

What kinds of dynamics are there? Lie pseudogroups, dynamical systems, and geometric integration

Robert I. McLachlan* G. R. W. Quispel†

Abstract

We classify dynamical systems according to the group of diffeomorphisms to which they belong, with application to geometric integrators for ODEs. This point of view unifies symplectic, Lie group, and volume-, integral-, and symmetry-preserving integrators. We review the Cartan classification of the primitive infinite-dimensional Lie pseudogroups (and hence of dynamical systems), and select the conformal pseudogroups for further study, i.e., those that contract volume or a symplectic structure at a constant rate. Their special properties are illustrated analytically (by a study of their behaviour with respect to symmetries) and numerically (by a geometric calculation of Lyapunov exponents). We also briefly discuss the nonprimitive pseudogroups.

1 Introduction

It is possible to make a primary classification of discrete-time dynamical systems¹ into three categories of increasing specificity[21]:

1. those which lie in a semigroup (for example, the set of all maps $\varphi : M \rightarrow M$, where M is the phase space);
2. those which lie in a symmetric space (for example, the diffeomorphisms closed under the composition $\varphi\psi^{-1}\varphi$, such as maps with time-reversal symmetry); and
3. those which lie in a group (for example, the group of all diffeomorphisms of phase space).

A ‘geometric’ numerical method for a differential equation is one which preserves some property of the flow of the differential equation. Two key examples are symplectic and volume-preserving integrators, which both provide excellent long-time stability [3, 21]. Notice that in each case, a subgroup of the group of diffeomorphisms of

*Institute of Fundamental Sciences, Massey University, Palmerston North, New Zealand (R.McLachlan@massey.ac.nz).

†Department of Mathematics, La Trobe University, Bundoora, Melbourne 3083, Australia (R.Quispel@latrobe.edu.au).

¹In this paper we consider only autonomous systems

M appears, namely the groups of symplectic and of volume-preserving maps. The questions we address in this paper are

1. What other such classes of dynamical systems are there? Is there a classification of dynamical systems?
2. For which of these can geometric integrators can be constructed?
3. Which other structures (e.g. symmetries and integrals) can be put into a common framework?

Such classifications are fundamental to the study of dynamics, because most generic phenomena (e.g. stability, codimension of bifurcations, dimension of invariant tori, Feigenbaum constants) depend on the class of systems considered. A two-level classification, first into semigroup/symmetric space/group, and then into their subspaces, seems a promising way to proceed.

We find that many proposed geometric integrators can be classified according to their diffeomorphism group. That is, one considers differential equations belonging to a Lie algebra \mathfrak{X} of vector fields on a manifold M whose flows lie in a subgroup \mathfrak{G} of the group of diffeomorphisms of M . Then a geometric integrator for the ODE $\dot{x} = f(x)$, $x \in M$, $f \in \mathfrak{X}$, is a map $\varphi_f \in \mathfrak{G}$. We call it a \mathfrak{G} -integrator.

The group structure not only influences the possible dynamics, it is also used in the construction of high-order integrators by composition [18, 38]. If $\varphi_{f_i} \in \mathfrak{G}$ for all i , then $\varphi_{f_1} \circ \varphi_{f_2} \circ \dots \in \mathfrak{G}$ (usually $f = \sum f_i$); \mathfrak{G} itself now plays no role in the design of particular composition methods.

The more general cases, of semigroups and symmetric spaces, we leave for the future [27].

There is no general theory of diffeomorphism groups. Instead, one considers the so-called *Lie* diffeomorphism groups, those that are the general solution of a set of PDEs. For example, on \mathbb{R} there are up to isomorphism only two such groups: the one defined by $\varphi' = 0$, with solution $\varphi(x) = x + a$ ($\mathfrak{G} \cong \mathbb{R}$ has dimension 1), and the one defined by $\varphi'' = 0$, with solution $\varphi(x) = ax + b$ ($\mathfrak{G} \cong \text{Aff}(1)$ has dimension 2).

If we allow the solutions to be merely *local* diffeomorphisms, then there is one more important case, that defined by $\varphi' \varphi''' - \frac{3}{2} \varphi''^2 = 0$, with solution $\varphi(x) = (ax + b)/(cx + d)$ ($\mathfrak{G} \cong SL(2)$ has dimension 3.) This situation is typical, leading to the study of Lie *pseudogroups*, sets of local diffeomorphisms closed under composition only when the composition is defined. The flows of a Lie algebra of vector fields generally form a pseudogroup, because for a fixed time the flow of a given vector field need not be defined for all $x \in M$.

