A Theoretical Framework for Backward Error Analysis on Manifolds

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Abstract

Backward Error Analysis (BEA) has been a crucial tool when analyzing long-time behavior of numerical integrators, in particular, one is interested in the geometric properties of the perturbed vector field that a numerical integrator generates. In this article we present a new framework for BEA on manifolds. We extend the previously known "exponentially close" estimates from $\mathbb{R}^n$ to smooth manifolds and also provide an abstract theory for classifications of numerical integrators in terms of their geometric properties. Classification theorems of type "symplectic integrators generate symplectic perturbed vector fields" are known to be true in $\mathbb{R}^n$. We present a general theory for proving such theorems on manifolds by looking at the preservation of smooth k-forms on manifolds by the pull-back of a numerical integrator. This theory is related to classification theory of subgroups of diffeomorphisms. We also look at other subsets of diffeomorphisms that occur in the classification theory of numerical integrators. Typically these subsets are anti-fixed points of group homomorphisms.

Dedicated to the memory of Jerrold E. Marsden.

1 Introduction

Let $\mathcal{M}$ be a smooth manifold, where, by smooth we throughout the paper mean C^∞. A smooth manifold is presumed to be finite-dimensional, while infinite-dimensional manifolds (when considered in Section 5) will always have the name "infinite", when addressed. Let $\mathfrak{X}(\mathcal{M})$ denote the set of smooth vector fields and let $X \in \mathfrak{X}(\mathcal{M})$. Consider the ordinary differential equation

$$\frac{d}{dt}y(t) = X_{y(t)}, \quad y(t) \in \mathcal{M}. \tag{1.1}$$

The flow map corresponding to X is denoted by $\theta_X : \mathbb{R} \times \mathcal{M} \to \mathcal{M}$. Also, we sometimes use the notation

$$\theta_X^{(q)}(t) = \theta_{X,t}(q) = \theta_X(t, q),$$

and if the vector field X is obvious we sometimes use θ instead of θ_X.

A numerical approximation to the solution of (1.1) can be found by constructing a family of diffeomorphisms $\{\Phi_h\}_{h\geq 0}$ and then (for each fixed h) one can obtain a sequence $\{q_{h,n}\}_{n\in\mathbb{N}}$, often referred to as the numerical solution, satisfying $q_{h,n+1} = \Phi_h(q_{h,n})$. We will throughout the paper denote the family $\{\Phi_h\}_{h\geq 0}$ by Φ_h. More formally we have the following:

Definition 1. *An integrator is a one-parameter family $\Phi_h : \mathcal{M} \to \mathcal{M}$ of diffeomorphisms that is smooth in h and satisfies $\Phi_0 = id$ (the identity mapping). If $X \in \mathfrak{X}(\mathcal{M})$ and*

$$\frac{d}{dh}\Big|_{h=0}\Phi_h(p) = X_p, \qquad p \in \mathcal{M},$$

then Φ_h is called an integrator for X. If, for any chart (U, φ) on $\mathcal{M}$, there exist a constant $C > 0$ such that, for $\hat{\Phi}_h = \varphi \circ \Phi_h \circ \varphi^{-1}$ and sufficiently small h

$$\|\hat{\Phi}_h(x) - \theta_{Y,h}(x)\| \leq Ch^{p+1}, \qquad x \in \varphi(U),$$

where Y is the vector field on $\varphi(U)$ induced by φ, the integrator Φ_h is said to be consistent with X of order p.

Remark 1 It follows immediately by smoothness and the Taylor theorem that if Φ_h is an integrator for X then Φ_h is consistent with X of order one.

If Φ_h is an integrator for the vector field X then, under suitable assumptions on Φ_h, one can guarantee that there is a metric d on $\mathcal{M}$ such that

$$d(q_n, \theta_{X,nh}(q_o)) \leq Ch^p, \qquad p \in \mathbb{N}, \quad C > 0,$$

at least for $nh \leq T$ for some $T > 0$ and sufficiently small h. The integer p is often referred to as the order of the numerical integrator.

The idea of backward error analysis is the following. Supposing that we have a numerical solution $\{q_{h,n}\}$ i.e. $q_{h,n+1} = \Phi_h(q_{h,n})$, could it be the case that the sequence $\{q_{h,n}\}$ is the "solution" to a different differential equation i.e. does there exist a vector field $\widetilde{X} \in \mathfrak{X}(\mathcal{M})$, a perturbation of X, such that

$$q_{h,n} = \theta_{\widetilde{X},nh}(q_0)? \tag{1.2}$$

If such a vector field exists, one can analyze the flow map $\theta_{\widetilde{X}}$ to gain information about the behavior of $\{q_{h,n}\}$. In most cases (1.2) may not be obtained, and one has to concentrate on constructing a family of vector fields $\widetilde{X}(h)$, depending on the parameter h, such that

$$d(q_{h,n}, \theta_{\widetilde{X}(h),nh}(q_0)) \leq f(h),$$

where $f : \mathbb{R} \to \mathbb{R}$ is continuous and $f(h) \to 0$ as $h \to 0$. Typically f could be $f(h) = Ch^s$ for some $C > 0$ and $s \in \mathbb{N}$. Or even better $f(h) = Ce^{-\gamma/h}$ for some $\gamma > 0$. The construction of the family of modified vector fields $\widetilde{X}(h)$ and the analysis of the corresponding flow map $\theta_{\widetilde{X}(h)}$ is known as Backward Error Analysis (BEA), and the family $\widetilde{X}(h)$ is often referred to as the modified or perturbed vector field.

2 Open problems and novelty of the paper

BEA is very well understood when $\mathcal{M} = \mathbb{R}^n$, and modified vector fields $\tilde{X}(h)$ are formally expressed as an infinite series

$$\widetilde{X}(h) = X_1 + hX_2 + h^2X_3 + \ldots, \tag{2.1}$$

where X_i is uniquely defined by Φ_h. Thus, it makes sense to talk about the modified (or perturbed) vector field generated by Φ_h. There are several articles on the subject, Hairer and Lubich [9], Calvo, Murua, and Sanz-Serna [4], Benettin and Giorgilli [3] and Reich [19]. The question, however is: what if we are not longer working in $\mathbb{R}^n$ but with some abstract manifold, can we still carry out the BEA? To illustrate the idea let us consider a simple example on an abstract manifold, in particular a matrix Lie group $\mathcal{G}$ with its corresponding Lie algebra $\mathfrak{g}$ (for references on Lie group problems see [12] and the references therein). Consider the equation

$$Y'(t) = AY(t), \qquad Y(0) = Y_0, \quad A \in \mathfrak{g}, \tag{2.2}$$

and let Φ_h be an integrator for the vector field $X \in \mathfrak{X}(\mathcal{G})$ defined by $X_Y = AY$. Then, it can be shown (with some appropriate assumptions on Φ_h, see Chapter IX in [10]) that there exists a sequence $\{A_j\}_{j \in \mathbb{N}} \subset \mathfrak{g}$ such that we can define a vector field $\widetilde{X}(h) \in \mathfrak{X}(\mathcal{G})$ by

$$\widetilde{X}(h)_Y = (A_1 + hA_2 + h^2A_3 + \ldots)Y, \tag{2.3}$$

where the series converges in the matrix norm on $\mathfrak{g}$. Moreover, if $\widetilde{Y}$ is a solution of

$$\widetilde{Y}'(t) = (A_1 + hA_2 + h^2 A_3 + \ldots)\widetilde{Y}(t), \qquad \widetilde{Y}(0) = Y_0,$$

then

$$\Phi_{nh}(Y_0) = \widetilde{Y}(nh), \quad \forall\, n \in \mathbb{N}, \qquad \widetilde{Y}(t) \in \mathcal{G}, \quad \forall\, t \in \mathbb{R}_+.$$

There are two important observation and also questions to address:

(i) It is possible to construct a modified vector field whose flow map will interpolate the numerical solution. However, the convergence in (2.3) is exceptional, and typically in the general case one must truncate a formal series to get a well defined vector field. However, how do we carry out the construction of such a series, and where do we truncate?

(ii) The solution of the modified equation shares a crucial property with the solution to the original problem. Namely, they are both in $\mathcal{G}$. In the general case we may ask the following: if the flow map of the original vector field has a certain property, under which conditions will the flow map of the modified vector field have the same properties?

The answers to these types of questions are the topic of this paper.

2.1 Extending estimates from $\mathbb{R}^n$ to manifolds

In the papers of Benettin and Giorgilli [3] , Hairer and Lubich [9] and Reich [19] the question of closeness of the numerical solution and the solution to the modified equation is addressed. In particular, it has been shown that for a suitable truncation of the series (2.1)

$$\|\theta_{\widetilde{X}(h),h}(q) - \Phi_h(q)\| \leq Che^{-\gamma/h}, \qquad q \in \mathcal{K}, \tag{2.4}$$

where C,$\gamma > 0$ and $\mathcal{K} \subset \mathbb{R}^n$ is compact. A crucial assumption for the previous estimate to be true is that both the vector field and the integrator Φ_h are analytic. In [9] Hairer and Lubich take (2.4) even further and show that (with some extra assumptions) variants of (2.4) are true even for multiple steps (not just one as (2.4) indicates). This ia a very powerful result as it suggests that the numerical solution is close to the true solution of the modified equation. This is all great, but what if $\mathbb{R}^n$ is replaced by a smooth manifold $\mathcal{M}$?

First, we are faced with the problem of constructing modified vector fields (as in (2.1)) on the manifold. This has been done by Reich in [18], Hairer, Lubich, Wanner in [10] and Hairer [8]. Although the techniques are different, they yield the same result. The technique used in [18] is based an the assumption that $\mathcal{M}$ is embedded in $\mathbb{R}^n$, and by using a tubular neighborhood technique, one extends the original vector field and integrator to a neighborhood around the manifold. By applying the standard technique from $\mathbb{R}^n$ to the extended vector field and integrator, one obtains the modified vector field on the manifold $\mathcal{M}$. The approach in [8] is similar, however, one assumes that the vector field is already defined on a neighborhood of the manifold. Hairer et al. [10] have a different strategy where the construction is done via charts and no extension of the vectorfield is needed.

Second, with the modified vector field established, do results of type (2.4) automatically follow (with the norm substituted by a metric of course)? (Note that this question is not addressed in [18, 10, 8]). This is a delicate question. It is tempting to try to use the already established techniques in $\mathbb{R}^n$, and typically for the long time estimates, the results of Hairer and Lubich [9]. However, to do so we must transform our problem to $\mathbb{R}^n$. One way to do this would be to follow the idea of Reich, via the tubular neighborhood, to obtain an extended vector field and integrator on a neighborhood of the manifold $\mathcal{M}$. Although tempting, this approach has a serious obstacle. Note that analyticity is crucial for results a la (2.4). The problem is that the mappings used in the extension approach are only C^∞, and hence analyticity is lost. Discouraged by that fact, one may try to emulate the ideas of Hairer et al. What if we simply use charts and do the analysis locally in $\mathbb{R}^n$? This would work because, by assuming that the manifold is analytic, the charts would be analytic. However, it is not enough to use charts and just quote the results by Hairer and Lubich [9] and deduce long term estimates on the manifold. The problem is that analysis in charts will only be local. To illustrate this issue we have chosen the following example:

Example 2.1. Let $\mathcal{M} = \mathbb{S}^2 \subset \mathbb{R}^3$, where $\mathbb{S}^2$ denotes the two sphere in $\mathbb{R}^3$. This is a compact manifold that can be given an analytic structure, however, it cannot be covered by only one chart. Suppose that we have an analytic vector field X on $\mathbb{S}^2$ and that Φ_h is an analytic integrator for X with corresponding modified vector field $\widetilde{X}(h)$ (to simplify the notation we will use the notation $\widetilde{X}$). Let $\{q_n\}_{n\in\mathbb{Z}_+}$ denote the numerical solution (e.g. $q_{n+1} = \Phi_h(q_n)$). Suppose that our task is to show that there is a metric d on $\mathbb{S}^2$ and constants $C, \gamma > 0$ such that

$$d(\theta_{\widetilde{X},nh}(q_0), q_n) \leq Ce^{-\gamma/h}, \tag{2.5}$$

however, we insist on using local charts and the techniques from Hairer and Lubich [9] directly (in those charts). We start by finding a chart (U, φ) such that $q_0 \in U$. Now suppose that $q_n \in U$ for $n \leq K$ for some $K > 0$. Now let $\hat{\Phi}_h : \varphi(U) \to \varphi(U)$ be defined by $\hat{\Phi}_h = \varphi \circ \Phi_h \circ \varphi^{-1}$, and let Y and $\widetilde{Y}$ be the vector fields on $\varphi(U)$ induced by φ and X and $\widetilde{X}$ respectively, e.g. $Y = \varphi_* X$ and $\widetilde{Y} = \varphi_* \widetilde{X}$ (see Section 3 for notation). Suppose that we have been able to show (using the vector space techniques in [9]) the existence of $C, \gamma > 0$ such that

$$\|\theta_{\widetilde{Y},nh}(\hat{q}_0) - \hat{q}_n\|_{\mathbb{R}^2} \leq Ce^{-\gamma/h}, \qquad n \leq K, \tag{2.6}$$

(where $\hat{q}_n = \varphi(q_n)$) however, for $N = K + 1$ then $q_{K+1} \notin U$. This forces us to change charts. So suppose that we can find a chart (V, ψ) such that $q_K \in U \cap V$ and $q_n \in V$ for $K \leq n \leq L$ for some $L > K$. Let $\tilde{\Phi}_h$, Z and $\widetilde{Z}$ be induced by (V, ψ) and Φ_h, X, $\widetilde{X}$ (similarly as above). To continue the analysis we first need to establish a bound on $\|\theta_{\widetilde{Z},Kh}(\tilde{q}_0) - \tilde{q}_K\|_{\mathbb{R}^2}$ (where $\tilde{q}_n = \psi(q_n)$). The only way we can do that is to use the already established (2.6). In particular, we have

$$\|\theta_{\widetilde{Z},Kh}(\tilde{q}_0) - \tilde{q}_K\|_{\mathbb{R}^2} = \|\psi \circ \varphi^{-1}(\theta_{\widetilde{Y},Kh}(\hat{q}_0)) - \psi \circ \varphi^{-1}(\hat{q}_K)\|_{\mathbb{R}^2},$$

however, to be able to use (2.6) we must establish that $\psi \circ \varphi^{-1}$ is Lipschitz continuous and a bound on the Lipschitz constant, say $C_{\psi\circ\varphi^{-1}}$. By invoking (2.6) we then get

$$\|\theta_{\widetilde{Z},Kh}(\tilde{q}_0) - \tilde{q}_K\|_{\mathbb{R}^2} \leq C_{\psi\circ\varphi^{-1}} Ce^{-\gamma/h}.$$

The problem now is that when continuing the analysis in the chart (V, ψ) we must take into account the accumulated error from the previous chart that depends on $C_{\psi\circ\varphi^{-1}}$ (and of course this constant may be greater than one). In fact, every time we would have to change charts we would get a contribution from the Lipschitz constant of the composite mapping. As we are interested in long term behavior we cannot restrict ourselves to the assumption that the numerical solution only changes charts finitely many times. And if we cannot do that, the type of analysis suggested in this example would yield estimates a la (2.5), however, with a constant C that grows every time the numerical solution changes chart. Such a result would be substantially less than optimal.

This leaves us with the following open question. How do we extend results a la (2.4) to manifolds? This question (and the answer) is one of the main themes of this paper. As we will see, abstractions of the ideas by Hairer and Lubich [9] and Reich [19, 18] will be crucial.

2.2 Extending classification theory from $\mathbb{R}^n$ to manifolds

A very important question to ask is: when will the flow map of the modified vector field have the same geometric properties as the original flow map? A typical question of this type would be: will the flow map of the modified vector field be symplectic provided that the original flow map is symplectic? The answer is yes, if the integrator is symplectic. Several other results regarding geometric properties of modified vector field can be found in [7], [10]. However, all these results are so far only valid when considering ODEs in $\mathbb{R}^n$, and we may therefore ask the same question as before: What if $\mathbb{R}^n$ is replaced by a manifold $\mathcal{M}$. There are some results in [10], however, these techniques work only for quite specific cases and are not suited for the general problems that we will consider here.

