2 x_2) \cdots \operatorname{cay}(\xi_n x_n)$$

The calculation of the differential of the mapping ϕ follows along the same lines as for ϕ in (13), except that some care most be taken in the 'elimination' of the dcays. Our calculation assumes that the basis elements of the Lie algebra satisfies the relation $x^3 = -x$, which is valid for instance for $\mathfrak{so}(n)$.

Hence, the result is:

$$\mathrm{d}\phi_u(v) = \sum_{k=1}^{n} \operatorname{Ad}_{\prod_{i=1}^{k-1} \operatorname{cay}(u_i x_i)} \frac{v_k}{1 + \frac{u_k^2}{4}} x_k \tag{15}$$

Inversion of (15) will follow along similar lines as in the inversion of (13). For details relating to this inversion, see [17].

4.2.5 Higher order diagonal Padé coordinates

Things are very simple for the Cayley transform. If we want to use higher order Padé approximations to the exponential map [3, 8], things get more complicated. The main reason for this is the non-commutativity of matrix multiplication.

The (p,p)-diagonal Padé approximant is defined as

$$R_{pp}(u) = \frac{N_{pp}(u)}{N_{pp}(-u)},$$

where

$$N_{pp}(u) = \sum_{j=0}^{p} c_j^{(p)} u^j = \sum_{j=0}^{p} \frac{(2p-j)!p!}{(2p)!j!(p-j)!} u^j.$$

From this, $\mathrm{dR}_{pp,u}(v)$ is readily being found to equal

$$\begin{aligned} \mathrm{dR}_{pp,u}(v) = N_{pp}(-u)^{-1} \Bigg(N_{pp}(-u) \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} N_{pp}(u+tv) \\ - N_{pp}(u) \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} N_{pp}(-u-tv) \Bigg) N_{pp}(u)^{-1}. \end{aligned} \tag{16}$$

Substituting for N_{pp} into (16), we get

$$\begin{aligned} N_{pp}(-u)\, \mathrm{dR}_{pp,u}(v) N_{pp}(u) = \\ \sum_{j=0}^{p} \sum_{m=0}^{p-1} \sum_{k=0}^{m} c_j^{(p)} c_{m+1}^{(p)} ((-1)^j + (-1)^m) u^{j+k} v u^{m-k}. \end{aligned} \tag{17}$$

Setting $p = 1$ in (17), we get the Cayley coordinate situation:

$$N_{11}(-u)\,\mathrm{dR}_{11,u}(v)N_{11}(u) = v$$

This expression can be inverted directly and we get

$$\mathrm{dR}_{11,u}^{-1}(v) = N_{11}(-u)\cdot v\cdot N_{11}(u),$$

which in expanded form is identical to (14).

For $p = 2$ we obtain

$$N_{22}(-u)\,\mathrm{dR}_{22,u}(v)N_{22}(u) = v - \frac{1}{12}u\cdot v\cdot u, \tag{18}$$

and for $p = 3$ we get

$$N_{33}(-u)\,\mathrm{dR}_{33,u}(v)N_{33}(u) = \\ v - \frac{1}{10}u\cdot v\cdot u + \frac{1}{60}(u^2\cdot v + u\cdot v\cdot u + v\cdot u^2) + \frac{1}{600}u^2\cdot v\cdot u^2. \tag{19}$$

For the general inversion of (17) to find dR_{pp}^{-1} we need to solve a linear matrix system in v. We will now demonstrate one such procedure for $\mathrm{dR}_{22,u}$ (See e.g. [10]). To find the inverse function $\mathrm{dR}_{22,u}^{-1}$ we realize, by examining (18), that we need to solve a matrix equation of the type

$$Z - XZX = W \tag{20}$$

for the matrix Z, where $X, Z, W \in \mathbb{R}^{n\times n}$. One way to solve equation (20) is to rewrite it as a linear system in Z. Assembling all the columns of a matrix A into a $n^2 \times 1$ vector and denoting it $\vec{a}$, we obtain the following equivalent linear system

$$(I_n \otimes I_n + X^T \otimes X)\vec{z} = \vec{w}, \tag{21}$$

where $\otimes$ denotes the Kronecker product, and I_n is the $n \times n$ identity matrix. This procedure generalizes easily to the dR_{pp}-case.

4.3 Numerical examples

We consider the following equation evolving in SO(3).

$$y'(t) = a(y(t))y(t) \tag{22}$$

Here, $a : \mathrm{SO}(3) \to \mathfrak{so}(3)$ is the following skew-symmetric matrix:

$$a(y) = \frac{1}{2}(y - y^T) \tag{23}$$

We solve the equation (22) with initial condition $y(0) = \mathtt{q}$, where `q` is the special orthogonal matrix obtained by the command `[q,r] = qr(magic(3))` in MATLAB. The equation is integrated from $t = 0$ to $t = 1$, with step sizes $h = [2^{-1}\ 2^{-2}\ 2^{-3}\ 2^{-4}\ 2^{-5}\ 2^{-6}\ 2^{-7}\ 2^{-8}]$.

We are interested in the flops impact the choice of different coordinate maps have for methods of different order. We consider local coordinates of the type exp, cay and R_{22}. In the numerical calculations we truncate the dexp^{-1}-series to the appropriate order, whereas for the dcay^{-1} and dR_{22}^{-1} we calculate these expressions exactly. The comparison is done for the following four Runge-Kutta methods: E1 - Eulers method (first order), ME2 - Modified Eulers method (second order), RK4 - 'The Runge-Kutta method' (fourth order), and butcher6 - Butchers sixth order method. The experiments were done using MATLAB and the *DiffMan* Toolbox.