Definition 1 [14, 35] *Let M be a manifold and let \mathfrak{G} be a set of local diffeomorphisms $\varphi : U_\varphi \rightarrow V_\varphi$ where U_φ, V_φ are open subsets of M . \mathfrak{G} is called a pseudogroup if the following hold:*

- (i) *The identity is in \mathfrak{G} .*
- (ii) *If $\varphi \in \mathfrak{G}$, then $\varphi|_U \in \mathfrak{G}$ for any open $U \subset U_\varphi$.*
- (iii) *If $\varphi \in \mathfrak{G}$, then $\varphi^{-1} : V_\varphi \rightarrow U_\varphi$ is in \mathfrak{G} .*
- (iv) *If φ and ψ are in \mathfrak{G} and $V_\varphi \subset U_\psi$, then $\psi \circ \varphi \in \mathfrak{G}$.*

(v) If φ is a local diffeomorphism of M such that each point in the domain of φ has a neighbourhood U such that $\varphi|_U \in \mathfrak{G}$, then $\varphi \in \mathfrak{G}$.

A pseudogroup \mathfrak{G} is called a Lie pseudogroup if its elements φ are the general solution of a set of PDEs in φ and its partial derivatives of some finite order.

The vector fields whose local flows are in \mathfrak{G} for sufficiently small times (the time depending on the local domain) form a Lie algebra, which we denote \mathfrak{X} . Vice versa, a Lie algebra of differentiable vector fields generates a pseudogroup. For any pseudogroup, the subset consisting of its elements which are global diffeomorphisms forms a group. For our applications, the distinction between local and global diffeomorphisms (i.e., between pseudogroups and groups of diffeomorphisms), is not crucial and will not be emphasized.

If a Lie pseudogroup \mathfrak{G} is finite-dimensional, then it is a Lie group. The flow of the ODE $\dot{x} = f(x, t)$, $f(\cdot, t) \in \mathfrak{X} \forall t$, belongs to \mathfrak{G} , where in this case \mathfrak{X} is a finite-dimensional Lie algebra. (For example, $\dot{x} = A(t)x$, where $x \in \mathbb{R}^n$ and $A(t) \in \mathfrak{so}(n)$; the flow is orthogonal.) The group orbit through the initial condition x_0 is a homogeneous space; the construction of \mathfrak{G} -integrators for ODEs on homogeneous spaces is an important part of geometric integration, for which an extensive and beautiful theory has been developed [28]. (See also Section 6, remark 7).

When M is 1-dimensional, the only infinite-dimensional pseudogroup on M is the set of all local diffeomorphisms. However, when M is 2-dimensional several new infinite-dimensional Lie pseudogroups appear. We let $M = \mathbb{R}^2$ and write $\varphi = (u(x, y), v(x, y))$.

Example 1 $\mathfrak{G} = \{\varphi : u_x = v_y, u_y = -v_x\}$ is defined by the Cauchy-Riemann equations, and may be identified with the complex locally analytic mappings, an infinite-dimensional group. Because the defining PDEs are linear, this group can be identified with its Lie algebra. Any differential equation $\dot{z} = f(z)$, $z \in \mathbb{C}$, f analytic, has a flow in \mathfrak{G} ; Euler's method in the variable z is a \mathfrak{G} -integrator.

Example 2 $\mathfrak{G} = \{\varphi : u_x v_y - u_y v_x = \det d\varphi = 1\}$, the area-preserving mappings, is also infinite-dimensional. Its Lie algebra is the divergence-free vector fields, elements of which have the form $\dot{x} = H_y(x, y)$, $\dot{y} = -H_x(x, y)$. Symplectic integrators such as the midpoint rule provide \mathfrak{G} -integrators.

Example 3 $\mathfrak{G} = \{\varphi : v_x = 0\} = \{\varphi : \varphi = (u(x, y), v(y))\}$ is infinite-dimensional. \mathfrak{G} -integrators have earlier been called "closed under restriction to closed subsystems" [2]. Note that all elements of φ leave the foliation $y = \text{const.}$ invariant. Such Lie pseudogroups are said to be *not primitive* and are not included in the standard classification. However, they do arise in geometric integration and we will consider them in Section 5.