Now consider a very basic example. Let $\rho : \mathcal{M} \to \mathcal{M}$ be a diffeomorphism on a smooth manifold $\mathcal{M}$ and denote the mapping

$$\Psi \mapsto \rho \circ \Psi \circ \rho^{-1}, \qquad \Psi \in \mathrm{Diff}(\mathcal{M}),$$

by σ. Note that this is a homomorphism on $\mathrm{Diff}(\mathcal{M})$ (the set of diffeomorphisms on $\mathcal{M}$, a more thorough definition follows below) since $\sigma(\Psi \circ \Phi) = \sigma(\Psi) \circ \sigma(\Phi)$, for $\Psi, \Phi \in \mathrm{Diff}(\mathcal{M})$. Suppose that $X \in \mathfrak{X}(\mathcal{M})$ is a vector field with flow map $\theta_{X,t}$ with the property that

$$\sigma(\theta_{X,t}) = \theta_{X,t}^{-1} = \theta_{X,-t}. \tag{2.7}$$

Suppose that we have an integrator Φ_h for X and that Φ_h satisfies $\sigma(\Phi_h) = \Phi_h^{-1}$. The question is then: Will the flow map $\theta_{\widetilde{X}(h),t}$ of the modified vector field $\widetilde{X}(h)$ satisfy

$$\sigma(\theta_{\widetilde{X}(h),t}) = \theta_{\widetilde{X}(h),t}^{-1} = \theta_{\widetilde{X}(h),-t}? \tag{2.8}$$

This has been considered in the $\mathbb{R}^n$ case when $\rho(x) = Tx$, $x \in \mathbb{R}^n$ and T is a linear operator in [7] and [19]. However, even the simplest case when $\mathcal{M}$ is a sphere and T is a unitary involution is not covered by the theory in [7] and [19]. One can off course ask a more general question: what if σ simply is a homomorphism such that (2.7) is satisfied? Would (2.8) follow? The existing theory is quite far from covering such a general question, even in $\mathbb{R}^n$, and of course not in the general setting.

Consider another basic example. Let μ be a volume form on a smooth manifold $\mathcal{M}$ and suppose that $X \in \mathfrak{X}(\mathcal{M})$ is a vector field whose flow map $\theta_{X,t}$ satisfy

$$\theta_{X,t}^{*}\mu = \mu,$$

(the notation $\theta_{X,t}^{*}$ denotes the standard pull back). Given an integrator Φ_h for X with the property that $\Phi_h^{*}\mu = \mu$. Does it follow that the flow map $\theta_{\widetilde{X}(h),t}$ of the modified vector field $\widetilde{X}(h)$ satisfy

$$\theta_{\widetilde{X}(h),t}^{*}\mu = \mu?$$

This question has been investigated in [7] and [19], however, only in the $\mathbb{R}^n$ case, and even the simplest example of a sphere will not be covered by the existing theory. The examples above are just two basic examples of what is not covered by the existing theory, and, in fact, there is a quite long list of open questions: Let $X \in \mathfrak{X}(\mathcal{M})$, with flow map $\theta_{X,t}$, for some smooth manifold $\mathcal{M}$. Suppose that Φ_h is an integrator for X with corresponding modified vector field $\widetilde{X}(h)$ and flow map $\theta_{\widetilde{X}(h),t}$.

(i) Let ω be a symplectic 2-form on $\mathcal{M}$. Suppose $\theta_{X,t}, \Phi_h \in S_1 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : \varphi^*\omega = \omega\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_1$?

(ii) Let ω be a symplectic 2-form on $\mathcal{M}$. Suppose $\theta_{X,t}, \Phi_h \in S_2 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : \varphi^*\omega = c\omega\,,\ c \in \mathbb{R}\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_2$?

(iii) Let μ be a volume form on $\mathcal{M}$. Suppose $\theta_{X,t}, \Phi_h \in S_3 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : \varphi^*\mu = \mu\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_3$?

(iv) Let μ be a volume form on $\mathcal{M}$. Suppose $\theta_{X,t}, \Phi_h \in S_4 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : \varphi^*\mu = c\mu\,,\ c \in \mathbb{R}\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_4$?

(v) Let α be a contact form. Suppose $\theta_{X,t}, \Phi_h \in S_5 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : (\varphi^*\alpha)_p = c_\varphi(p)\alpha_p\,, c_\varphi \in C^\infty(\mathcal{M})\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_5$?

(vi) Let $f \in C^\infty(\mathcal{M})$. Suppose $\theta_{X,t}, \Phi_h \in S_6 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : f \circ \varphi = f\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_6$?

(vii) Let $\sigma : \mathrm{Diff}(\mathcal{M}) \to \mathrm{Diff}(\mathcal{M})$ be a homomorphism. Suppose $\theta_{X,t}, \Phi_h \in S_7 = \{\varphi \in \mathrm{Diff}(\mathcal{M}) : \sigma(\varphi) = \varphi^{-1}\}$. Does it follow that $\theta_{\widetilde{X}(h),t} \in S_7$?

It seems to be a dearth of literature on these basic questions and we therefore consider it an important task to develop an abstract framework that can handle these issues. Before embarking on such a challenge let us ask the question: Can we build this on the existing frameworks? The novel ideas by Reich [19] are of a very abstract nature and are well suited for further developments. It is the notion of the "Tangent Space at the Identity" of $\mathrm{Diff}(\mathcal{M})$ that is the crucial tool that can be used in an abstract framework . As we will see in Example 6.2 and Remark 5 the framework in [19] is not complete, even in $\mathbb{R}^n$, however, it can be completed and made abstract. In order to do the abstraction we feel it is natural to go to the source of such techniques, namely, the work by Ebin and Marsden [6] on infinite-dimensional manifolds, in particular, infinite-dimensional subgroups of $\mathrm{Diff}(\mathcal{M})$. Our framework is very much inspired by their work.

The theory in this paper may seem involved at first glance, and it may be appropriate to ask: are such technical abstractions really necessary? A question like that must be viewed in the light of the questions we are asking. Note that the questions in (i)-(vii) above are very general, in particular (vii). As in most cases in mathematics, general questions may have to be treated with abstract framework (that may happen to be involved). To answer the initial question, the answer is yes, as the Remark 7 shows.

3 Background and notation

We will first introduce some notation. If $\mathcal{M}$ and $\mathcal{N}$ are smooth manifolds and $F : \mathcal{M} \to \mathcal{N}$ is a smooth map, we will adopt the notation from [13] and denote the derivative, or the tangent mapping $T_pF : T_p\mathcal{M} \to T_p\mathcal{N}$, by F_* e.g. for $x \in T_p\mathcal{M}$ we let $F_*x = T_pFx$. The derivative of a function $F : \mathbb{R}^n \to \mathbb{R}^m$ will be denoted by DF, and similarly derivatives of higher order will be denoted by D^rF. As usual we identify $D^rF(x)$ with $L^r_{\mathrm{sym}}(\mathbb{R}^n, \mathbb{R}^m)$, the set of symmetric r linear mappings from $\mathbb{R}^n \times \cdots \times \mathbb{R}^n$ (r-times) to $\mathbb{R}^m$. The set of smooth k-forms on $\mathcal{M}$ will be denoted by $\Omega^k(\mathcal{M})$.

Given a vector field X with corresponding flow map $\theta_X : I \times \mathcal{M} \to \mathcal{M}$, where I is an open interval of $\mathbb{R}$, we will allow slight misuse of notation by letting $\theta_X(t, s, p)$ denote the flow of X at time t that takes the value p at time s. We also adopt the Einstein summation convention, meaning that $\sum_i x^i E_i$ will be denoted by $x^i E_i$, hence omitting the summation sign.

Throughout this section $\mathcal{M} = \mathbb{R}^n$ and we will review some of the well known results that will be crucial for our developments in the upcoming sections. Let Φ_h be an integrator on $\mathbb{R}^n$, and suppose that Φ_h is consistent of order p with $X \in \mathfrak{X}(\mathbb{R}^n)$. As discussed in the introduction, the idea is to look for a family of vector fields $\widetilde{X}(h)$ such that $\Phi_h \approx \theta_{\widetilde{X}(h),h}$ and thus the study of the numerical solution reduces to the study of the flow $\theta_{\widetilde{X}(h)}$. The family of modified vector fields $\widetilde{X}(h)$ is formally defined in terms of an asymptotic expansion in the step size h; i.e.,

$$\widetilde{X}(h) = X_1 + hX_2 + h^2X_3 + \ldots$$

The infinite sequence of vector fields $\{X_i\}_{i=1,\ldots,\infty}$ can be obtained by using the Taylor series expansion of the one-step method Φ_h i.e.,

$$\Phi_h = id + h\Phi_1 + h^2\Phi_2 + \ldots,$$

where id is the identity map and the Φ_js are smooth mappings, and then compare this series with the expansion of the flow map $\theta_{h,\widetilde{X}(h)}$. The vector fields X_i are chosen such that these two series coincide term by term. We will follow the recursive approach by Reich [19] when defining the vector fields X_i, as this approach is advantageous when one wants to study the geometric properties of the modified vector field as done in Section 5.

The recursive construction is as follows. Let Φ_h be an integrator for the smooth vector field X. Suppose that we have obtained $\{X_j\}_{j=1}^{i}$, and we want to determine X_{i+1}. Let

$$Y_i(h) = \sum_{j=1}^{i} h^{j-1} X_j.$$

Suppose that $\{X_j\}_{j=1}^{i}$ has been chosen such that the distance between $\Phi_h(q)$ and $\theta_{h,Y_i(h)}(q)$ is $\mathcal{O}(h^{i+1})$ for all $q \in \mathbb{R}^n$. Now define

$$Y_{i+1}(h) = Y_i(h) + h^i X_{i+1}, \qquad X_{i+1}(q) = \lim_{h\to 0} \frac{\Phi_h(q) - \theta_{h,Y_i(h)}(q)}{h^{i+1}}, \quad q \in \mathbb{R}^n. \tag{3.1}$$

Note that the limit exists by the choice of $Y_i(h)$. This definition of $Y_{i+1}(h)$ generates a flow map that is $\mathcal{O}(h^{i+2})$ away from Φ_h. Indeed, by Taylor's theorem and the definition of $Y_{i+1}(h)$ we get

$$\theta_{h,Y_{i+1}(h)}(q) - \theta_{h,Y_i(h)}(q) = h^{i+1} X_{i+1}(q) + \mathcal{O}(h^{i+2})$$

and

$$\theta_{h,Y_i(h)}(q) - \Phi_h(q) = h^{i+1} X_{i+1}(q) + \mathcal{O}(h^{i+2}).$$

Thus,

$$\begin{aligned} \theta_{h,Y_{i+1}(h)}(q) - \Phi_h(q) &= \theta_{h,Y_i(h)}(q) + h^{i+1} X_{i+1}(q) - \Phi_h(q) + \mathcal{O}(h^{i+2}) \\ &= \mathcal{O}(h^{i+2}). \end{aligned} \tag{3.2}$$

Letting $X_1 = X$ the construction is complete. Note that it is easy to see that $X_i = 0$ for $i = 2, \ldots, p$ when Φ_h is of order p.

As mentioned above there are several important results regarding BEA in $\mathbb{R}^n$, and for an excellent review we refer to [10]. Some of the results in [19] are of crucial importance for the following arguments and we will give a short summary. Let $\mathcal{B}_r(x) \subset \mathbb{C}^n$ be the open complex ball of radius r around $x \in \mathbb{R}^n$. Let also $\|\cdot\|$ denote the max norm on $\mathbb{C}^n$. Let $\mathcal{K} \subset \mathbb{R}^n$ be a compact subset and define, for $Z \in \mathfrak{X}(\mathbb{R}^n)$ and $r > 0$,

$$\|Z\|_r = \sup_{x \in \mathcal{B}_r\mathcal{K}} \|Z_x\|, \quad \text{where} \quad \mathcal{B}_r\mathcal{K} = \bigcup_{x_0 \in \mathcal{K}} \mathcal{B}_{r(x_0)}.$$

Lemma 3.1. *(Reich) Let Φ_h be an integrator for $X \in \mathfrak{X}(\mathbb{R}^n)$. Suppose that the vector field X is real analytic in an open set $\mathcal{U} \subset \mathbb{R}^n$ and that there is a compact subset $\mathcal{K} \subset \mathcal{U}$ and constants K, $R > 0$ such that $\|X\|_R \leq K$. Suppose also that the mapping $h \mapsto \Phi_h(x)$ is real analytic for all $x \in \mathcal{U}$. Then there exist $M \geq K$ such that*

$$\|\Phi_\tau - id\|_{\alpha R} \leq |\tau| M \leq (1-\alpha)R \quad \textit{for} \quad |\tau| \leq \frac{(1-\alpha)R}{M},$$

where $\alpha \in [0, 1)$.

Theorem 3.2. *(Reich) Let the assumptions of Lemma 3.1 be satisfied and let Φ_h be consistent of order p with X . Then, the family $\{X_i\}$ defined in (3.1) is analytic and, for all integers $m \geq p+1$, there exists $C > 0$, such that, for $\widetilde{X}(h)_m = X_1 + hX_2 + h^2X_3 + \ldots + h^{m-1}X_m$, we have*

$$\sup_{x \in \mathcal{K}} \|\Phi_h(x) - \theta_{\widetilde{X}_m,h}(x)\| \leq Ch\Big(\frac{h(m-p+1)M}{R}\Big)^m,$$

where X_j is defined as in (3.1). Also,

$$\sup_{x \in \mathcal{K}} \|X_j(x)\| \leq C\left(\frac{(j-p)M}{R}\right)^{j-1}, \qquad j \geq p+1.$$

Remark 2 Note that Theorem 3.2 is not quoted directly as stated in [19], but the bounds presented here come from equation (4.17) and (4.13) in the proof of Theorem 2 in [19]. Note that the results in Lemma 3.1 and Theorem 3.2 are stated in $\mathbb{R}^n$, however, they will be useful in the proofs below as we will use these estimates in local coordinates.

4 Backward error analysis on manifolds

This section is devoted to answering the questions posed in Section 2.1. The following theorem is a generalization of Theorem 2 in [19] and Theorem 1 in [9].

Theorem 4.1. *Let $\mathcal{M}$ be a smooth manifold, $X \in \mathfrak{X}(\mathcal{M})$ and let Φ_h be an integrator that is consistent with X of order p. Then there exists a family of smooth vector fields $\{X_j\}_{j\in\mathbb{N}}$ on $\mathcal{M}$, where each X_j is uniquely determined by Φ_h, with the following properties:*

(i) There is a metric d on $\mathcal{M}$ such that if $\mathcal{K} \subset \mathcal{M}$ is a compact subset and for any $N \in \mathbb{N}$ such that $\widetilde{X}_N(h) = X_1 + hX_2 + \dots h^{N-1}X_N$ there exists a $C_N > 0$, depending on N, such that for sufficiently small $h > 0$ we have

$$d(\theta_{\widetilde{X}_N,h}(q), \Phi_h(q)) \leq C_N h^{N+1}, \qquad q \in \mathcal{K},$$

where $\theta_{\widetilde{X}_N}$ is the flow map of $\widetilde{X}_N(h)$.

(ii) If $\mathcal{M}$, X are analytic and $h \mapsto \Phi_h(q)$ is analytic for q in compact $\mathcal{K} \subset \mathcal{M}$, then there exists an integer k (depending on h) and $C, \gamma > 0$ such that for $\widetilde{X}(h) = X_1 + hX_2 + \dots h^{k-1}X_k$ it follows that, for sufficiently small h,

$$d(\Phi_h(q), \theta_{\widetilde{X},h}(q)) \leq Che^{-\gamma/h}, \tag{4.1}$$

for all $q \in K$, where d is the same metric as in (i). Also, there exists a finite collection $\mathcal{F}$ of charts on $\mathcal{M}$, covering $\mathcal{K}$, and a constant $C > 0$ such that if $(U, \varphi) \in \mathcal{F}$ and Y, $\widetilde{Y}(h)$ are the vector field induced by φ and X, $\widetilde{X}(h)$ respectively then

$$\sup_{x\in\varphi(U)} \|Y(x) - \widetilde{Y}(h)(x)\| \leq Ch^p, \qquad \sup_{x\in\varphi(U)} \|DY(x) - D\widetilde{Y}(h)(x)\| \leq Ch^p. \tag{4.2}$$

Proof. The construction of $\{X_j\}$ is as follows: For any chart (U, φ), let $\hat{\Phi}_h = \varphi \circ \Phi_h \circ \varphi^{-1}$ and let Y be the vector field induced by φ. Doing the calculations in (3.1) and (3.2) with $\hat{\Phi}_h$ and θ_Y we obtain a family of smooth vector fields $\{Y_j\}$ on $\varphi(U)$, and hence also a family $\{\varphi_*^{-1}Y_j\}$ on U. It is easy to see, using the fact that Y_j is uniquely defined by $\hat{\Phi}_h$, that $\{\varphi_*^{-1}Y_j\}$ is independent of the choice of charts. Thus, we obtain a family of global smooth vector fields $\{X_j\}$ from the local construction. Also, each X_j is uniquely determined by Φ_h. (This construction can also be found in Theorem 5.1 Chap. IX.5 in [10]).