In Figure 1 we see four plots, one for each of the methods. Along the horizontal axis is the flops count as measured by MATLAB, and along the vertical axis is the global error in the solution for $t = 1$. In the figure, exp coordinates are denoted by a continuous line with circles, cay coordinates are denoted by a dotted line, and R_{22} coordinates by a dash-dotted line.

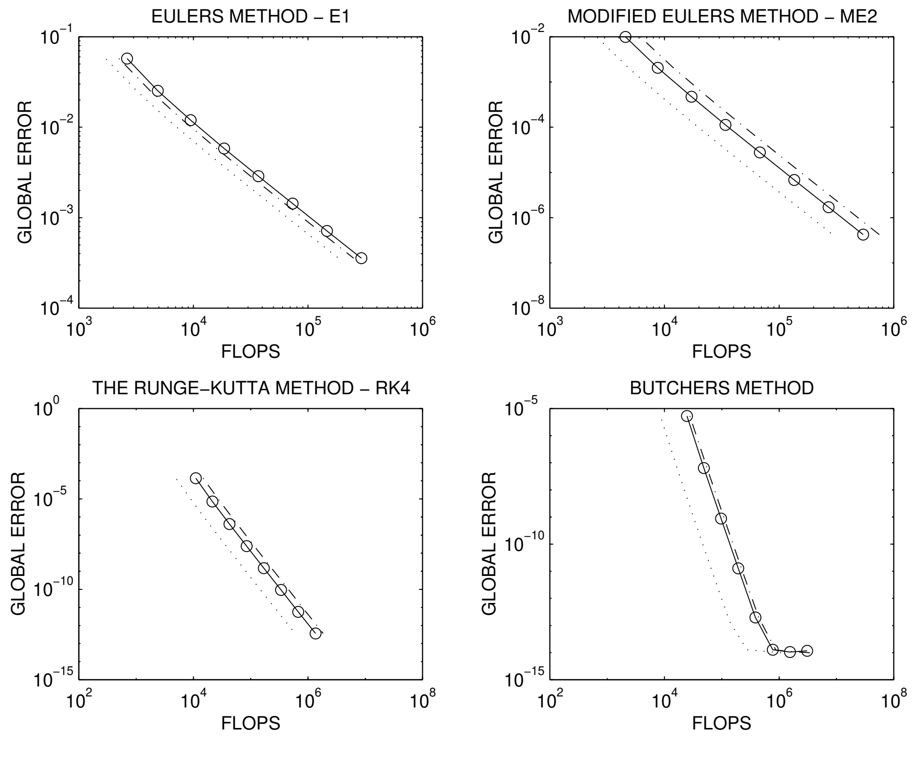

Figure 1: Global error versus flops count.

From the plots we can conclude that the Cayley coordinates does constitute a saving in this particular problem for all the different methods. It should be warned, however, that the Cayley coordinates do run into trouble if -1 is an eigenvalue of $y(t)$. In case of the R_{22} coordinates we have to solve a linear system in each step in order to determine R_{22}^{-1}. This is expensive and does not compare with the exponential coordinates, unless for very high order methods.

5 Conclusion

We have constructed a local group action on the Lie algebra $\mathfrak{g}$ equivalent in the sense of equivariance to the group action on the manifold $\mathcal{M}$. Hence, this gives us the following group action diagram:

$$
\begin{tikzcd}
\mathfrak{g} \arrow[r, "f"] & G \arrow[r, "\Phi_p"] & \mathcal{M} \\
\mathfrak{g} \arrow[r, "f"'] \arrow[u, "\mathrm{B}_g"] & G \arrow[r, "\Phi_p"'] \arrow[u, "L_g"'] & \mathcal{M} \arrow[u, "\Phi_g"']
\end{tikzcd}
$$

Accompanying the above finite picture of the situation, there is also an infinitesimal diagram:

$$
\begin{tikzcd}
\mathrm{T}\mathfrak{g} \arrow[r, "\mathrm{T}f"] & \mathrm{T}G \arrow[r, "\mathrm{T}\Phi_p"] & \mathrm{T}\mathcal{M} \\
\mathfrak{g} \arrow[r, "f"'] \arrow[u, "\mathrm{df}_u^{-1}(\xi)"] & G \arrow[r, "\Phi_p"'] \arrow[u, "\mathrm{T}R_p(\xi)"'] & \mathcal{M} \arrow[u, "\xi_{\mathcal{M}}(p)"']
\end{tikzcd}
$$

Every vector field locally written in the form of an infinitesimal generator on the manifold $\mathcal{M}$ can be transformed to an equivalent vector field on the Lie algebra $\mathfrak{g}$. These vector fields are $\Phi_p \circ f$-related. We emphasize that all the above constructions are local in nature, since we are considering local coordinate maps on the Lie group manifold.

Addressing the aspects of developing object oriented software what we have obtained is a nice separation of 'how' a differential equation is defined on the domain, verses 'what', in terms coordinates, is used in the numerical integrator. In other words, a differential equation can be defined in a coordinate-free manner, independently of the actual coordinates used to coordinatize the Lie group in the numerical method.

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