Definition 2 [14] A pseudogroup \mathfrak{G} is called transitive if for all $x, y \in M$ there exists $\varphi \in \mathfrak{G}$ such that $\varphi(x) = y$. A foliation of M is invariant under \mathfrak{G} if φ permutes the leaves of the foliation for all $\varphi \in \mathfrak{G}$ (i.e., if \mathfrak{G} maps leaves to leaves). A foliation of M is fixed under \mathfrak{G} if φ maps each leaf to itself for all $\varphi \in \mathfrak{G}$. A pseudogroup \mathfrak{G} is called primitive if it leaves no nontrivial foliation invariant.

Note that a primitive Lie pseudogroup must be transitive, for otherwise its orbits would be an invariant foliation. This is not true for pseudogroups of non-Lie type.

Example 4 $\mathfrak{G} = \{\varphi : \varphi(x+1, y) = \varphi(x, y) + (1, 0)\}$, the mappings which have a discrete translation symmetry $(x, y) \mapsto (x+1, y)$. Given an ODE with such a symmetry, we may want to construct a \mathfrak{G} -integrator for it, namely one that has the same symmetry. This group is primitive and transitive. However, it cannot be defined by PDEs because the constraint is not local; it is not a Lie pseudogroup. Another example of a diffeomorphism group which is not a Lie pseudogroup was provided by Lie himself: in $\{\varphi : u(x, y) = f(x), v(x, y) = f(y)\}$, one cannot eliminate f in favour of the derivatives of u and v .

Example 5 The local diffeomorphisms with given invariant sets (for example, a given list of fixed points and periodic orbits) form a pseudogroup which is not of Lie type, although as in the previous example, we would like to construct \mathfrak{G} -integrators. Fixed-point-preserving integrators are known [36].

Example 6 Let $M = \mathbb{R}^n$, let G be a Lie subgroup of $GL(n)$, and let \mathfrak{G} be the Lie pseudogroup consisting of all local diffeomorphisms whose derivative lies in G for all $x \in M$. It can be finite or infinite dimensional. For $G = Sp(n)$, \mathfrak{G} is the infinite-dimensional set of symplectic maps; but for $G = SO(n)$, \mathfrak{G} is finite dimensional. For, writing $f_i(x) \frac{\partial}{\partial x_i}$ for an element of the Lie algebra of \mathfrak{G} , we have

$$f_{i,j} + f_{j,i} = 0 \Rightarrow f_{i,jk} = f_{i,kj} = -f_{k,ij} = -f_{k,ji} = f_{j,ki} = f_{j,ik} = -f_{i,jk} = 0,$$

so the general solution is $f(x) = Ax + b$ for $A \in \mathfrak{so}(n)$, $b \in \mathbb{R}^n$.

Therefore, one should understand the relationship between the G and the dimension of \mathfrak{G} . It depends on the *order* of the Lie algebra \mathfrak{g} of G , essentially the highest degree in the power series of a vector field in \mathfrak{X} which is not determined by the terms of lower degree. The calculation above shows that $\mathfrak{so}(n)$ has degree 1. It turns out that \mathfrak{g} has infinite order if it contains an element of rank one; this simplifies the classification of the infinite-dimensional \mathfrak{G} a good deal. If the order of \mathfrak{g} is finite, or if it is infinite but \mathfrak{g} has no element of rank one (complex matrix Lie algebras being the main example) and M is compact, then \mathfrak{G} is a finite-dimensional Lie group [14].

Cartan developed a structure theory of Lie pseudogroups and gave a classification of the complex primitive infinite-dimensional Lie pseudogroups, finding 6 classes [5]. In the 1960s, gaps in his proof were discovered which were rectified by Singer and Sternberg [33], allowing a complete proof by Guillemin, Quillen, and Sternberg [11]. Their method allowed the classification of the real pseudogroups by Shnider [32]. Amazingly, on any real manifold M there are only 14 possible classes of such pseudogroups; the assumptions of locality reduce everything to the consideration of groups of formal power series. The key reference for diffeomorphism groups is Kobayashi [14], although it predates the modern work on the classification. There is very little in print since the 1960s that refers to the classification. It seems that since limited progress was being made on the nontransitive case, interest in the general theory waned; research has focussed instead on the analytic and group-theoretic properties of the classical diffeomorphism groups [1, 29].