To show (i), note that, by compactness of $\mathcal{K}$, consistency of Φ_h and the fact that $\theta_{X,0} = \Phi_0 = id$, we can find a finite collection $\mathcal{F} = \{(U_j, \varphi_j)\}$ of charts such that there are open sets $V_j \subset U_j$ and $h_0 > 0$, such that $\theta_{X,h}(V_j) \subset U_j$ and $\Phi_h(V_j) \subset U_j$, for $h < h_0$ (for some $h_0 > 0$) and $\{V_j\}$ covers $\mathcal{K}$. We may also assume without loss of generality that φ_j^{-1} is defined on $\overline{\varphi_j(U_j)}$.

To get the desired metric and bound that we asserted, we use the Whitney Embedding Theorem to obtain a diffeomorphism $F : \mathcal{M} \to \mathcal{N} \subset \mathbb{R}^m$ for some $m \geq 2n$, where $\mathcal{N}$ is an embedded submanifold and $n = \dim(\mathcal{M})$. By the choice of $\mathcal{F}$ above we have that if $p \in \mathcal{K}$ then $q = \varphi(p)$ for some $(U, \varphi) \in \mathcal{F}$, and, by letting $\widetilde{X}_N = X_0 + hX_1 + \dots h^N X_N$ and by a little manipulation and the calculation in (3.1) and (3.2), we get that

$$\|F \circ \Phi_h(p) - F \circ \theta_{\widetilde{X}_N,h}(p)\| = \|F \circ \varphi^{-1}(\hat{\Phi}_h(q)) - F \circ \varphi^{-1}(\theta_{\widetilde{Y}_N,h}(q))\| \leq C_N h^N \tag{4.3}$$

where C_N bounds the Lipschitz's constant of all $\underline{F \circ \varphi^{-1}}$ and $\widetilde{Y}_N(h) = Y + hY_1 + \dots h^N Y_N$. Note that $F \circ \varphi^{-1}$ is Lipschitz by smoothness and since $\overline{\varphi(U)}$ is compact and can be assumed without loss of generality to be convex. Also, since $\mathcal{N}$ is embedded, it has the subspace topology and hence it inherits a metric from $\mathbb{R}^m$ which again leads to a metric d on $\mathcal{M}$ induced by F.

To show (ii), notice that we may, by arguing as in the proof of (i) and possibly changing $\mathcal{F}$, where $\mathcal{F}$ is as in the proof of (i), assume that for each $(U, \varphi) \in \mathcal{F}$ there is an $r_\varphi > 0$ such that $B_{r_\varphi}(0)$ is properly contained in $\varphi(U)$,

$$\theta_{X,h}(\varphi^{-1}(B_{r_\varphi}(0))) \subset U, \quad \Phi_h(\varphi^{-1}(B_{r_\varphi}(0))) \subset U, \quad h \leq h_0,$$

and $\bigcup_{(U,\varphi)\in\mathcal{F}}\varphi^{-1}(B_{r_\varphi}(0))$ is an open cover of $\mathcal{K}$. Let $(U,\varphi)\in\mathcal{F}$ and let Y be the induced vector field on $V=\varphi(U)$ of X by φ, and let $\widetilde{\mathcal{K}}=\overline{B_{r_\varphi}(0)}$. From the previous discussion it follows that there exists an $R_\varphi>0$ such that the complexification of Y is defined on $\mathcal{B}_{R_\varphi}\widetilde{\mathcal{K}}$ and by continuity $\|Y\|_{R_\varphi}\le K_\varphi$ for some $K_\varphi>0$. Now consider the integrator on V defined by $\tilde{\Phi}_h=\varphi\circ\Phi_h\circ\varphi^{-1}$. We can now apply Lemma 3.1 and Theorem 3.2 to obtain constants M_φ, $C_\varphi>0$ such that

$$\widetilde{Y}_m=Y_1+hY_2+h^2Y_3+\ldots+h^{m-1}Y_m,\qquad m\ge p+1,$$

where Y_j is the vector field on $\varphi(U)$ induced by X_j and φ. We have the estimates

$$\|\hat{\Phi}_h(x)-\theta_{\tilde{Y}_m,h}(x)\|\le C_\varphi h\Big(\frac{h(m-p+1)M_\varphi}{R_\varphi}\Big)^m,\qquad x\in\widetilde{\mathcal{K}},\tag{4.4}$$

$$\|Y_j(x)\|\le C_\varphi\left(\frac{(j-p)M_\varphi}{R_\varphi}\right)^{j-1},\qquad x\in\widetilde{\mathcal{K}},\quad j\ge p+1.\tag{4.5}$$

To get the metric and the desired bounds, let

$$M=\max\{M_\varphi:\varphi\in\mathcal{F}\},\quad C=\max\{C_\varphi:\varphi\in\mathcal{F}\},\quad R=\min\{R_\varphi:\varphi\in\mathcal{F}\}.$$

To show (4.1), we can now use the same approach as in (i) and apply (4.4) to get

$$d(\Phi_h(q),\theta_{\widetilde{X}_m,h}(q))\le\tilde{C}h\Big(\frac{h(m-p+1)M}{R}\Big)^m,\qquad q\in\mathcal{K},$$

where $\tilde{C}$ is a constant depending on C and the Lipchitz constants of $F\circ\varphi^{-1}$. (F is here as in the proof of (i)). To get the desired bound we choose m to be the integer part of $\mu=\frac{R}{hMe}+p-1$. Hence, we get

$$\begin{aligned}d(\Phi_h(q),\theta_{\widetilde{X}_m,h}(q))&\le\tilde{C}he^{-m}\\&\le\tilde{C}he^{-\mu+1}\\&\le\tilde{C}he^{-p}e^{-\gamma/h},\qquad q\in\mathcal{K},\end{aligned}$$

where $\gamma=R/(Me)$.

To show (4.2), note that by analyticity and Cauchy's integral formula, it follows by (4.5) (by possibly changing C) that

$$\max\left(\|Y_j(x)\|,\|DY_j(x)\|\right)\le C\left(\frac{(j-p)M}{R}\right)^{j-1},\qquad x\in\widetilde{\mathcal{K}},\quad j\ge p+1.$$

Thus, since Φ_h is of order p

$$\begin{aligned}\max(\|Y_j(x)-\widetilde{Y}_j(h)(x)\|,&\|DY_j(x)-D\widetilde{Y}_j(h)(x)\|)\\&\le C\sum_{j=p+1}^{m}\left(\frac{hM(j-p)}{R}\right)^{j-1}\\&=C\left(\frac{hM}{R}\right)^p\sum_{j=p+1}^{m}(j-p)^p\left(\frac{hM(j-p)}{R}\right)^{j-1-p}\\&\le C\left(\frac{hM}{R}\right)^p\sum_{j=p+1}^{m}\frac{(j-p)^p}{e^{j-p-1}}\left(\frac{j-p}{m-p+1}\right)^{j-1-p}\\&\le C\left(\frac{hM}{R}\right)^p d_pK,\end{aligned}\tag{4.6}$$

where d_p bounds $\frac{(j-p)^p}{e^{j-p-1}}$ and K bounds $\sum_{j=p+1}^{m}\left(\frac{j-p}{m-p+1}\right)^{j-1-p}$. Also, in the second to last inequality we have used the fact that

$$h\le\frac{R}{Me(m-p+1)}.$$

The theorem follows. $\square$

Remark 3 The computation in (4.6) is almost word for word taken from the last computations in the proof of Theorem 2 in [19].

The idea is now to use this result and follow the ideas in the proof of Corollary 2 (p. 444) in [9] applied to a general manifold setting. This corollary is using Lady Widermere's fan, and that technique requires vector space operations. Hence, unfortunately, the corollary cannot be applied directly, but after a series of preparations we can follow the analysis in [9] closely.

Let us first recall some basic facts from differential geometry that will be useful in the following argument. By the normal space to an embedded submanifold $\mathcal{M} \subset \mathbb{R}^n$ at x we mean the subspace $N_x\mathcal{M} \subset T\mathbb{R}^n$ consisting of all vectors that are orthogonal to $T_x\mathcal{M}$ with respect to the Euclidean dot product. The normal bundle of $\mathcal{M}$ is the subset $N\mathcal{M} \subset T\mathbb{R}^n$ defined by

$$N\mathcal{M} = \coprod_{x\in\mathcal{M}} N_x\mathcal{M} = \{(x,v) \in T\mathbb{R}^n : x \in \mathcal{M}, v \in N_x\mathcal{M}\}.$$

Define a map $E : N\mathcal{M} \to \mathbb{R}^n$ by

$$E(x,v) = x + v, \tag{4.7}$$

where we have done the usual identification. A tubular neighborhood of $\mathcal{M}$ is a neighborhood U of $\mathcal{M}$ in $\mathbb{R}^n$ that is the diffeomorphic image under E of an open subset $\mathcal{V} \subset N\mathcal{M}$ of the form

$$\mathcal{V} = \{(x,v) \in N\mathcal{M} : |v| < \delta(x)\}$$

for some positive continuous function $\delta : \mathcal{M} \to \mathbb{R}$. A useful fact that will come in handy in the next theorem is that every embedded submanifold of $\mathbb{R}^n$ has a tubular neighborhood.

Theorem 4.2. *Let $\mathcal{M}$ be a smooth manifold and $X \in \mathfrak{X}(\mathcal{M})$ with flow map θ_X that exists for all $t \in \mathbb{R}$ and all $p \in \mathcal{M}$. Let Φ_h be an integrator that is consistent of order r with X. Let $\{q_{h,n}\}_{n\in\mathbb{Z}_+}$ be the numerical solution produced by Φ_h recursively and let $\{X_i\}$ be the family of vector fields from Theorem 4.1. Suppose that there is a compact set $\mathcal{K} \subset \mathcal{M}$, $h_0 > 0$ and $T \leq \infty$ such that $\{q_{h,n}\}_{n\leq T/h} \subset \mathcal{K}$ for all $h \leq h_0$. For any integer $s \geq r+1$, let $\widetilde{X}(h) = X_1 + hX_2 + \ldots h^{s-1}X_s$. Suppose also that*

$$\bigcup_{t\leq T, h\leq h_0, s<\infty} \theta_{\widetilde{X}(h),t}(\{q_{h,n}\}_{n\leq T/h}) \subset \mathcal{K}, \tag{4.8}$$

and that for any finite collection $\mathcal{F}$ of charts covering $\mathcal{K}$ then $\theta_{X,t}$ has uniformly bounded spacial derivatives for all $|t| \leq T$ in any charts belonging to $\mathcal{F}$. (To simplify notation we will simply denote $q_{h,n}$ by q_n.)

(i) Then there are constants $L > 0$ and $C_s > 0$ (depending on s) such that

$$d(\theta_{\widetilde{X}(h),nh}(q_0), q_n) \leq h^{s+1}C_s\left(\frac{e^{Lh^{r+1}n}-1}{e^{Lh^{r+1}}-1}\right), \qquad nh \leq T.$$

(ii) If $\mathcal{M}$, X and $h \mapsto \Phi_h(p)$ are analytic and $\widetilde{X}(h)$ is as in (ii) of Theorem 4.1, then there exist constants $L > 0$ and $C > 0$ such that

$$d(\theta_{\widetilde{X},nh}(q_0), q_n) \leq he^{-\gamma/h}C\left(\frac{e^{Lh^{r+1}n}-1}{e^{Lh^{r+1}}-1}\right), \qquad nh \leq T.$$

Proof. We will show that there are constants $C > 0$ and $L > 0$ such that

$$d(\theta_{\widetilde{X},t}(p), \theta_{\widetilde{X},t}(q)) \leq Ce^{Lh^r t}d(p,q), \qquad t \leq T, \quad p,q \in \{q_{h,n}\}_{n\leq T/h}, \tag{4.9}$$

where d is the same metric as in Theorem 4.1. Now, suppose for the moment that (4.9) is true. Recall that $\{q_{h,n}\}_{n\in\mathbb{Z}_+}$ is the numerical solution obtained recursively by Φ_h and let $t_k = kh$.

Also, to avoid cluttered notation we will use just $\widetilde{X}$ for $\widetilde{X}(h)$. Then

$$\begin{aligned} d(\theta_{\widetilde{X},t_n}(q_0),q_n) &\leq \sum_{k=1}^{n} d(\theta_{\widetilde{X}}(t_n,t_{k-1},q_{k-1}),\theta_{\widetilde{X}}(t_n,t_k,q_k)) \\ &\leq \sum_{k=1}^{n} Ce^{Lh^r(t_n-t_k)} d(\theta_{\widetilde{X}}(t_k,t_{k-1},q_{k-1}),\theta_{\widetilde{X}}(t_k,t_k,q_k)) \\ &= \sum_{k=1}^{n} Ce^{Lh^r(t_n-t_k)} d(\theta_{\widetilde{X},h}(q_{k-1}),q_k), \end{aligned}$$

where the second inequality follows from (4.9) and the last equality follows from the fact that $\theta_{\widetilde{X}}(t_k,t_k,q_k) = q_k$ and $\theta_{\widetilde{X}}(t_k,t_{k-1},q_{k-1}) = \theta_{\widetilde{X},h}(q_{k-1})$. Thus, using Theorem 4.1, we get the two cases

(i) $d(\theta_{\widetilde{X},t_n}(q_0),q_n) \leq C_1 h^{s+1}\sum_{k=0}^{n-1} e^{Lh^r kh} = h^{s+1}C_1\left(\frac{e^{Lh^{r+1}n}-1}{e^{Lh^{r+1}}-1}\right)$,

(ii) $d(\theta_{\widetilde{X},t_n}(q_0),q_n) \leq C_2 h e^{-\gamma/h}\sum_{k=0}^{n-1} e^{Lh^r kh} = C_2 h e^{-\gamma/h}\left(\frac{e^{Lh^{r+1}n}-1}{e^{Lh^{r+1}}-1}\right)$,

where C_1 and C_2 are the constants from Theorem 4.1 (i) and (ii) respectively. Also, the last inequalities in cases (i) and (ii) come from the standard techniques used to prove convergence of one step methods (details can be found on p. 161 [11]). Thus, to conclude, we only need to show (4.9). To do that we will transform our problem from the manifold setting into a vector space environment and then follow the analysis in Corollary 2 [9] quite closely.

By Whitney's embedding theorem we obtain a smooth embedding $F : \mathcal{M} \to \mathbb{R}^m$, for $m \geq 2n$, where $n = \dim(\mathcal{M})$. Let $\mathcal{N} = F(\mathcal{M})$. Now, F, X and $\widetilde{X}$ induce vector fields on $\mathcal{N}$, namely, $F_* X_{F^{-1}(\cdot)}$ and $F_* \widetilde{X}_{F^{-1}(\cdot)}$. With a slight misuse of notation we will also denote these vector fields by X and $\widetilde{X}$ respectively. Our first goal is to extend X and $\widetilde{X}$ to a neighborhood around $\mathcal{N}$.

Let U be a tubular neighborhood of $\mathcal{N}$ i.e. $\mathcal{N} \subset U \subset \mathbb{R}^m$ where U is open in $\mathbb{R}^m$ and diffeomorphic to an open set $\mathcal{V} \subset N\mathcal{N}$ of the form

$$\mathcal{V} = \{(x,v) \in N\mathcal{N} : |v| < \delta(x)\} \tag{4.10}$$

for some positive continuous function $\delta : \mathcal{N} \to \mathbb{R}$. Note that diffeomorphism mentioned above $E : \mathcal{V} \to U$ is defined as in (4.7). For $(x,v) \in N\mathcal{N}$ we identify $T_{(x,v)}N\mathcal{N}$ with $T_x\mathcal{N} \times \mathbb{R}^{m-n}$ and define the vector fields Z and $\widetilde{Z}$ by

$$Z_{(x,v)} = (X_x, 0) \in T_x\mathcal{N} \times \mathbb{R}^{m-n}, \qquad \widetilde{Z}_{(x,v)} = (\widetilde{X}_x, 0) \in T_x\mathcal{N} \times \mathbb{R}^{m-n}. \tag{4.11}$$

Now Z and $\widetilde{Z}$ are obviously smooth, thus, we can define smooth vector fields Y and $\widetilde{Y}$ on U by $Y = E_* Z_{E^{-1}(\cdot)}$ and $\widetilde{Y} = E_* \widetilde{Z}_{E^{-1}(\cdot)}$. We are now in the position where we can apply the ideas from the proof of Corollary 2 [9]. But before we do so we need to establish two facts.

Claim I. There exists a smooth vector field $\widehat{Y}$ on U such that $Y - \widetilde{Y} = h^r \widehat{Y}$. Indeed, by the construction of $\widetilde{X}$, and the fact that Φ_h is of order r, it follows that there is a vector field $\widehat{X}$ on $\mathcal{N}$ such that

$$\widehat{X} = h^{-r}(X - \widetilde{X}). \tag{4.12}$$

Thus, for $x \in U$, we have

$$\begin{aligned} Y_x - \widetilde{Y}_x &= E_*(Z_{E^{-1}(x)} - \widetilde{Z}_{E^{-1}(x)}) \\ &= E_*\Big((X_{\pi(E^{-1}(x))},0) - (\widetilde{X}_{\pi(E^{-1}(x))},0)\Big) \\ &= h^r E_*(\widehat{X}_{\pi(E^{-1}(x))},0), \end{aligned} \tag{4.13}$$

where $\pi : N\mathcal{N} \to \mathcal{N}$ is the canonical projection. Thus, by letting $\widehat{Y} = E_*(Z_{E^{-1}(\cdot)} - \widetilde{Z}_{E^{-1}(\cdot)})$ the assertion follows.

Claim II. There is a compact set $\widetilde{\mathcal{K}} \supset F(\mathcal{K})$ such that the interior $\widetilde{\mathcal{K}}^o \supset F(\mathcal{K})$ is open in U, and there is a constant $M > 0$ such that (independently of h) we have

$$\sup_{z \in \widetilde{\mathcal{K}}} \left\| \widehat{Y}(z) \right\| \leq M, \qquad \sup_{z \in \widetilde{\mathcal{K}}} \left\| D\widehat{Y}(z) \right\| \leq M, \tag{4.14}$$

$$\sup_{z \in \widetilde{\mathcal{K}}} \left\| \frac{\partial}{\partial z} \theta_Y(t,s,z) \right\| \leq M, \qquad \sup_{z \in \widetilde{\mathcal{K}}} \left\| \frac{\partial^2}{\partial z^2} \theta_Y(t,s,z) \right\| \leq M, \qquad s < t \leq T. \tag{4.15}$$

Let $\mathcal{F}$ be the collection of charts referred to in Theorem 4.1 (ii). It is easy to see that we may without loss of generality assume that $\mathcal{F}$ is a family of charts on $\mathcal{N}$, covering $F(\mathcal{K})$, with the properties stated in Theorem 4.1 (ii). Now, for $(V,\varphi) \in \mathcal{F}$, define $U_\varphi = \{x \in U : \pi(E^{-1}(x)) \in V\}$, where $\pi : N\mathcal{N} \to \mathcal{N}$ is the canonical projection. Observe that U_φ is obviously open in $\mathbb{R}^m$ and also

$$F(\mathcal{K}) \subset \bigcup_{(V,\varphi) \in \mathcal{F}} U_\varphi$$

(this is clear by the definition of E). Let $\widetilde{\mathcal{K}}$ be a compact set with the properties that $\widetilde{\mathcal{K}}^o$ is open in $\mathbb{R}^m$ and

$$F(\mathcal{K}) \subset \widetilde{\mathcal{K}}^o \subset \widetilde{\mathcal{K}} \subset \bigcup_{(V,\varphi) \in \mathcal{F}} U_\varphi.$$

Note that (4.15) follows immediately from the assumption about uniformly bounded spacial derivatives of $\theta_{X,t}$ in any charts belonging to $\mathcal{F}$. To see (4.14), for $(V,\varphi) \in \mathcal{F}$ let $F_\varphi : U_\varphi \times \mathbb{R}^n \to \mathbb{R}^m$ be defined by

$$F_\varphi(x,v) = T_{E^{-1}(x)}E \cdot (T_a\varphi^{-1} \cdot v, 0), \qquad a = \varphi \circ \pi(E^{-1}(x)),$$

where

$$T_{E^{-1}(x)}E : T_{\pi(E^{-1}(x))}\mathcal{N} \times \mathbb{R}^{m-n} \to \mathbb{R}^m$$

and $A \cdot y$ denotes that the operator A acts linearly on y. Then by (4.13) we get

$$Y_x - \widetilde{Y}_x = h^r F_\varphi(x, \widehat{X}_\varphi(\rho(x))), \qquad \rho(x) = \varphi \circ \pi(E^{-1}(x)), \quad x \in U_\varphi,$$

where $\widehat{X}_\varphi$ is the vector field on $\varphi(V)$ induced by $\widehat{X}$ and φ, ($\widehat{X}$ is defined in (4.12)). Hence,

$$\begin{aligned} &D(Y - \widetilde{Y})(x) \cdot y \\ &\qquad = h^r DF_\varphi(x, \widehat{X}_\varphi(\rho(x))) \cdot (y, D\widehat{X}_\varphi(\rho(x)) \cdot D\rho(x) \cdot y), \quad x \in U_\varphi,\, y \in \mathbb{R}^m. \end{aligned}$$

By Theorem 4.1 (ii) it follows that there is a constant K such that

$$\sup_{y \in \varphi(V)} \|\widehat{X}_\varphi(y)\| \leq K, \qquad \sup_{y \in \varphi(V)} \|D\widehat{X}_\varphi(y)\| \leq K,$$

uniformly for all sufficiently small h and all $\varphi \in \mathcal{F}$. This allows us to find a constant bounding $\|DF_\varphi(x, \widehat{X}_\varphi(\rho(x)))\|$, $\|D\widehat{X}_\varphi(\rho(x))\|$ and $\|D\rho(x)\|$ for all $x \in U_\varphi$ and $\varphi \in \mathcal{F}$. Since $\{U_\varphi\}_{\varphi \in \mathcal{F}}$ covers $\widetilde{K}$ we, deduce that $\|D\widehat{Y}(x)\|$ is bounded uniformly for all sufficiently small h and for all $x \in \widetilde{\mathcal{K}}$. Similar reasoning gives a bound on $\|\widehat{Y}(x)\|$ for small h and all $x \in \widetilde{\mathcal{K}}$.

Note that we may without loss of generality assume that $\widetilde{\mathcal{K}}$ is convex. Indeed, if that is not the case choose a compact set $\widehat{\mathcal{K}}$ whose interior is open and an open set $\widehat{U}$ such that $F(\mathcal{K}) \subset \widehat{\mathcal{K}}^o \subset \widehat{\mathcal{K}} \subset \widehat{U} \subset \widetilde{\mathcal{K}}$, and an $f \in C^\infty(\mathbb{R}^m)$ such that $0 \leq f(x) \leq 1$, $\operatorname{supp}(f) \subset \widehat{U}$ and f is equal to one on $\widehat{\mathcal{K}}$. Define $Y_f = fY$, $\widetilde{Y}_f = f\widetilde{Y}$ and $\widehat{Y}_f = f\widehat{Y}$. Now Claim I and Claim II are still valid (possibly with different constants) for these vector fields and since they are globally defined $\widetilde{\mathcal{K}}$ could be chosen to be convex.

Now, using Claim I and the Alekseev-Gröbner formula (p. 96, [11]) (recall that $\theta_X(t,s,p)$ denotes the flow of X at time t that takes the value p at time s, see Section 3) we get, for $p \in F(\{q_{h,n}\}_{n \leq T/h})$, that

$$\theta_{\widetilde{Y}}^{(p)}(t) = \theta_Y^{(p)}(t) + h^r \int_0^t \frac{\partial}{\partial z} \theta_Y(t,s,\theta_{\widetilde{Y}}^{(p)}(s)) \widehat{Y}(\theta_{\widetilde{Y}}^{(p)}(s))\, ds, \qquad t \leq T.$$

Note that the latter expression is justified by the assumption on global existence of θ_X and (4.8). Hence, by using the above expression also for $q \in F(\{q_{h,n}\}_{n \leq T/h})$, subtracting the two equations and applying Claim II (this is where convexity is crucial) it follows that

$$\|\theta_{\widetilde{Y}}^{(p)}(t) - \theta_{\widetilde{Y}}^{(q)}(t)\| \leq M\|p-q\| + h^r \int_0^t 2M^2 \|\theta_{\widetilde{Y}}^{(p)}(t) - \theta_{\widetilde{Y}}^{(q)}(t)\|, \qquad t \leq T.$$

Letting $L = 2M^2$ and by appealing to the Gronwall lemma [11] gives

$$\|\theta_{\widetilde{Y}}^{(p)}(t) - \theta_{\widetilde{Y}}^{(q)}(t)\| \leq Ce^{Lh^r t}\|p-q\|, \qquad t \leq T.$$

Hence, since $\mathcal{M}$ inherits a metric from $\mathcal{N}$ similarly to what is done in the proof of Theorem 4.1 we obtain (4.9), and we are done. □

5 Geometry in infinite dimensions

Given an integrator Φ_h, Theorem 4.1 and Theorem 4.2 assures us that there is a unique family of vector fields $\{X_i\}$ such that for some properly chosen N, the vector field $\widetilde{X}_N(h) = X_1 + hX_2 + \ldots + h^{N-1}X_N$ will have a flow map $\theta_{\widetilde{X}_N(h),t}$ that is close to the integrator (in the sense described in Theorem 4.1 and Theorem 4.2). Thus it makes sense to talk about the perturbed or modified vector field induced by Φ_h. In the following we will refer to $\widetilde{X}_N(h)$ as the perturbed or modified vector field and to simplify the notation we will denote the perturbed vector field by $\widetilde{X}(h)$. It is of great importance in order to understand the behavior of the numerical approximation that we understand the behavior of $\theta_{\widetilde{X}(h),t}$. A convenient tool for analyzing $\theta_{\widetilde{X}(h),t}$ is the theory of classifications of diffeomorphisms.

Definition 2. *Let $\mathcal{M}$ be a smooth manifold. Define*

$$\mathrm{Diff}(\mathcal{M}) = \{\varphi \in C^\infty(\mathcal{M}, \mathcal{M}) : \varphi \text{ is a bijection, } \varphi^{-1} \in C^\infty(\mathcal{M}, \mathcal{M})\}.$$

In the following we will consider subsets of $\mathrm{Diff}(\mathcal{M})$ with certain geometric properties. We are interested in determining under which conditions geometric properties of the flow map of the original vector field will be preserved by the flow map of the perturbed vector field. In other words, if the flow map $\theta_{X,t}$ of a vector field X is in some subset $S \subset \mathrm{Diff}(\mathcal{M})$, under which conditions will $\theta_{\widetilde{X}(h),t} \in S$? To answer the previous question it is convenient to look at $\mathrm{Diff}(\mathcal{M})$ as a manifold itself, in particular as an infinite dimensional manifold.

5.1 Cartan's subgroups

Diffeomorphism groups and subgroups occur frequently in classical mechanics and are therefore a crucial concept in Geometric Integration. The theory of such groups originate, from the work of Lie and Cartan [5], in particular Cartan gave a classification of the complex primitive infinite-dimensional diffeomorphism groups, finding six classes. We will give a brief review here and refer to [14] for a more detailed discussion. The diffeomorphism groups of Cartan are as follows:

- $\mathrm{Diff}(\mathcal{M})$, the group of all diffeomorphisms on $\mathcal{M}$.
- The diffeomorphisms preserving a symplectic 2-form ω on $\mathcal{M}$, that is the set of diffeomorphisms φ such that $\varphi^*\omega = \omega$.
- The diffeomorphisms preserving a volume form μ on $\mathcal{M}$, that is the set of diffeomorphisms φ such that $\varphi^*\mu = \mu$.
- The diffeomorphisms preserving a given contact 1-form α up to a scalar function, that is the set of diffeomorphisms φ such that $(\varphi^*\alpha)_p = c_\varphi(p)\mu$.
- The group of diffeomorphisms preserving a given symplectic form ω up to an arbitrary constant multiple, that is the set of diffeomorphisms φ such that $\varphi^*\omega = c_\varphi\omega$.

- The group of diffeomorphisms preserving a given volume form μ up to an arbitrary constant multiple, that is the set of diffeomorphisms φ such that $\varphi^*\mu = c_\varphi \mu$.

These subgroups serve as a motivation for most of the theory in the upcoming sections.

5.2 Infinite-dimensional manifolds

We will give a short review of the basic definitions of infinite-dimensional manifolds, their tangent bundle and tangent spaces. For a more thorough treatment of the subject we refer to [15]. For an informal introduction of the concept of vector fields belonging to some Lie algebra generated by a group of diffeomorphisms we refer to [2].

Definition 3. *A Hausdorff space $\mathcal{M}$ is called a C^∞-manifold modeled on a separable locally convex topological vector space E if $\mathcal{M}$ is covered by an indexed family $\{U_\alpha : \alpha \in A\}$ of open subsets of $\mathcal{M}$ satisfying the following:*

(i) For each U_α, there is an open subset $V_\alpha \subset E$ and a homeomorphism $\varphi_\alpha : V_\alpha \to U_\alpha$.

(ii) If $U_\alpha \cap U_\beta \neq \emptyset$ then $\varphi_\beta^{-1} \circ \varphi_\alpha$ is a C^∞ diffeomorphism of $\varphi_\alpha^{-1}(U_\alpha \cap U_\beta)$ onto $\varphi_\beta^{-1}(U_\alpha \cap U_\beta)$. The maps $\varphi_\beta^{-1} \circ \varphi_\alpha$ are called coordinate transformations.

(iii) The indexed family A is the maximal one among indexed families satisfying (i) and (ii) above.

$\mathcal{M}$ is called a Frechet, Banach or Hilbert manifold if E itself is a Frechet, Banach or Hilbert space respectively.

Throughout the paper we will use the name E-manifold to describe a C^∞-manifold modeled on a separable locally convex topological vector space E. With a smooth structure on $\mathcal{M}$ we can define the tangent bundle and the tangent space. First we need to introduce an equivalence relation.

Definition 4. *Let $\mathcal{M}$ be an E-manifold. Let $x \in V_\alpha$ and $y \in V_\beta$. Then x and y are equivalent ($x \sim y$) if and only if x and y are contained in the domains of $\varphi_\beta^{-1} \circ \varphi_\alpha$, $\varphi_\alpha^{-1} \circ \varphi_\beta$ and $\varphi_\beta^{-1} \circ \varphi_\alpha(x) = y$.*

Now, for an infinite-dimensional manifold $\mathcal{M}$ covered by $\{U_\alpha = \varphi_\alpha^{-1}(V_\alpha) : \alpha \in A\}$ we may view $\mathcal{M}$ as $\{V_\alpha : \alpha \in A\}$ glued together with the equivalence relation from Definition 4. This gives rise to the following definition of the tangent bundle and the tangent space.

Definition 5. *The tangent bundle $T\mathcal{M}$ of an E-manifold $\mathcal{M}$ is the collection $\{V_\alpha \times E : \alpha \in A\}$ glued according to the following equivalence relation:*

$$(x, u) \in V_\alpha \times E \quad \text{and} \quad (y, v) \in V_\beta \times E$$

are equivalent if and only if $x \sim y$ and $(\varphi_\beta^{-1} \circ \varphi_\alpha)_* u = v$.

Definition 6. *Define the mapping π of $\bigcup_{\alpha \in A} V_\alpha \times E$ onto $\bigcup_{\alpha \in A} V_\alpha$ by $\pi(x, u) = x$. Since $(x, u) \sim (y, v)$ yields $\pi(x, u) = \pi(y, v)$, then π naturally defines a mapping (which we will, by slight abuse of notation, denote by the same symbol) π of $T\mathcal{M}$ onto $\mathcal{M}$. This map is called the projection of the tangent bundle. Then the tangent space of $\mathcal{M}$ at p is defined as*

$$T_p\mathcal{M} = \pi^{-1}(p).$$

5.3 The smooth structure of $C^k(\mathcal{M})$, $H^s(\mathcal{M})$ and $\mathrm{Diff}(\mathcal{M})$

Before we define $C^k(\mathcal{M})$ and $H^s(\mathcal{M})$ and show how to make them into manifolds, we need to discuss how to make Banach and Hilbert spaces out of sections of vector bundles. We will follow [16] (Chap. IV) quite closely. Firstly, we need to define an inner product and norm on

$L^k_{\mathrm{sym}}(\mathbb{R}^n, \mathbb{R}^m)$. Let $\{e_j\}$ be an orthonormal basis for $\mathbb{R}^n$ and define, for $T, S \in L^k_{\mathrm{sym}}(\mathbb{R}^n, \mathbb{R}^m)$, the inner product and norm

$$\langle T, S\rangle = \langle T(e_{i_1}, \ldots, e_{i_k}), S(e^{i_1}, \ldots, e^{i_k})\rangle, \qquad \|T\| = \langle T, T\rangle^{1/2}.$$

(Recall the Einstein summation convention here (discussed in Section 3). In particular, the above inner product is a sum over all indices). Secondly, let $\mathcal{M}$ be a compact manifold and let $\pi : E \to \mathcal{M}$ be a smooth vector bundle over $\mathcal{M}$ of rank m. Now, for smooth $f : \mathcal{N} \to \mathcal{M}$, where $\mathcal{N}$ is a smooth manifold, we let $\pi' : f^*E \to \mathcal{N}$ denote the pull back bundle and $\Gamma(E)$ denote the set of all smooth sections of E.