We give the classification here briefly, and outline how each case (and three important families of nonprimitive subgroups) arises in geometric integration. In each case it is crucial to consider whether the structure is presented in its local canonical form, the general form being usually much harder to preserve in an integrator. In Sections 3 and 4 we consider the conformal symplectic and conformal volume preserving Lie pseudogroups in more detail, providing \mathfrak{G} -integrators and evidence of their usefulness for these dissipative systems.

Our integrators are based on splitting and composition [18, 38]. In the simplest instance of this technique one writes $f = \sum f_i$ as a sum of vector fields (possible here since $f \in \mathfrak{X}$, a linear space) with simple flows, and lets $\varphi_\tau = \prod_i \exp(\tau f_i)$, a first-order \mathfrak{G} -integrator with time step τ . Then the order can be increased by composition: $\psi_\tau = \varphi_{\tau/2} \varphi_{-\tau/2}^{-1}$ is a second-order \mathfrak{G} -integrator and $\psi_{\alpha\tau}^n \psi_{(1-2n\alpha)\tau} \psi_{\alpha\tau}^n$ ($n \geq 1$, $\alpha = 1/(2n - (2n)^{1/3})$) is a 4th-order \mathfrak{G} -integrator. Note that $1 - 2n\alpha < 0$, so the central stage involves integrating the vector fields f_i backwards in time. The use of negative time steps is unavoidable if one wants a composition of flows to have order greater than 2, but it is not a problem here since $\exp(\tau f_i)$ and $\exp(-\tau f_i)$ both lie in \mathfrak{G} . (It *is* a problem if the set of dynamical systems under consideration forms only a semigroup and not a group.) Therefore the conformal symplectic and conformal volume preserving systems provide rare examples of dissipative systems for which high-order composition methods can be used.

2 The primitive infinite-dimensional pseudogroups

A primitive infinite-dimensional pseudogroup \mathfrak{G} on a real manifold M must be one of the following.

1. $\mathfrak{G} = \text{Diff}(M)$, the pseudogroup of all local diffeomorphisms of M . Almost any one-step integrator lies in \mathfrak{G} , provided the time step is small enough and depends smoothly on x .
2. $\mathfrak{G} = \text{Diff}_{\text{Sp}}(M)$, the local diffeomorphisms preserving a symplectic 2-form ω . Its Lie algebra consists of the locally Hamiltonian vector fields, X such that $i_X \omega$ is closed. \mathfrak{G} -integrators are called symplectic integrators. They have only been generally constructed in two cases, when ω is the canonical symplectic 2-form on \mathbb{R}^n and when M is a coadjoint orbit of a Lie algebra (Lie-Poisson integrators [10]). To further classify these pseudogroups depends on classifying the symplectic forms on M , which is an open problem.
3. $\mathfrak{G} = \text{Diff}_{\text{Vol}}(M)$, the local diffeomorphisms preserving a volume form μ on M . Its Lie algebra consists of the divergence-free vector fields, X such that $\text{div}_\mu X = 0$. If M is compact, then all volume forms are equivalent up to a constant [25]. Volume-preserving integrators have been considered both in the canonical case $M = \mathbb{R}^n$, $\mu = dx_1 \dots dx_n$ [9], and in the general case [30].
4. $\mathfrak{G} = \text{Diff}_{\text{Contact}}(M)$, the local diffeomorphisms preserving a contact 1-form α up to a scalar function. Contact integrators for the canonical case $\alpha = dx_0 + \sum x_{2i} dx_{2i+1}$ have been constructed by Feng [8]. A non-canonical example is provided by a Hamiltonian vector field restricted to an energy surface;

the theorem of Ge [10] on energy-symplectic integrators shows that we should not expect to be able to construct \mathfrak{G} -integrators in this case.