We can now make subspaces of $\Gamma(E)$ into Banach and Hilbert spaces. Let $\Gamma(\mathcal{B}_n, \mathbb{R}^m)$ denote the vector space of all functions from the closed n-ball $\mathcal{B}_n \subset \mathbb{R}^n$ with radius one into $\mathbb{R}^m$, regarded as the set of sections of the product bundle $\mathcal{B}_n \times \mathbb{R}^m$ over $\mathcal{B}_n$. Now cover $\mathcal{M}$ with finitely many charts $\{(U_i, \varphi_i)\}_{i=1}^r$ such that $\varphi_i(U_i) = \mathcal{B}_n$, and choose trivializations Ψ_i on $(\varphi_i^{-1})^*E$ such that $\Psi_i : \pi'^{-1}(\mathcal{B}_n) \to \mathcal{B}_n \times \mathbb{R}^m$. Define the linear mapping

$$F : \Gamma(E) \to \bigoplus_{i=1}^r \Gamma(\mathcal{B}_n, \mathbb{R}^m), \quad F(\xi) = (\xi_1, \ldots \xi_r), \quad \xi_i(x) = \Psi_i(\xi \circ \varphi_i^{-1}(x)) \tag{5.1}$$

and define the norm $\|\cdot\|_{\mathcal{B},k}$ and inner product $\langle \cdot, \cdot\rangle_{\mathcal{H},k}$ in the following way. For $u = (u_1, \ldots, u_r), v = (v_1, \ldots, v_r) \in \bigoplus_{i=1}^r \Gamma(\mathcal{B}_n, \mathbb{R}^m)$, let

$$\begin{aligned} |u|_{\mathcal{B},k} &= \max_{1\leq j\leq k} \sum_{i=1}^r \sup_{x\in\mathcal{B}_n} \|D^j u_i(x)\| \\ \langle u, v\rangle_k &= \max_{1\leq j\leq k} \sum_{i=1}^r \int_{\mathcal{B}_n} \langle D^j u_i(x), D^j v_i(x)\rangle \, dx, \end{aligned} \tag{5.2}$$

and for $\xi, \eta \in \Gamma(E)$

$$\|\xi\|_{\mathcal{B},k} = |F(s)|_{\mathcal{B},k}, \qquad \langle \xi, \eta\rangle_{\mathcal{H},k} = \langle F(\xi), F(\eta)\rangle_k.$$

Let $C^k(E) = \overline{\Gamma(E)}$ and $H^s(E) = \overline{\Gamma(E)}$, where the closures are in the norms $\|\cdot\|_{\mathcal{B},k}$ and $\|\cdot\|_{\mathcal{H},s}$ respectively. These Banach and Hilbert spaces will be useful in the next developments.

Given two smooth manifolds, $\mathcal{M}$ and $\mathcal{N}$, let $C^k(\mathcal{M}, \mathcal{N})$ denote the set of mappings from $\mathcal{M}$ to $\mathcal{N}$ such that their derivatives (in any local coordinates) of order $\leq k$ exist and are continuous. Also, if $s > \dim(\mathcal{M})/2$ we let $H^s(\mathcal{M}, \mathcal{N})$ denote the set of mappings from $\mathcal{M}$ to $\mathcal{N}$ with square integrable (in charts) derivatives (in the distributional sense) of order $\leq s$. We will show how to make $C^k(\mathcal{M})$ and $H^s(\mathcal{M})$ (where $C^k(\mathcal{M})$ and $H^s(\mathcal{M})$ are short for $C^k(\mathcal{M}, \mathcal{M})$ and $H^s(\mathcal{M}, \mathcal{M})$) into a Banach and Hilbert manifold respectively. The description will be rather brief and we refer to [6] and [15] for a more detailed discussion.

First one needs candidates for the charts on $C^k(\mathcal{M})$. Let $f \in C^k(\mathcal{M})$ and define

$$T_f C^k(\mathcal{M}) = \{g \in C^k(\mathcal{M}, T\mathcal{M}) : \pi \circ g = f\},$$

where $\pi : T\mathcal{M} \to \mathcal{M}$ is the canonical projection. Note that $T_f C^k(\mathcal{M})$ can naturally be identified with $C^k(f^*(T\mathcal{M}))$ with the norm as discussed above, and hence we have the desired Banach space. Similar reasoning applies to $H^s(\mathcal{M})$ by replacing $C^k(f^*(T\mathcal{M}))$ with $H^s(f^*(T\mathcal{M}))$.

As we will only need a chart around the identity in the following arguments, we will show how to construct the chart for $f = \mathrm{id}$ and refer to [6] [15] [20] for the general case. Let $\exp_q$ denote the Riemannian exponential map $\exp_q : T_q\mathcal{M} \to \mathcal{M}$ (note that $\exp_q$ is defined on all of $T_q\mathcal{M}$ since $\mathcal{M}$ is compact). Define $\mathrm{Exp} : \mathrm{T}\mathcal{M} \to \mathcal{M} \times \mathcal{M}$, by

$$\mathrm{Exp}(v_q) = (q, \exp_q(v_q)).$$

Now Exp is a diffeomorphism from a neighborhood $\mathcal{N}(\mathcal{M} \times \{0\})$ of $\mathcal{M} \times \{0\} \subset T\mathcal{M}$ (where we have allowed a minor misuse of notation using $\mathcal{M} \times \{0\}$) to a neighborhood $\mathcal{U}(\Delta)$ of the diagonal $\Delta \subset \mathcal{M} \times \mathcal{M}$. This defines a neighborhood $\mathcal{V}(\mathrm{id})$ around id, namely,

$$\mathcal{V}(\mathrm{id}) = \{f \in C^k(\mathcal{M}) : \mathrm{Gr}(f) \subset \mathcal{U}(\Delta)\}, \tag{5.3}$$

where $\mathrm{Gr}(f)$ is the graph of f. Similarly, we define a neighborhood $\mathcal{W}(\zeta_0)$ of the zero section $\zeta_0 : \mathcal{M} \to T\mathcal{M}$ by

$$\mathcal{W}(\zeta_0) = \{X \in T_{\mathrm{id}} C^k(\mathcal{M}) : X(\mathcal{M}) \subset \mathcal{N}(\mathcal{M} \times \{0\})\}$$

We can now define the chart $(\omega_{\mathrm{Exp}}, \mathcal{V}(\mathrm{id}))$ by

$$\begin{aligned} \omega_{\mathrm{Exp}}(f) &= \mathrm{Exp}^{-1} \circ (\mathrm{id}, f), \qquad & f \in \mathcal{V}(\mathrm{id}), \\ \omega_{\mathrm{Exp}}^{-1}(X) &= \mathrm{Pr}_2 \circ \mathrm{Exp} \circ X, \qquad & X \in \mathcal{W}(\zeta_0), \end{aligned} \tag{5.4}$$

where $\mathrm{Pr}_2 : \mathcal{M} \times \mathcal{M} \to \mathcal{M}$ is the projection onto the second factor.

Using this differentiable structure, $C^k(\mathcal{M})$ becomes a Banach manifold [6], [15] and similarly we can make a Hilbert manifold of $H^s(\mathcal{M})$. The brief discussion above can be summarized in the following theorem [20].

Theorem 5.1. *Let $\mathcal{M}$ be a compact Riemannian manifold. Then, with the differential structure suggested above, $C^k(\mathcal{M})$, where $k \geq 1$, and $H^s(\mathcal{M})$, where $s > \dim(\mathcal{M})/2$, become Banach and Hilbert manifolds respectively. Also*

$$T_{\mathrm{id}} C^k(\mathcal{M}) = \mathfrak{X}^k(\mathcal{M}), \qquad T_{\mathrm{id}} H^s(\mathcal{M}) = \mathfrak{X}^s_H(\mathcal{M}),$$

where $\mathfrak{X}^k(\mathcal{M})$ denotes the set of vector fields whose derivatives (in local coordinates) of order $\leq k$ exist and are continuous, and $\mathfrak{X}^s_H(\mathcal{M})$ denotes the set of vector fields such that the derivatives (in the distributional sense) of order $\leq s$ in local coordinates exist and are square integrable.

Actually, the differentiable structure suggested above is independent of the choice of Riemannian metric on $\mathcal{M}$, however, that fact will not be central in the upcoming discussions. Throughout this paper $C^k(\mathcal{M})$ and $H^s(\mathcal{M})$ are understood to have the differential structure as presented above. The following property of integrators, stated in Theorem 5.2, is quite convenient and will be a crucial ingredient in some of the later sections. The key is really that for an integrator Φ_h on a smooth compact manifold $\mathcal{M}$, there is a difference between the mappings

$$\mathbb{R} \ni h \mapsto \Phi_h \in C^k(\mathcal{M}), \qquad \mathbb{R} \ni h \mapsto \Phi_h(q) \in \mathcal{M}, \quad q \in \mathcal{M}. \tag{5.5}$$

And of course there is a difference between the derivatives

$$\frac{d}{dh}\Big|_{h=0} \Phi_h \in \mathfrak{X}^k(\mathcal{M}), \qquad \frac{d}{dh}\Big|_{h=0} \Phi_h(q) \in T_q\mathcal{M}. \tag{5.6}$$

Note that it is not clear that the properties of an integrator are sufficient for the existence of the derivative in the first part of (5.6), and this must be established. Also, if the derivative exist, even though the mappings in (5.5) are different, could it be true that for $q \in \mathcal{M}$ we have $\left(\frac{d}{dh}\big|_{h=0} \Phi_h\right)(q) = \frac{d}{dh}\big|_{h=0} \Phi_h(q)$?

Theorem 5.2. *Let $\mathcal{M}$ be a compact n dimensional manifold and let Φ_h be an integrator on $\mathcal{M}$. Then there exist neighborhoods $U \subset C^k(\mathcal{M})$ and $\tilde{U} \subset H^s(\mathcal{M})$ of* id *(the identity), where $k \geq 1$ and $s > n/2$, such that the mappings $\mathbb{R} \ni h \mapsto \Phi_h \in U$ and $\mathbb{R} \ni h \mapsto \Phi_h \in \tilde{U}$ are smooth for sufficiently small h. Also,*

$$\left(\frac{d}{dh}\Big|_{h=0} \Phi_h\right)(q) = \frac{d}{dh}\Big|_{h=0} \Phi_h(q), \qquad q \in \mathcal{M}.$$

Proof. We will first establish the existence of U and then prove that $h \mapsto \Phi_h \in U$ is smooth. Note that by the reasoning in Section 5.3 there is a neighborhood $U \subset C^k(\mathcal{M})$, containing the identity, defined by

$$U = \{f \in C^k(\mathcal{M}) : \mathrm{Gr}(f) \in \mathcal{U}(\Delta)\},$$

where $\mathcal{U}(\Delta)$ is defined as in (5.3), such that $(\mathcal{V}, \omega_{\mathrm{Exp}})$ is a local chart around id, and ω_{Exp} is defined in (5.4). We claim that $\Phi_h \in U$ for all sufficiently small h. Indeed, this is true, for since $\mathcal{U}(\Delta)$ is a neighborhood of the diagonal $\Delta \in \mathcal{M} \times \mathcal{M}$ (in the product topology), and by compactness of $\mathcal{M}$, it suffices to show that for $r, s > 0$ and $q \in \mathcal{M}$, there is an h_0 such that $\Phi_h(B_r(q)) \subset B_{r+s}(q)$ for $h < h_0$, where $B_r(q)$ denotes the open ball of radius r around q with respect to some metric d on $\mathcal{M}$. Let $X \in \mathfrak{X}(\mathcal{M})$ be defined by $X_p = \frac{d}{dh}\big|_{h=0}\Phi_h(p)$. Then there is a $h_0 > 0$ such that

$$\theta_{X,h}(B_r(q)) \subset B_{r+s}(q), \qquad h \leq h_0. \tag{5.7}$$

Now, since $\Phi : \mathbb{R} \times \mathcal{M} \to \mathcal{M}$ is smooth, and by the classical convergence analysis of integrators in $\mathbb{R}^n$ and compactness of $\mathcal{M}$, it follows that there is a $C > 0$ such that $d(\theta_{X,h}(q), \Phi_h(q)) \leq Ch$ (where d is the metric on $\mathcal{M}$) for $h \leq \tilde{h}$ for some $\tilde{h} > 0$. Thus, using (5.7), the assertion follows.

Consider the smooth mapping $\omega_{\mathrm{Exp}} \circ \Phi : \mathbb{R} \times \mathcal{M} \to T\mathcal{M}$ as a time-dependent smooth vector field. Choose charts $\{(U_i, \varphi_i)\}$ and trivializations $\{\Psi_i\}$ and define F as in (5.1). To prove that $h \mapsto \Phi_h$ is differentiable, we need to show that there is a vector field $Y \in \mathfrak{X}(\mathcal{M})$ such that

$$\lim_{t\to 0} \frac{1}{t} |F(\omega_{\mathrm{Exp}} \circ \Phi)(h+t, \cdot) - F(\omega_{\mathrm{Exp}} \circ \Phi)(h, \cdot) - tF(Y)|_{\mathcal{B},k} = 0,$$

where $|\cdot|_{\mathcal{B},k}$ is defined as in (5.2), and

$$\lim_{t\to 0} \frac{1}{t} |F(\omega_{\mathrm{Exp}} \circ \Phi)(h+t, \cdot) - F(\omega_{\mathrm{Exp}} \circ \Phi)(h, \cdot) - tF(Y)|_{s} = 0,$$

where $|\cdot|_s$ is the norm induced by $\langle \cdot, \cdot \rangle_s$ defined in (5.2). We claim that he vector field defined by $Y_p = \frac{d}{du}\big|_{u=h}(\omega_{\mathrm{Exp}} \circ \Phi)(u, p)$ is the right candidate (obviously $Y \in \mathfrak{X}(\mathcal{M})$). Letting ξ_i be a local representative of $\omega_{\mathrm{Exp}} \circ \Phi$ with respect to Ψ_i and φ_i as in (5.1), it suffices to show that

$$\lim_{t\to 0} \max_{0\leq l \leq k} \sup_{x \in \mathcal{B}_n} \frac{1}{t} \|D^l \xi_i(h+t, x) - D^l \xi_i(h, x) - tD^l \frac{d}{du}\Big|_{u=h} \xi_i(u, x)\| = 0 \tag{5.8}$$

and

$$\begin{aligned} \lim_{t\to 0} \max_{0\leq l \leq s} \frac{1}{t} \int_{\mathcal{B}_n} \Big\langle & D^l \xi_i(h+t, x) - D^l \xi_i(h, x) - tD^l \frac{d}{du}\Big|_{u=h} \xi_i(u, x), \\ & D^l \xi_i(h+t, x) - D^l \xi_i(h, x) - tD^l \frac{d}{du}\Big|_{u=h} \xi_i(u, x) \Big\rangle \, dx = 0. \end{aligned} \tag{5.9}$$