5. $\mathfrak{G} = \text{Diff}_{\text{CSp}}(M)$, the local diffeomorphisms preserving a symplectic form ω up to a constant multiple. That is, $\varphi^*\omega = c_\varphi\omega$, where the constant c_φ depends on $\varphi \in \mathfrak{G}$. We study ODEs and integrators for this *conformal symplectic* pseudogroup in Section 4.
6. $\mathfrak{G} = \text{Diff}_{\text{CVol}}(M)$, the local diffeomorphisms preserving a volume form μ up to a constant multiple. That is, $\varphi^*\mu = c_\varphi\mu$, where the constant c_μ depends on $\varphi \in \mathfrak{G}$. We study this *conformal volume preserving* case in Section 3.
- 7–12. When M also has a complex structure, there are the pseudogroups obtained by considering the complex analytic local diffeomorphisms which also lie in one of the groups 1–6. We call these, e.g., $\text{CDiff}_{\text{CVol}}(M)$, the complex analytic local diffeomorphisms preserving a (real) volume form up to a (complex) constant. (There are also two new cases, which are subgroups of the conformal pseudogroups—see items 13 and 14.) If we require that the diffeomorphisms be globally defined, i.e., holomorphic, then these pseudogroups are finite-dimensional Lie groups when M is compact or when $M = \mathbb{C}$ and have been extensively studied [14]. On the other hand, $\text{CDiff}(\mathbb{C}^2)$ is infinite-dimensional, since it contains $x' = x, y' = y + f(x)$, $x, y \in \mathbb{C}$. Complex symplectic maps are occasionally studied [37].
13. $\mathfrak{G} = \text{CDiff}_{\text{CSp}'}(M)$, the complex analytic local diffeomorphisms preserving a real symplectic form up to a real multiple of $e^{ic_\varphi z}$, where c_φ is a real constant depending on $\varphi \in \mathfrak{G}$, and z is a complex constant independent of φ .
14. $\mathfrak{G} = \text{CDiff}_{\text{CVol}'}(M)$, the complex analytic local diffeomorphisms preserving a real volume form up to a real multiple of $e^{ic_\varphi z}$, where c_φ is a real constant depending on $\varphi \in \mathfrak{G}$, and z is a complex constant independent of φ .

The theory of dynamical systems mostly studies Diff (general invertible dynamics), CDiff (some complex dynamics), Diff_{Sp} (Hamiltonian dynamics), and Diff_{Vol} (volume-preserving dynamics). In particular, conformal dynamics, which can be dissipative, is not widely studied in its own right. (One reference is [26], which classifies the quadratic conformal symplectic maps.) Nevertheless, these systems have some interesting features that are not shared by nearby systems, whose preservation can lead to superior integrator performance.

When M is a complex manifold, $\text{Diff}(M)$ has only 6 primitive infinite-dimensional subgroups, namely items 7–12 above. Cases 13 and 14 are excluded because the 2-parameter subgroup $\{\exp(tX) : t \in \mathbb{C}\}$ must be in \mathfrak{G} when M is complex; but when M is a real manifold with a complex structure, we only need that $\{\exp(tX) : t \in \mathbb{R}\} \subset \mathfrak{G}$, which it is in these cases.

3 Conformal volume-preserving dynamics

Let μ be a volume element on a manifold M . We wish to study the vector fields X whose local time- t flow lies in $Diff_{CVol}(M)$. That is,

$$\exp(tX)^*\mu = c(t)\mu.$$

(See, e.g., [17] for the notation.) Differentiating with respect to time,

$$\dot{c}(0)\mu = \mathfrak{L}_X\mu := (\operatorname{div}_\mu X)\mu = di_X\mu + i_Xd\mu = di_X\mu$$

Therefore, $\operatorname{div}_\mu X = \dot{c}(0)$ must be constant, and if $\dot{c}(0) \neq 0$, μ must be exact, which we now assume. (In particular, M cannot be compact.) Let $\mu = d\alpha$ and let X_c be the unique solution of $i_{X_c}\mu = \alpha$. Then $X = X_0 + cX_c$, where $\operatorname{div}_\mu X_0 = 0$ and $\operatorname{div}_\mu X_c = 1$. We can write

$$i_{X_0}\mu = d\beta + [\gamma],$$

where β is an $n - 2$ -form and $[\gamma] \in H^{n-1}(M)$.

On \mathbb{R}^n with the Euclidean volume form, this gives a representation of the constant-divergence vector fields as, e.g.,

$$\begin{aligned} X &= X_0 + X_c \\ &= \sum_i \left(\sum_j \frac{\partial \beta_{ij}}{\partial x_j} - \frac{c}{n} x_i \right) \frac{\partial}{\partial x_i}, \end{aligned} \tag{1}$$

where $\beta_{ij}(x) = -\beta_{ji}(x)$. This is a natural representation if we wish to construct geometric integrators using splitting and composition, because the dissipative part X_c can be integrated exactly. The divergence-free part can be integrated by any volume-preserving integrator, e.g. by splitting. This approach has the advantage that volume evolves at exactly the correct rate.