To see (5.8), let $\tilde{t} = (t, 0, \ldots, 0)$ and let $\tilde{D}$ denote the total derivative on the space $C^1(R^{n+1}, R^n)$ Then, by Taylor's Theorem [1] and smoothness of ξ_i it follows that

$$\begin{aligned} \xi_i(h+t, x) - \xi_i(h, x) - t\frac{d}{du}\Big|_{u=h} \xi_i(u, x) & \\ &= \xi_i(h+t, x) - \xi_i(h, x) - \tilde{D}\xi_i(h, x)(\tilde{t}) \\ &= \tilde{D}^2 \xi_i(h, x)(\tilde{t}, \tilde{t}) + R(h, x, \tilde{t})(\tilde{t}, \tilde{t}), \end{aligned}$$

where both $\tilde{D}^2\xi_i$ and R are smooth. Hence

$$\lim_{t\to 0} \max_{0\leq l \leq k} \sup_{x \in \mathcal{B}_n} \frac{1}{t} \|D^l \tilde{D}^2 \xi_i(h, x)(\tilde{t}, \tilde{t}) + D^l R(h, x, \tilde{t})(\tilde{t}, \tilde{t})\| = 0,$$

where $D^l \tilde{D}^2 \xi_i(h, x)(\tilde{t}, \tilde{t})$ and $D^l R(h, x, \tilde{t})(\tilde{t}, \tilde{t})$ and are the l-th derivatives of

$$x \mapsto \tilde{D}^2 \xi_i(h, x)(\tilde{t}, \tilde{t}) \quad \text{and} \quad x \mapsto R(h, x, \tilde{t})(\tilde{t}, \tilde{t})$$

respectively, and we have shown (5.8). Now, (5.9) follows by similar reasoning. To show that $h \mapsto \Phi_h$ is infinitely smooth we observe that $\omega_{\mathrm{Exp}} \circ \Phi$ is infinitely smooth and since $Y_p = \frac{d}{du}\big|_{u=h}(\omega_{\mathrm{Exp}} \circ \Phi)(u, p)$ we may argue as above using Taylor's theorem and deduce smoothness. We are now done with the first part of the proof. Since we have established above that for $q \in \mathcal{M}$ we have

$$\left(\frac{d}{dh}\Big|_{h=0} \Phi_h\right)(q) = \frac{d}{dh}\Big|_{h=0} (\omega_{\mathrm{Exp}} \circ \Phi)(h, q),$$

the last assertion of the theorem is straightforward, as seen by the following calculation

$$\begin{aligned}\left(\frac{d}{dh}\Big|_{h=0}\Phi_h\right)(q) &= \frac{d}{dh}\Big|_{h=0}(\omega_{\mathrm{Exp}}\circ\Phi)(h,q)\\ &= \frac{d}{dh}\Big|_{h=0}\exp_q^{-1}(\Phi_h(q))\\ &= (\exp_q^{-1})_*\frac{d}{dh}\Big|_{h=0}\Phi_h(q)\\ &= \frac{d}{dh}\Big|_{h=0}\Phi_h(q).\end{aligned}$$

□

Let $\mathcal{D}^1(\mathcal{M})$ be the set of C^1 diffeomorphisms on $\mathcal{M}$ (a compact manifold) and let $\mathrm{Diff}^s(\mathcal{M}) = \mathcal{D}^1(\mathcal{M}) \cap H^s(\mathcal{M})$, for $s > \dim(\mathcal{M})/2 + 1$, Then $\mathrm{Diff}^s(\mathcal{M})$ is open in $H^s(\mathcal{M})$ ([6] p. 107) and

$$\mathrm{Diff}^s(\mathcal{M}) = \{\psi \in H^s(\mathcal{M}) : \psi \,\text{is bijective, } \psi^{-1} \in H^s(\mathcal{M})\}. \tag{5.10}$$

Since $\mathrm{Diff}^s(\mathcal{M})$ is an open subset of $H^s(\mathcal{M})$, it naturally inherits its smooth manifold structure from $H^s(\mathcal{M})$. Throughout the paper $\mathrm{Diff}^s(\mathcal{M})$ will denote the set in (5.10) with this smooth structure. We immediately get the following.

Corollary 5.3. *Let $\mathcal{M}$ be a compact manifold and let Φ_h be an integrator on $\mathcal{M}$. Then there exists a neighborhood $U \subset \mathrm{Diff}^s(\mathcal{M})$, where $s > \dim(\mathcal{M})/2 + 1$, such that the mapping $\mathbb{R} \ni h \mapsto \Phi_h \in U$ is smooth for sufficiently small h and*

$$\left(\frac{d}{dh}\Big|_{h=0}\Phi_h\right)(q) = \frac{d}{dh}\Big|_{h=0}\Phi_h(q), \qquad q \in \mathcal{M}.$$

Proof. Follows immediately from Theorem 5.2 □

The next theorem describes the smoothness of the group operations: multiplication and invertion on $\mathrm{Diff}^s(\mathcal{M})$.

Theorem 5.4. *[20] For $s > \dim(\mathcal{M})/2 + 1$ it follows that $\mathrm{Diff}^s(\mathcal{M})$ is a smooth infinite-dimensional manifold and a Lie group in the following sense: For $g \in \mathrm{Diff}^s(\mathcal{M})$, right multiplication is C^∞ as a map*

$$R_g : \mathrm{Diff}^s(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M}), \qquad R_g(f) = f \circ g.$$

Left multiplication is C^k as a map

$$L_g : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M}), \qquad L_g(f) = g \circ f.$$

The group multiplication μ is C^k as a map

$$\mu : \mathrm{Diff}^{s+k}(\mathcal{M}) \times \mathrm{Diff}^s(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M}), \qquad \mu(f,g) = f \circ g.$$

The inversion ν is C^k as a map

$$\nu : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M}), \qquad \nu(f) = f^{-1}.$$

5.4 Alternative definition of the tangent space at the identity

Similarly to the discussion in the previous section one may consider submanifolds of $\mathrm{Diff}^s(\mathcal{M})$. We thus consider a symplectic 2-form on $\mathcal{M}$ and let

$$S = \{\varphi \in \mathrm{Diff}^s(\mathcal{M}) : \varphi^*\omega = \omega\}. \tag{5.11}$$

Then, according to [6], if $s > \frac{1}{2}\dim(\mathcal{M}) + 1$ then S is a closed submanifold of $\mathrm{Diff}^s(\mathcal{M})$ and

$$T_{\mathrm{id}}S = \{X \in \mathfrak{X}^s_H(\mathcal{M}) : \mathcal{L}_X\omega = 0\}, \tag{5.12}$$

where $\mathcal{L}_X\omega$ denotes the Lie derivative of ω with respect to X.

Returning to Cartans subgroups of $\mathrm{Diff}(\mathcal{M})$, we are interested in determining the tangent spaces at the identity for these subgroups of $\mathrm{Diff}(\mathcal{M})$. But not only that, we will see in the upcoming discussion that there are subsets of $\mathrm{Diff}(\mathcal{M})$ without group structure that may be of interest in geometric integration. The problem we are faced with when focusing on finding $T_{\mathrm{id}}S$ for some subset $S \subset \mathrm{Diff}(\mathcal{M})$, is that, to be rigorous (according to Definition 6), we must impose a smooth structure on S. This can be quite technical and sometimes may be impossible. Note that the crucial assumption in defining a smooth structure on $\mathrm{Diff}^s(\mathcal{M})$ has been compactness of $\mathcal{M}$, and this is an assumption we would like to remove. Also, we are interested in very specific subsets of $\mathrm{Diff}(\mathcal{M})$, namely subsets of one-parameter diffeomorphisms (integrators and flow maps).

Our goal is therefore to find a definition of the tangent space at the identity of subsets of integrators and flow maps that is independent of the choice of smooth structure on the set, and also coincides with the usual definition on well-known examples. Note that by our definition of integrator, it is superfluous to talk about integrators and flow maps, as a flow map is an integrator.

Suppose that we should choose a heuristically and more intuitive definition of the tangent space at the identity of (5.11) to obtain (5.12). A natural definition would be to consider the collection of derivatives at zero of smooth curves $\mathbb{R} \ni t \mapsto f(t) \in S$, where $f(0) = \mathrm{id}$ i.e.

$$T_{\mathrm{id}}S = \{X \in \mathfrak{X}(\mathcal{M}) : X = \frac{d}{dt}\Big|_{t=0} f(t),\ f(t) \in S,\ f(0) = \mathrm{id}\}.$$

Thus, if we consider the set $\tilde{S} \subset S$ defined by $\tilde{S} = \{\Phi_h \in S : \Phi_h \text{ is an integrator}\}$, a natural definition of the tangent space at the identity of $\tilde{S}$ is

$$T_{\mathrm{id}}\tilde{S} = \{X \in \mathfrak{X}(\mathcal{M}) : X = \frac{d}{dt}\Big|_{h=0} \Phi_h,\ \Phi_h \in \tilde{S}\},$$

where $\frac{d}{dt}\big|_{h=0}\Phi_h$ would have been well defined by Corollary 5.3 had we considered the smooth structure discussed in Section 5.3. But this definition is based on an underlying smooth structure on S since the derivative $\frac{d}{dt}\big|_{h=0}\Phi_h$ is defined as the derivative of the mapping $h \mapsto \Phi_h \in \tilde{S}$. To get rid of that extra technicality we suggest the following

$$T_{\mathrm{id}}\tilde{S} = \{X \in \mathfrak{X}(\mathcal{M}) : X_q = \frac{d}{dh}\Big|_{h=0} \Phi_h(q),\ \Phi_h \in \tilde{S},\ q \in \mathcal{M}\}.$$

This definition does not depend on any smooth structure on S, it only depends on the smooth structure on $\mathcal{M}$ as we take the derivative of the mapping $h \mapsto \Phi_h(q) \in \mathcal{M}$.

Note that it is not clear that with the latter definition that $T_{\mathrm{id}}\tilde{S} = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}$, (even though that is the case, see Section 6) but if we consider the following subset of $\tilde{S}$, namely, $\hat{S} = \{\theta_t \in S : \theta_t \text{ is a flow map}\}$, then obviously, by the formula for the Lie derivative

$$T_{\mathrm{id}}\hat{S} = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}.$$

Thus our definition is compatible with (5.11) and (5.12). To be more formal, by the reasoning above, we suggest the following definition.

Definition 7. *Let $S \subset \mathrm{Diff}(\mathcal{M})$ be a set of integrators. Define the tangent space at the identity by*

$$T_{\mathrm{id}}S = \{X \in \mathfrak{X}(\mathcal{M}) : X_q = \frac{d}{dh}\Big|_{h=0} \Phi_h(q),\ \Phi_t \in S,\ q \in \mathcal{M}\}.$$

Note that the idea of defining the tangent space at the identity in this way was first (at least to our knowledge) introduced by Reich in [19] for $\mathcal{M} = \mathbb{R}^n$. The requirement that $\mathcal{M} = \mathbb{R}^n$

is irrelevant for the definition, however, and Reich should be credited for introducing such an important tool. Note also that the name "tangent space" used here is a slight abuse of language as there is no restriction on S and therefore $T_{\text{id}}S$ may not be a vector space e.g. consider $S = \{\Phi_h\}$ containing only one element. Then the vector field X defined by $X_q = \frac{d}{dt}\big|_{h=0}\Phi_h(q)$ is in $T_{\text{id}}S$ but tX, for $t \in \mathbb{R}$, may not be in $T_{\text{id}}S$ as Φ_h may not be a flow map.

Remark 4 Note that if $A = T_{id}S$ there may exist $\tilde{S}$ such that $S \neq \tilde{S}$ and $A = T_{id}\tilde{S}$. Consider the following short argument. Let $\mathcal{M} = \mathbb{R}^n$ and let ω be a symplectic 2-form on $\mathcal{M}$. Let $A = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}$ and

$$S = \{\theta_t \in \mathrm{Diff}(\mathcal{M}) : \theta_t^*\omega = \omega,\, \theta_t \text{ is a flow map}\}.$$

Then $A = T_{id}S$. Let $X \in A$ and let the integrator Φ_h be Euler's method applied to X and let $\tilde{S} = S \cup \Phi_h$. By consistency we have $\frac{d}{dh}\big|_{h=0}\Phi_h(x) = X_x$. Hence $T_{id}\tilde{S} = A$.

Throughout the paper we will be concerned with the question: Given $S \subset \mathrm{Diff}(\mathcal{M})$ and $X \in T_{id}S$ will the flow map $\theta_{X,t} \in S$. Note that this obviously not automatic as S may contain only one element that is not a flow map (only an integrator). It is therefore important to establish conditions on S such that the answer to the question above is affirmative. We will first define a notion of closedness of S that does not depend on any smooth structure (and topology) of $\mathrm{Diff}(\mathcal{M})$ (it only depends of the topology on $\mathcal{M}$).

Definition 8. *Let $S \subset \mathrm{Diff}(\mathcal{M})$ be a semi group. Then S is said to be closed iff for any integrator $\Phi_h \subset S$, then*

$$\Psi_h(p) = \lim_{n\to\infty} \Phi_{h/n} \circ \cdots \circ \Phi_{h/n}(p), \quad (n \textit{ times}) \quad p \in \mathcal{M},$$

exists and $\Psi_h \in S$.

Proposition 5.5. *Let $S \subset \mathrm{Diff}(\mathcal{M})$ be a semi group. Then S is closed iff for every $X \in T_{id}S$ then the flow map $\theta_{X,t} \in S$.*

Proof. Let $X \in \mathfrak{X}(\mathcal{M})$ be the vector field generated by Φ_h (i.e. $X_p = \frac{d}{dh}\big|_{h=0}\Phi_h(p)$). Note that if $\mathcal{M} = \mathbb{R}^n$, it follows by the standard convergence proof of one-step methods [11] that

$$\Psi_h(p) = \lim_{n\to\infty} \Phi_{h/n} \circ \cdots \circ \Phi_{h/n}(p), \quad (n \text{ times}) \quad p \in \mathcal{M}, \tag{5.13}$$

exists and also $\Psi_h = \theta_{X,h}$ (the flow map of X). To extend this result to a smooth manifold we may use exactly the same embedding technique from the proof of Theorem 4.2 via the tubular neighborhood as in (4.10) and eventually define a vector field as in (4.11) and then apply the result in (5.13). We omit the details, however, conclude that (5.13) is valid for arbitrary smooth manifolds. Note that since (5.13) is valid regardless of any assumptions on the closedness of S, the assertion of the proposition follows. ☐

6 Classification theory of integrators

In the following we will assume that $X \in A \subset \mathfrak{X}(\mathcal{M})$ where A is a vector subspace of the infinite-dimensional Lie algebra of vector fields on $\mathcal{M}$. In addition we will assume that there is a closed semigroup $S \subset \mathrm{Diff}(\mathcal{M})$ such that $A = T_{id}S$. We will show that if the integrator $\Phi_h \in S$ then the perturbed vector field $\widetilde{X}(h) \in A$.

Theorem 6.1. *Suppose that $X \in A \subset \mathfrak{X}(\mathcal{M})$ where A is a linear subspace. Let $S \subset Diff(\mathcal{M})$ be a semigroup that is closed in the sense of Definition 8 such that $A = T_{id}S$. Suppose also that the integrator $\Phi_h \in S$ for all h. Then the perturbed vector field $\widetilde{X}(h) \in A$ and the flow map $\theta_{\widetilde{X},h}$ of $\widetilde{X}(h)$ is also in S.*

Proof. Let $\{X_j\}$ be the family of vector fields from Theorem 4.1. It suffices to show that $X_j \in A$ for all $j \in \mathbb{N}$. We do so by induction. Suppose that $X_j \in A$ for $i \leq j$. We will show that $X_{j+1} \in A$. To to that we need to show that there is a one-parameter family of diffeomorphisms $\Psi_h \in S$ such that, for $p \in \mathcal{M}$, we have $X_{j+1}(p) = \frac{d}{dh}\big|_{h=0}\Psi_h(p)$. Let $\widetilde{X}_j = X_1 + hX_2 + \ldots + h^{j-1}X_j$. We claim that

$$\Psi_h = \theta^{-1}_{\widetilde{X}_j,h^{1/(1+j)}} \circ \Phi_{h^{1/(1+j)}}$$

is the right candidate. Note that it is not clear (because of the root) that Ψ_h is smooth at $h = 0$, but that is part of the proof. However, $\Psi_h \in S$, indeed, by the induction assumption and the assumption that A is a vector space we have $\theta^{-1}_{\widetilde{X}_j,t} = \theta_{-\widetilde{X}_j,t} \in S$, so since $\Phi_h \in S$ and by the semigroup hypothesis the assertion follows. Let (U, φ) be a chart on $\mathcal{M}$, and let $\tilde{Y}_j$ and $\{Y_j\}$ be the vector fields induced by φ, $\widetilde{X}_j$ and $\{X_j\}$. By the construction of $\{X_j\}$ it suffices to show that $\frac{d}{dh}\big|_{h=0}\widehat{\Psi}_h(x) = Y_{j+1}(x)$, where $\widehat{\Psi}_h$ is a local representative of Ψ_h with respect to φ, and $x \in \varphi(U)$. To see this, note that by the construction of $\{X_j\}$ and Taylor's theorem it follows that

$$\widehat{\Phi}_h(x) = \theta_{\widetilde{Y}_j,h}(x) + h^{j+1}Y_{j+1}(x) + h^{j+2}Z(x, h),$$

where $\widehat{\Phi}_h$ is the local representative of Φ_h with respect to φ and Z is some smooth mapping. This gives, again by Taylor's theorem, that there is a smooth mapping $R : \mathbb{R}^n \times \mathbb{R}^n \to L^2_{\mathrm{sym}}(\mathbb{R}^n)$ such that

$$\begin{aligned} \theta^{-1}_{\widetilde{Y}_j,h} \circ \widehat{\Phi}_h(x) &= \theta^{-1}_{\widetilde{Y}_j,h}(\theta_{\widetilde{Y}_j,h}(x) + h^{j+1}Y_{j+1}(x) + h^{j+2}Z(x, h)) \\ &= x + D\theta^{-1}_{\widetilde{Y}_j,h}(x)W(x, h) + D^2\theta^{-1}_{\widetilde{Y}_j,h}(x)(W(x, h), W(x, h)) \\ &\qquad + R(\theta_{\widetilde{Y}_j,h}(x), W(x, h))(W(x, h), W(x, h)), \end{aligned} \tag{6.1}$$

where $W(x, h) = h^{j+1}Y_{j+1}(x) + h^{j+2}Z(x, h)$. It is easy to see (by smoothness) that

$$\begin{aligned} &\|D^2\theta^{-1}_{\widetilde{Y}_j,h}(x)(W(x, h), W(x, h)) \\ &\qquad + R(\theta_{\widetilde{Y}_j,h}(x), W(x, h))(W(x, h), W(x, h))\| = \mathcal{O}(h^{j+2}), \qquad h \to 0. \end{aligned}$$

And also, since $\theta^{-1}_{\widetilde{Y}_j,h}$ is a flow map, it follows that $D\theta^{-1}_{\widetilde{Y}_j,h}(x) = I + \mathcal{O}(h)$ as $h \to 0$. Hence

$$\theta^{-1}_{\widetilde{Y}_j,h} \circ \widehat{\Phi}_h(x) = x + h^{j+1}Y_{j+1}(x) + \mathcal{O}(h^{j+2}), \qquad h \to 0.$$

Hence,

$$Y_{j+1}(x) = \lim_{h\to 0} \frac{\theta^{-1}_{\widetilde{Y}_j,h^{1/(1+j)}} \circ \widehat{\Phi}_{h^{1/(1+j)}}(x) - x}{h} = \frac{d}{dh}\Big|_{h=0}\hat{\Psi}_h(x).$$

The fact that $X_1 = X \in A$ completes the induction and we are done. □

In a later section we will treat the case where S is not a subgroup, but has some other structure. However, a natural question to ask is: does S have to have any structure at all? The answer is affirmative as the following example shows.

Example 6.2. We follow the reasoning in Remark 4 and let ω be a symplectic 2-form on $\mathcal{M} = \mathbb{R}^n$. Also, we have the subspace $A = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}$ and

$$S = \{\theta_t \in \mathrm{Diff}(\mathcal{M}) : \theta_t^*\omega = \omega,\ \theta_t \text{ is a flow map}\}.$$

Then $A = T_{id}S$. If $X \in A$ and Φ_h is Euler's method (forward Euler) applied to X and we let $\tilde{S} = S \cup \Phi_h$ then

$$\frac{d}{dh}\Big|_{h=0}\Phi_h(x) = X_x \quad \text{and} \quad T_{id}\tilde{S} = A.$$

Thus, if we relax the semigroup hypothesis in Theorem 6.1 and assume no structure on the set, then $\tilde{S}$ is a set and $T_{id}\tilde{S} = A$ so, if Theorem 6.1 was true without the semigroup assumption, the perturbed vector field of Euler's method would be symplectic. It is easy to find examples of symplectic vector fields such that the perturbed vector field of Euler's method is not symplectic and thus we have a contradiction.

Subsets of $\mathrm{Diff}(\mathcal{M})$	Subsets of $\mathfrak{X}(\mathcal{M})$
Let $\omega \in \Omega^2(\mathcal{M})$ be symplectic. $\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : \Phi_h^*\omega = \omega\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = 0\}$
$\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : \Phi_h^*\omega = c_{\Phi_h}\omega\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\omega = \beta_X\omega\}$
Let $\mu \in \Omega^n(\mathcal{M})$ be a volume form. $\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : \Phi_h^*\mu = \mu\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\mu = 0\}$
$\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : \Phi_h^*\mu = c_{\Phi_h}\mu\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\mu = \beta_X\mu\}$
Let $\alpha \in \Omega^1(\mathcal{M})$ be a contact form. $\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : (\Phi_h^*\alpha)_p = c_{\Phi_h}(p)\alpha_p\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : (\mathcal{L}_X\alpha)_p = \beta_X(p)\alpha_p\}$
Let $f \in C^\infty(\mathcal{M})$. $\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : f \circ \Phi_h = f\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : f_*X = 0\}$
Let $\sigma : \mathrm{Diff}(\mathcal{M}) \to \mathrm{Diff}(\mathcal{M})$ be a smooth homomorphism. $\{\Phi_h \in \mathrm{Diff}(\mathcal{M}) : \sigma(\Phi_h) = \Phi_h^{-1}\}$	$\{X \in \mathfrak{X}(\mathcal{M}) : \sigma_*X = -X\}$

Table 1: Subsets of diffeomorphisms with corresponding candidates for the tangent spaces at the identity.

Remark 5 Note that Theorem 6.1 is just Theorem 1 in [19] with $\mathbb{R}^n$ replaced by a general manifold $\mathcal{M}$ and the additional assumption that S is a semigroup. The previous example shows that Theorem 1 in [19] is incomplete. Note also that Theorem 1 was also originally formulated in a technical report [17] in the language of groups of diffeomorphisms and Lie algebras of vector fields.

We are now ready to make use of Theorem 6.1 in analyzing geometric properties of the perturbed vector field. To be able to utilize Theorem 6.1 we therefore need to determine the tangent space at the identity for the desired subsets of $\mathrm{Diff}(\mathcal{M})$. Table 6 shows several subsets of $\mathrm{Diff}(\mathcal{M})$, that may be of some interest in Geometric Integration, with corresponding subspaces that are candidates for being the tangent space at the identity for the corrsponding subsets. We intend to prove that these subspaces actually are the correct tangent spaces.

As Table 6 shows, the Lie derivative is crucial in computing the tangent space at the identity in several interesting examples. The following result is therefore crucial

Proposition 6.3. *Let $\mathcal{M}$ be a smooth manifold and let Φ_t be an integrator. Suppose that $X = \mathfrak{X}(\mathcal{M})$ and $\frac{d}{dt}\big|_{t=0}\Phi_t(p) = X_p$ for $p \in \mathcal{M}$. Let τ be a smooth covariant k-tensor field on $\mathcal{M}$. Then*

$$(\mathcal{L}_X\tau)_p = \lim_{t\to 0}\frac{\Phi_t^*(\tau_{\Phi_t(p)}) - \tau_p}{t}.$$

Proof. Let θ_t be the flow map of X. Then, for $p \in \mathcal{M}$ we have

$$(\mathcal{L}_X\tau)_p = \lim_{t\to 0}\frac{\theta_t^*(\tau_{\theta_t(p)}) - \tau_p}{t},$$

thus the assertion will be evident if we can show that there is a $C > 0$ such that for $X_1, \ldots X_k \in T_p\mathcal{M}$ we have

$$|\Phi_t^*(\tau_{\Phi_t(p)})(X_1, \ldots X_k) - \theta_t^*(\tau_{\theta_t(p)})(X_1, \ldots X_k)| \leq Ct^2, \tag{6.2}$$

for sufficiently small t. We will prove this. Let (U, φ) be a chart containing p then, in these coordinates, τ will have the form

$$\tau = \tau_{i_1 \ldots i_k} dx^{i_1} \otimes \ldots \otimes dx^{i_k},$$

where $\tau_{i_1 \ldots i_k} : \mathcal{M} \to \mathbb{R}$ is a smooth function.

Note that the assertion (6.2) becomes evident were we to show that there is a $C > 0$ such that

$$|\tau_{i_1\dots i_k}(\Phi_t(p)) - \tau_{i_1\dots i_k}(\theta_t(p))| \le Ct^2 \tag{6.3}$$

and

$$\begin{aligned}|dx^{i_1}\big|_{\theta_t(p)}\otimes \dots \otimes dx^{i_k}\big|_{\theta_t(p)}&((\theta_t)_*X_1,\dots,(\theta_t)_*X_k) \\ - dx^{i_1}\big|_{\Phi_t(p)} \otimes \dots \otimes dx^{i_k}\big|_{\Phi_t(p)}&((\Phi_t)_*X_1,\dots,(\Phi_t)_*X_k)| \le Ct^2\end{aligned} \tag{6.4}$$

for sufficiently small t. Let $\tilde{\theta}_t = \varphi \circ \theta_t \circ \varphi^{-1}$ and let $\{e_j\}$ be the usual basis for $\mathbb{R}^n$ such that $\frac{\partial}{\partial x_j} = \varphi_*^{-1} e_j$. Also, let $X_l = a_l^j \frac{\partial}{\partial x_j}$, where $1 \le l \le k$. Then

$$\begin{aligned} dx^{i_1}\big|_{\theta_t(p)} \otimes \dots \otimes & dx^{i_k}\big|_{\theta_t(p)}((\theta_t)_*X_1,\dots,(\theta_t)_*X_k) \\ &= dx^{i_1}\big|_{\theta_t(p)} \otimes \dots \otimes dx^{i_k}\big|_{\theta_t(p)}(a_1^j(\theta_t)_*\frac{\partial}{\partial x_j}\Big|_p,\dots,a_k^j(\theta_t)_*\frac{\partial}{\partial x_j}\Big|_p) \\ &= dx^{i_1}\big|_{\theta_t(p)} \otimes \dots \otimes dx^{i_k}\big|_{\theta_t(p)}(a_1^j\varphi_*^{-1}(\tilde{\theta}_t)_*e_j,\dots,a_k^j\varphi_*^{-1}(\tilde{\theta}_t)_*e_j) \\ &= dx^{i_1}\big|_{\theta_t(p)} \otimes \dots \otimes dx^{i_k}\big|_{\theta_t(p)}(a_1^j\varphi_*^{-1}b_j^\mu(t)e_\mu,\dots,a_k^j\varphi_*^{-1}b_j^\mu(t)e_\mu) \\ &= (a_1^j b_j^\mu(t)\delta_\mu^{i_1})\dots(a_k^j b_j^\mu(t)\delta_\mu^{i_k}) \\ &= (a_1^j b_j^{i_1}(t))\dots(a_k^j b_j^{i_k}(t)), \end{aligned}$$

where $b_j^\mu : \mathbb{R} \to \mathbb{R}$, $b_j^\mu(t)e_\mu = (\tilde{\theta}_t)_*e_j$ and δ_μ^i is the Kronecker delta. Let $\tilde{\Phi}_t = \varphi \circ \Phi_t \circ \varphi^{-1}$. Then by exactly the same calculation as above we get

$$dx^{i_1}\big|_{\Phi_t(p)} \otimes \dots \otimes dx^{i_k}\big|_{\Phi_t(p)}((\Phi_t)_*X_1,\dots,(\Phi_t)_*X_k) = (a_1^j c_j^{i_1}(t))\dots(a_k^j c_j^{i_k}(t)),$$

where $c_j^\mu : \mathbb{R} \to \mathbb{R}$ and $c_j^\mu(t)e_\mu = (\tilde{\Phi}_t)_*e_j$. Thus, to show (6.4) we only need to show that $c_j^\mu(t) - b_j^\mu(t) = \mathcal{O}(t^2)$, which is easily seen to follow if $\|(\tilde{\Phi}_t)_* - (\tilde{\theta}_t)_*\| = \mathcal{O}(t^2)$. To see the latter; note that, by our assumption and by Taylor's theorem, we have $\tilde{\Phi}_t(x) = x + t\widetilde{X}(x) + t^2Y_1(x)$ and $\tilde{\theta}_t(x) = x + t\widetilde{X}(x) + t^2Y_2(x)$, where $\widetilde{X}$ is the vector field induced by X and φ, and $Y_i : \mathbb{R}^n \to \mathbb{R}^n$ is smooth. Hence, taking derivative with respect to x and possibly restricting to a compact domain yield the assertion. Note that (6.3) follows by the fact that $\tilde{\Phi}_t(x) - \tilde{\theta}_t(x) = \mathcal{O}(t^2)$ and smoothness of $\tau_{i_1\dots i_k}$. □

Throughout this section we will use (as opposed to the notation in section 5.3) the notation $C^\infty(\mathcal{N})$ for $C^\infty(\mathcal{N},\mathbb{R})$ when $\mathcal{N}$ is a smooth manifold.

Corollary 6.4. *Let $\tau \in \Omega^k(\mathcal{M})$ be a smooth k-form. Let*

$$S_1 = \{\Phi_t : \Phi_t^*\tau = \tau\}, \quad S_2 = \{\Phi_t : \Phi_t^*\tau = c_\Phi(t)\tau,\ c_\Phi \in C^\infty(\mathbb{R})\}$$

and $S_3 = \{\Phi_t : (\Phi_t^*\tau)_p = c_\Phi(t,p)\tau,\ c_\Phi \in C^\infty(\mathbb{R}\times\mathcal{M})\}$. Also, let

$$A_1 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\tau = 0\}, \quad A_2 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\tau = \alpha_X\tau,\ \alpha_X \text{ constant}\}$$

and $A_3 = \{X \in \mathfrak{X}(\mathcal{M}) : \mathcal{L}_X\tau = \alpha_X\tau,\ \alpha_X \in C^\infty(\mathcal{M})\}$. Then $T_{id}S_1 = A_1$, $T_{id}S_2 = A_2$ and $T_{id}S_3 = A_3$

Proof. Let $\Phi_t \in S_2$ and $X = \frac{d}{dt}\big|_{t=0}\Phi_t$. Then, by Proposition, 6.3

$$\mathcal{L}_X\tau = \lim_{t\to 0}\frac{\Phi_t^*(\tau_{\Phi_t(p)}) - \tau_p}{t} = c_\Phi'(0)\tau_p,$$

where the last equality follows by our assumption, so $X \in A$ and hence $T_{id}S_2 \subset A_2$. The inclusions $T_{id}S_1 \subset A_1$ and $T_{id}S_3 \subset A_3$ follow similarly. As for the other inclusion, let $X \in A_2$

and θ_t be the flow map of X. Then, for $p \in \mathcal{M}$ and $X_1, \ldots, X_n \in T_p\mathcal{M}$ we have the following differential equation

$$\begin{aligned}\frac{d}{dt}\Big|_{t=t_0} \theta_t^*(\tau_{\theta_t(p)})(X_1, \ldots, X_n) &= \theta_{t_0}^* \left((\mathcal{L}_X\tau)_{\theta_{t_0}(p)}\right)(X_1, \ldots, X_n) \\ &= \alpha_X(\theta_{t_0}(p)) \left(\theta_{t_0}^* \tau_{\theta_{t_0}(p)}\right)(X_1, \ldots, X_n).\end{aligned}$$

Thus, $\theta_t^*(\tau_{\theta_t(p)})(X_1, \ldots, X_n)$ must satisfy

$$\theta_t^*(\tau_{\theta_t(p)})(X_1, \ldots, X_n) = e^{\beta_X(t,p)}\tau_p(X_1, \ldots, X_n),$$

where $\beta_X(t,p) = \int_0^t \alpha_X(\theta_s(p))\, ds$. Hence, $\theta_t \in S_2$. The inclusions $A_1 \subset T_{id}S_1$ and $A_3 \subset T_{id}S_3$ follow similarly. □

Corollary 6.5. *Let $X \in \mathfrak{X}(\mathcal{M})$ and $\tau \in \Omega^k(\mathcal{M})$. Let Φ_h be an integrator for X.*

(i) If $\mathcal{L}_X\tau = 0$ and $\Phi_h^*\tau = \tau$ then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}}\tau = 0$.

(ii) If $\mathcal{L}_X\tau = \alpha_X\tau$ and $\Phi_h^*\tau = c_\Phi(h)\tau$, where c is smooth, then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}}\tau = \alpha_{\widetilde{X}}\tau$.

(iii) If $\mathcal{L}_X\tau = \alpha_X\tau$ where $\alpha_X \in C^\infty(\mathcal{M})$ $(\Phi_h^*\tau)_p = c_\Phi(h,p)\tau$, $c_\Phi \in C^\infty(\mathbb{R}\times\mathcal{M})\}$, then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}}\tau = \alpha_{\widetilde{X}}\tau$ where $\alpha_X \in C^\infty(\mathcal{M})$

Proof. Note that the sets S_1, S_2, S_3 from Corollary 6.4 are easily seen to be groups and they are in fact closed in the sense of Definition 8 (this is easily seen from the proof of Corollary 6.4 and the statement of Proposition 5.5). The corresponding sets A_1, A_2, A_3 are vector spaces, a fact easily seen from Cartan's formula. Thus, the assertion follows by Theorem 6.1. □

We can now prove the main theorem.