The group property directly confers a major advantage on \mathfrak{G} -integrators. Namely, any composition of flows, even for negative time steps, lies in the group. This is essential in attaining orders higher than 2. For contrast, for general dissipative systems (e.g. those that contract volume [22] or have a Lyapunov function), this is not possible: the dynamics lie only in a semigroup, which is left by negative time steps.

The two most famous conformal volume-preserving dynamical systems are the Lorenz system in \mathbb{R}^3 and the Hénon map in \mathbb{R}^2 . Their conformal property has often been remarked on and used in studies (see, e.g., [16]). For example, it implies that the sum of the Lyapunov exponents is equal to $\operatorname{div}_\mu X$, which can be used as a check on a calculation or to avoid calculating all exponents. A system which contracts some volume element cannot have a completely unstable fixed point (one with $\dim W^u = n$), a topological invariant of this class of systems. However, the conformal property is not believed to be a decisive factor in controlling the dynamics in the way that volume preservation itself is. The volume contraction is so strong that all nearby systems may have similar dynamics. Even if this is true, there can still be an advantage in preserving the same structure preserved by the actual flow. $Diff_{CVol}(M)$ has infinite codimension in $Diff(M)$ and staying in it may confer some advantage.

To examine this question, we have calculated the Lyapunov exponents of the Lorenz attractor using geometric and non-geometric integrators. The phase space

is \mathbb{R}^3 with coordinates (x, y, z) , and the system is (using a different splitting from Eq. (1))

$$\begin{aligned} \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} &= X_c + X_0 \\ &= \begin{pmatrix} -\sigma & \sigma & 0 \\ r & -1 & 0 \\ 0 & 0 & -b \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ -xz \\ xy \end{pmatrix} \end{aligned}$$

Here X_0 is in fact a Poisson system with Hamiltonian $y^2 + z^2$ and Casimir x ; its flow is a rotation in the y - z plane. X_c is linear and can be integrated exactly. We consider the \mathfrak{G} -integrator

$$\varphi_\tau = \exp(\tau X_0) \exp(\tau X_c)$$

where τ is the time step. This is only a first order method, but because it is smoothly conjugate to the second-order leapfrog method,

$$\exp(-\frac{1}{2}\tau X_0) \varphi_\tau \exp(\frac{1}{2}\tau X_0) = \exp(\frac{1}{2}\tau X_0) \exp(\tau X_c) \exp(\frac{1}{2}\tau X_0),$$

it yields $\mathcal{O}(\tau^2)$ estimates of the Lyapunov exponents. (This feature alone strongly recommends the geometric integrator.) We regard $\varphi_\tau : x_k \mapsto x_{k+1}$ as a given map with known derivative A_k whose exponents are to be calculated. Note that $\det A_k = \exp(\tau(-\sigma - 1 - b)) =: e^{\tau c}$, as for the exact flow. We use the discrete QR method [7] for calculating the exponents [7]. Let $Q_0 \in SO(n)$ and

$$Q_{k+1}R_{k+1} = A_k Q_k, \quad k = 0, 1, 2, \dots,$$

where the left hand side is the QR -factorization of the right hand side. Then the Lyapunov exponents are given by

$$\sigma_i = \lim_{k \rightarrow \infty} \frac{1}{k} \sum_{j=1}^k \ln(R_j)_{ii}.$$

Since $\det Q_k = \det Q_{k+1} = 1$, we have $\det R_{k+1} = \det A_k = e^{\tau c}$. Thus, at each time step the expansion rates $(R_k)_{ii}$ have exactly the correct product, and the estimates of the Lyapunov exponents on any finite time interval have exactly the correct sum c .

For a non-geometric method, we used the second-order Taylor series method [12]. Its discretization error was found to be roughly comparable to that of the geometric leapfrog method on the attractor.

The errors due to the necessary finite-time cutoff are estimated by dividing the samples into (e.g. 10) segments and computing the standard deviation of the estimates on each segment. The sample interval can be chosen long enough to avoid short-time correlations, but the complicated long-time nature of the time series make it difficult to get more sophisticated error estimates. For the 'classical' Lorenz parameters we can compare to the calculation of Sprott [34], which is accurate to 3 significant figures. We also tested another set of parameters, those used in [7].

The results are shown in Table 3. Both methods give second order accurate exponents, but the geometric method

Table 1: Calculation of the Lyapunov exponents of the Lorenz attractor. The total integration time is T , the time step is τ ; estimated finite- T errors in the final digits are shown in parenthesis.

Method	T	τ	σ_1	σ_2	σ_3
(a) $\sigma = 10, r = 28, b = 8/3$ (classical case)					
Sprott [34]			0.906	0	-14.572
\mathfrak{G} -integrator: stable for $\tau < 0.12$, max. error $\sim 8\tau^2$					
	10^5	0.01	0.9060(4)	$-1(1) \times 10^{-5}$	-14.5726(4)
	5000	0.05	0.9264(20)	$7(50) \times 10^{-5}$	-14.5930(20)
Taylor series integrator: stable for $\tau < 0.033$, max. error $\sim 730\tau^2$					
	5000	0.01	0.9083(17)	$4(60) \times 10^{-5}$	-14.4997(17)
(b) $\sigma = 16, r = 40, b = 4$					
Dieci et al. [7]			1.36006	0.00570	-22.36576
\mathfrak{G} -integrator: stable for $\tau < 0.075$, max. error $\sim 34\tau^2$					
	5000	0.01	1.3742(30)	0.0020(20)	-22.3763(30)
	5000	1/30	1.4089(30)	0.0004(20)	-22.4092(30)
Taylor series integrator: stable for $\tau < 0.017$, max. error $\sim 2900\tau^2$					
	5000	0.01	1.3799(20)	0.0001(4)	-22.0816(20)

- (i) takes 0.66 of the time per time step;
- (ii) is stable for time steps up to 4 times larger; and
- (iii) computes exponents with errors about 1% the size

compared to the Taylor series method. That is, its effective error constant is about 0.0066 that of the Taylor series method, or, it runs about 12 times faster for the same error. The sampling errors are not reduced, so that long runs are still required for accurate exponents.

This example does not fully test the structural stability of conformal volume preserving dynamics. In particular, such systems in \mathbb{R}^3 have only one independent Lyapunov exponent σ_1 ; the others are $\sigma_2 = 0$ and $\sigma_3 = c - \sigma_1$. However, the numerical evidence is very strong and suggests that, e.g., the errors in the largest negative exponent reported in [7] may be due to the integrator and not to the method of computing the exponents themselves.

4 Conformal symplectic dynamics

One finds the vector fields as in the last section. Let ω be a symplectic 2-form on a manifold M . We wish to study the vector fields X whose local time- t flow lies in

$Diff_{\text{Sp}}(M)$. That is,

$$\exp(tX)^*\omega = c(t)\omega.$$

Differentiating with respect to time,

$$\dot{c}(0)\omega = \mathcal{L}_X\omega = di_X\omega + i_Xd\omega = di_X\omega$$

Therefore, if $\dot{c}(0) \neq 0$, $\omega = -d\theta$ must be exact, which we now assume. (As before, M cannot be compact.) If also $H^1(M) = 0$, then all conformal Hamiltonian vector fields can be defined by

$$i_X\omega = dH + c\theta$$

for some ‘‘Hamiltonian’’ function H and some constant c . (We have chosen the signs here so that $c > 0$ corresponds to dissipation in simple mechanical systems.) On any M we can write $X = X_0 + cX_c$, where X_0 is locally Hamiltonian and X_c is a fixed vector field satisfying $i_{X_c}\omega = \theta$. Notice, however, that $\dot{H} = ci_X\theta$ need not be zero, and in fact can change sign.

In the canonical case, $M = \mathbb{R}^{2n}$, $\theta = pdq$, $\omega = dq \wedge dp$, giving the conformal Hamiltonian system

$$\dot{q} = H_p, \quad \dot{p} = -H_q - cp. \quad (2)$$

For $H = \frac{1}{2}\|p\|^2 + V(q)$, these are mechanical systems with linear dissipation. (The conformal nature of such systems, and the symmetry of their Lyapunov exponents, was studied in [6].) This is a special case of Rayleigh dissipation, for which $\dot{p} = -H_q - cR(q)p$ where $R(q)$ specifies a Riemannian metric on the configuration space. So to obtain a conformal system, this metric must be compatible with the symplectic structure. We suspect that, since this form of dissipation is special mathematically (forming a Lie pseudogroup), it must be special physically too.