Theorem 6.6. *Let $X \in \mathfrak{X}(\mathcal{M})$ with corresponding flow map θ_t, and let Φ_h be a numerical integrator for X with corresponding perturbed vector field $\widetilde{X}(h)$ and flow map $\tilde{\theta}_t$. Then*

(i) if ω is a symplectic 2-form on $\mathcal{M}$ such that $\theta_t^*\omega = \omega$ and $\Phi_h^*\omega = \omega$ then the perturbed vector field $\widetilde{X}(h)$ is symplectic i.e. it satisfies $\mathcal{L}_{\widetilde{X}(h)}\omega = 0$, and $\tilde{\theta}_t^*\omega = \omega$.

(ii) if μ is a volume form on $\mathcal{M}$ such that $\theta_t^*\mu = \mu$ and $\Phi_h^*\mu = \mu$ then the perturbed vector field $\widetilde{X}(h)$ is divergence-free i.e. it satisfies $\operatorname{div}\widetilde{X}(h) = 0$, and $\tilde{\theta}_t^*\mu = \mu$.

(iii) if ω is a symplectic 2-form on $\mathcal{M}$ such that $\theta_t^*\omega = \alpha(t)\omega$ and $\Phi_h^*\omega = \beta(h)\omega$, where $\alpha, \beta : \mathbb{R} \to \mathbb{R}$ are smooth, then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}(h)}\omega = \rho\omega$, where ρ is a real constant and $\tilde{\theta}_t^*\omega = \tilde{\alpha}(t)\omega$, where $\tilde{\alpha}$ is smooth.

(iv) if μ is a volume form on $\mathcal{M}$ such that $\theta_t^*\mu = \alpha(t)\mu$ and $\Phi_h^*\mu = \beta(h)\mu$, where $\alpha, \beta : \mathbb{R} \to \mathbb{R}$ are smooth, then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}(h)}\mu = \rho\mu$, where ρ is a real constant and $\tilde{\theta}_t^*\mu = \tilde{\alpha}(t)\mu$, where $\tilde{\alpha}$ is smooth.

(v) if τ is a contact 1-form on $\mathcal{M}$ such that $(\theta_t^*\tau)_p = \alpha(t,p)\tau$ and $(\Phi_h^*\tau)_p = \beta(h,p)\tau$, where $\alpha, \beta \in C^\infty(\mathbb{R}\times\mathcal{M})$ then the perturbed vector field $\widetilde{X}(h)$ satisfies $\mathcal{L}_{\widetilde{X}(h)}\tau = \rho\tau$, where $\rho \in C^\infty(\mathcal{M})$ and $\tilde{\theta}_t^*\tau = \tilde{\alpha}(t,p)\tau$, where $\alpha \in C^\infty(\mathbb{R}\times\mathcal{M})$.

(vi) if $f : \mathcal{M} \to \mathbb{R}$ is a smooth function such that $f_*X = 0$ and $f \circ \Phi_h = f$. Then the perturbed vector field $\widetilde{X}(h)$ satisfies $f_*\widetilde{X}(h) = 0$ and $f \circ \tilde{\theta}_t = f$.

Proof. (i)–(v) follow from corollary 6.5 and its proof as well as Theorem 6.1. To show (vi), note that

$$S = \{\varphi_t : f \circ \varphi_t = f\}$$

is obviously a closed semigroup in the sense of Definition 8 and it is easily seen that

$$T_{id}S = \{X \in \mathfrak{X}(\mathcal{M}) : f_* X = 0\}$$

and the latter is a vector space. Hence, appealing to Theorem 6.1 yields our assertion. □

Remark 6 Note that (i) in Theorem 6.6 is important for the study of integration of Hamiltonian vector fields, however, symplectic vector fields are only locally Hamiltonian. It is therefore of interest to understand when one can expect to get globally Hamiltonian modified vector fields. It is well known [13] that every locally Hamiltonian vector field on $\mathcal{M}$ is globally Hamiltonian if and only if $H^1_{dR}(\mathcal{M}) = 0$, where $H^1_{dR}(\mathcal{M})$ denotes the 1st de Rham cohomology group of the manifold.

7 Smooth homomorphisms and their anti fixed points

In the previous section we considered subsets of $\mathrm{Diff}(\mathcal{M})$ that are semigroups. It turns out that there are interesting examples that do not fit into the previous framework. One of these examples are anti-fixed points of smooth homomorphisms and this is the theme in this section. By a smooth homomorphism we mean a C^1 mapping $\sigma : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M})$, (recall (5.10) for the definition of $\mathrm{Diff}^s(\mathcal{M})$) where $s > \frac{1}{2}\dim(\mathcal{M})+1$ and $k \geq 0$, such that $\sigma(\Psi \circ \Phi) = \sigma(\Psi) \circ \sigma(\Phi)$. An anti-fixed point of σ is an element $\Phi \in \mathrm{Diff}(\mathcal{M})$ such that $\sigma(\Phi) = \Phi^{-1}$. Recall also $\mathfrak{X}^{s+k}_H(\mathcal{M})$ from Theorem 5.1.

An example of such a smooth homomorphism is the following. Let $\rho : \mathcal{M} \to \mathcal{M}$ be a diffeomorphism and denote the mapping

$$\Psi \mapsto \rho \circ \Psi \circ \rho^{-1} \tag{7.1}$$

by σ. Note that this is a homomorphism on $\mathrm{Diff}(\mathcal{M})$, since $\sigma(\Psi \circ \Phi) = \sigma(\Psi) \circ \sigma(\Phi)$. Also, by Theorem 5.4, σ is C^k as a map

$$\sigma : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M}).$$

Theorem 7.1. *Let $\mathcal{M}$ be a compact manifold, $s > \frac{1}{2}\dim(\mathcal{M})+1$ and $k \geq 0$. Let $X \in \mathfrak{X}(\mathcal{M})$ with corresponding flow map θ_t and let Φ_h be an integrator for X. Let $\sigma : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M})$ be a C^1 group homomorphism and define*

$$S = \{\varphi \in \mathrm{Diff}^{s+k}(\mathcal{M}) : \sigma(\varphi) = \iota(\varphi^{-1})\},$$

$$A = \{X \in \mathfrak{X}^{s+k}_H(\mathcal{M}) : \sigma_* X = -\iota_* X\},$$

where $\iota : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^s(\mathcal{M})$ is the inclusion map. Suppose that $\theta_t \in S$. If $\Phi_h \in S$ then the modified vector field $\widetilde{X}(h) \in A$ and $\tilde{\theta}_t \in S$, where $\tilde{\theta}_t$ is the flow map of $\widetilde{X}(h)$.

Proof. The proof is similar to the proof of Theorem 6.1. Let

$$\tilde{S} = \{\Phi_h \in S : \Phi_h \text{ is an integrator}\}, \qquad \tilde{A} = A \cap \mathfrak{X}(\mathcal{M}).$$

We will first show that $\tilde{A} = T_{id}\tilde{S}$. To see that $T_{id}\tilde{S} \subset \tilde{A}$, let $\Psi_h \in \tilde{S}$ be an integrator. To get the desired inclusion we have to show that

$$\sigma_*\left(\frac{d}{dh}\Big|_{h=0} \Psi_h\right) = -\frac{d}{dh}\Big|_{h=0} \Psi_h, \tag{7.2}$$

where $\frac{d}{dh}\big|_{h=0} \Psi_h$ is well defined because of Corollary 5.3.

To see this, for any chart (U, φ) let $\tilde{\Psi}_h = \varphi \circ \Psi_h \circ \varphi^{-1}$. Let $Y = \frac{d}{dh}\big|_{h=0}\Psi_h$ and $\tilde{Y}$ be the vector field induced by φ and Y. By Taylor's Theorem and a little manipulation we have $\tilde{\Psi}_h^{-1}(y) = y - h\tilde{Y}(y) + \mathcal{O}(h^2)$, where $y \in \varphi(U)$, and thus, by Corollary 5.3, $\frac{d}{dh}\big|_{h=0}\Psi_h^{-1} = -Y$. Hence, we have

$$\sigma_* Y = \frac{d}{dh}\Big|_{h=0}\sigma(\Psi_h) = \frac{d}{dh}\Big|_{h=0}\Psi_h^{-1} = -Y,$$

and this yields (7.2). To get the inclusion $T_{id}\tilde{S} \supset \tilde{A}$ we must show that for $Y \in \tilde{A}$ the corresponding flow map satisfies $\sigma(\theta_{Y,t}) = \theta_{Y,t}^{-1}$. To see that, note that by Corollary 5.3 $t \mapsto \theta_{Y,t} \in \mathrm{Diff}^{s+k}(\mathcal{M})$ is smooth so $t \mapsto \sigma(\theta_{Y,t}) \in \mathrm{Diff}^s(\mathcal{M})$ is smooth and

$$\frac{d}{dt}\Big|_{t=0}\sigma(\theta_{Y,t}) = \sigma_* \frac{d}{dt}\Big|_{t=0}\theta_{Y,t} = \sigma_* Y = -Y.$$

Thus, $\sigma(\theta_{Y,t})$ is the flowmap of $-Y$ and hence $\sigma(\theta_{Y,t}) = \theta_{-Y,t} = \theta_{Y,t}^{-1}$. Note that we have shown more than just $\tilde{A} = T_{id}\tilde{S}$, we have also shown that for $X \in \tilde{A}$ then the flow map $\theta_{X,t} \in \tilde{S}$.

We can now proceed as in the proof of Theorem 6.1. The Theorem will follow if we can show that $\widetilde{X}(h) \in A$. The proof is by induction. Now for sufficiently small $h > 0$ let $\widetilde{X}_i(h) = X_1 + hX_1 + \ldots + h^{i-1}X_i$ where X_j is constructed as in the proof of Theorem 4.1. Suppose $\widetilde{X}_j \in \tilde{A}$ for all $j \leq i$ for some j. We will show that $X_{i+1} \in \tilde{A}$, thus we need to show that $\sigma_*(X_{i+1}) = -X_{i+1}$, which we will do.

Let θ_i be the flow map of $\widetilde{X}_i(h)$. Let $\widehat{\theta}_{i,t} = \theta_{i,t^{1/(1+i)}}$ and $\widehat{\Phi}_t = \Phi_{t^{1/(1+i)}}$. We will need the following fact

$$X_{i+1} = \frac{d}{dt}\Big|_{t=0}\hat{\theta}_{i,t}^{-1} \circ \hat{\Phi}_t \quad \text{and} \quad -X_{i+1} = \frac{d}{dt}\Big|_{t=0}\hat{\theta}_{i,t} \circ \hat{\Phi}_t^{-1}. \tag{7.3}$$

Suppose for a moment that (7.3) is true. Then

$$\begin{aligned}
\sigma_*(X_{i+1}) &= \sigma_*(\frac{d}{dt}\Big|_{t=0}\hat{\theta}_{i,t}^{-1} \circ \hat{\Phi}_t) \\
&= \frac{d}{dt}\Big|_{t=0}\sigma(\hat{\theta}_{i,t}^{-1} \circ \hat{\Phi}_t) \\
&= \frac{d}{dt}\Big|_{t=0}\sigma(\hat{\theta}_{i,t}^{-1}) \circ \sigma(\hat{\Phi}_t) \\
&= \frac{d}{dt}\Big|_{t=0}\hat{\theta}_{i,t} \circ \hat{\Phi}_t^{-1} = -X_{i+1},
\end{aligned}$$

where the second to last equality follows by the induction hypothesis on X_i and the proved fact that $\tilde{A} = T_{id}\tilde{S}$. Thus, to conclude the argument we only have to show (7.3).

It suffices to show (7.3) in local coordinates. Let (U, φ) be a chart on $\mathcal{M}$, and let $\tilde{\Phi}_h = \varphi \circ \Phi_h \circ \varphi^{-1}$ and $\tilde{\theta}_{i,h} = \varphi \circ \theta_{i,h} \circ \varphi^{-1}$. Let $\widehat{X}_{i+1}$ be the vector field on $\varphi(U)$ induced by X_{i+1} and φ. By the construction of $\widetilde{X}_i(h)$ it follows that for $y \in \varphi(U)$ we have

$$\tilde{\Phi}_h(y) = \tilde{\theta}_{i,h}(y) + h^{i+1}\widehat{X}_{i+1}(y) + \mathcal{O}(h^{i+2}),$$

$$\Phi_h^{-1}(y) = \tilde{\theta}_{i,h}^{-1}(y) - h^{i+1}\widehat{X}_{i+1}(y) + \mathcal{O}(h^{i+2}).$$

So, by arguing as in the proof of Theorem 6.1, we get

$$\tilde{\theta}_{i,h}^{-1} \circ \tilde{\Phi}_h(y) = y + h^{i+1}\widehat{X}_{i+1}(y) + \mathcal{O}(h^{i+2})$$

$$\tilde{\theta}_{i,h} \circ \tilde{\Phi}_h^{-1}(y) = y - h^{i+1}\widehat{X}_{i+1}(y) + \mathcal{O}(h^{i+2}).$$

Let $t = h^{i+1}$. Then

$$\widetilde{X}_{i+1} = \lim_{t \to 0}\frac{\tilde{\theta}_{i,t^{(1/1+i)}}^{-1} \circ \tilde{\Phi}_{t^{(1/1+i)}} - id}{t} = \frac{d}{dt}\Big|_{t=0}\tilde{\theta}_{i,t^{(1/1+i)}}^{-1} \circ \tilde{\Phi}_{t^{(1/1+i)}}.$$

And similarly we get $-\widetilde{X}_{i+1} = \frac{d}{dt}\Big|_{t=0}\tilde{\theta}_{i,t^{(1/1+i)}} \circ \tilde{\Phi}_{t^{(1/1+i)}}^{-1}$, proving (7.3). The fact that $\widetilde{X}_1 = X \in A$ completes the induction. □

Corollary 7.2. *Let $\mathcal{M}$ be a compact manifold. Let $X \in \mathfrak{X}(\mathcal{M})$ and let Φ_t be a numerical integrator for X. Suppose that σ is defined as in (7.1) and that $\sigma(\theta_{X,h}) = \theta_{X,h}^{-1}$ and $\sigma(\Phi_h) = \Phi_h^{-1}$ then the perturbed vector field $\widetilde{X}(h)$ of Φ_h satisfies $\sigma_* \widetilde{X}(h) = -\widetilde{X}(h)$ and $\sigma(\tilde{\theta}_{X,t}) = \tilde{\theta}_{X,t}^{-1}$, where $\tilde{\theta}$ is the flow of $\widetilde{X}(h)$.*

Proof. Follows from Theorems 5.4 and 7.1. □

Remark 7 Note that there is a difference in the prerequisites needed for Theorem 7.1 and Theorem 6.6. In particular, Theorem 7.1 must use the existence of some smooth structure on $\mathrm{Diff}(\mathcal{M})$, however, Theorem 6.6 does not rely on this. Recall that the essence of Theorem 7.1 and its proof is

$$\sigma : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^{s}(\mathcal{M}),$$

a C^1 group homomorphism and also

$$S = \{\varphi \in \mathrm{Diff}^{s+k}(\mathcal{M}) : \sigma(\varphi) = \iota(\varphi^{-1})\}, \quad A = \{X \in \mathfrak{X}_H^{s+k}(\mathcal{M}) : \sigma_* X = -\iota_* X\},$$

where $\iota : \mathrm{Diff}^{s+k}(\mathcal{M}) \to \mathrm{Diff}^{s}(\mathcal{M})$ is the inclusion map. Now by letting

$$\tilde{S} = \{\Phi_h \in S : \Phi_h \text{ is an integrator}\}, \qquad \tilde{A} = A \cap \mathfrak{X}(\mathcal{M}),$$

one shows that $\tilde{A} = T_{id}\tilde{S}$. It is in this process the results in 5.3 are absolutely necessary. Note that the tangent map σ_* (or the derivative) is not even defined without a smooth structure on $\mathrm{Diff}(\mathcal{M})$. The necessity of the framework in 5.3 may not be clear at first glance when considering question (vii) from Section 2.2, however, after realizing that $\tilde{A} = T_{id}\tilde{S}$ and that the modified vector field is in A provided that the integrator is in S, this becomes clear. Comparing with Theorem 6.6 one realizes that the smooth structure of $\mathrm{Diff}(\mathcal{M})$ is not needed at all. However, the formula for the Lie-derivative in Proposition 6.3 is absolutely crucial.

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