For the general conformal Hamiltonian system (2), the energy obeys $\dot{H} = -cp^t H_p$ which can have any sign. The system can have a ‘‘conformal symplectic attractor’’ analogous to the Lorenz attractor. For simple mechanical systems, however, $H = \frac{1}{2}\|p\|^2 + V(q)$, and $\dot{H} = -c\|p\|^2 \leq 0$. The energy becomes a Lyapunov function and all orbits tend to fixed points.

The eigenvalues of the Jacobian of X (and hence the Lyapunov exponents of X) occur in pairs with sum $-c$; the spectrum is constrained to the same degree as that of Hamiltonian systems. Consider an invariant set (fixed point, periodic orbit etc.) with stable manifold W^s and unstable manifold W^u . Their dimensions obey

$$\dim W^s \begin{cases} \leq \dim W^u & \text{for } c > 0, \\ \geq \dim W^u & \text{for } c < 0, \\ = \dim W^u & \text{for } c = 0. \end{cases} \quad (3)$$

Since these dimensions are invariant under homeomorphisms, the inequality (3) is a topological invariant. A system in which one of these three conditions did not hold for all invariant manifolds could not be conformal symplectic. Conformal symplectic systems also have characteristic properties in the presence of symmetries (see Section 4.2). We do not have a complete characterisation of their dynamics, however; in particular, it is not clear whether the flow on a strange attractor is influenced by the symplectic structure beyond merely having its dimension bounded.

As before, geometric integrators can be constructed by splitting: X_c can be integrated exactly, and a symplectic integrator applied to X_0 . Alternatively, since X_c is

linear, one can split off the entire linear part of X and integrate it exactly. As with conformal volume preserving systems, the order can be increased by composition.

Interestingly, the symplectic Runge-Kutta methods are not conformal symplectic, as the following example illustrates.

Example 7 Consider a linear canonical 4-dimensional system with $H = \frac{1}{2}(q_1^2 + p_1^2)$ and let the map φ be the midpoint rule with time step 2τ . The map φ is linear and one can calculate

$$\varphi^* \omega \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial p_1} \right) = \frac{1 + c\tau + \tau^2}{1 - c\tau + \tau^2}$$

and

$$\varphi^* \omega \left(\frac{\partial}{\partial q_2}, \frac{\partial}{\partial p_2} \right) = \frac{1}{1 - c^2\tau^2}.$$

The integrator φ is conformal symplectic iff these two are equal for all τ , which is true iff $c = 0$.

4.1 Calculation of Lyapunov exponents

For a numerical example we consider two linearly repelling Duffing oscillators,

$$\left. \begin{aligned} \dot{q}_i &= p_i \\ \dot{p}_i &= q_i - q_i^3 + \beta_i(q_1 - q_2) + \gamma \cos t - cp_i \end{aligned} \right\} i = 1, 2$$

where $\beta_1 = -\beta_2 := \beta > 0$. The time- 2π flow of the system is a conformal symplectic map. For small values of β the attractor is only slightly perturbed from the attractor of the standard $\beta = 0$ Duffing oscillator. As β increases an interesting new state appears in which one oscillator traces out a motion close to the $\beta = 0$ attractor, while keeping the second at arms length. This state has a single positive Lyapunov exponent, suggesting that the second oscillator is slaved to the first. (Although, from the symmetry of the problem, the two can change places.) We took $\gamma = 0.5$, $\beta = 0.1$, $c = 0.25$ and calculated the Lyapunov exponents of this state using geometric and nongeometric integrators.

As before, the geometric integrator is the standard composition $\exp(\tau A)\exp(\tau B)$, where now A contains all the linear terms (including the damping), and B contains only the nonlinear potential, with frozen time. It leads to second order estimates of the exponents. The nongeometric integrator is the second order Taylor series method, which has truncation errors about the same size as the geometric leapfrog method. We expect that other standard integrators give similar results.

We digress to discuss the calculation of Lyapunov exponents σ_i for (conformal) symplectic maps. Recall that these should have constant pairwise sums, and since the QR -algorithm calculates them in descending order, we expect $\sigma_i + \sigma_{n+1-i} = -c$. Consider the first step $Q_1 R_1 = A_1 Q_0$. Here, A_1 is (conformal) symplectic, but there is no reason for R_1 to be, and hence the exponents need not sum correctly. Now the QR factorization corresponds to the Iwasawa decomposition of both of the Lie groups $GL(n)$ and $SL(n)$, and hence is appropriate for both general and (conformal) volume preserving systems, but *not* of $CSp(n)$ (the conformal symplectic matrices). The factors Q_1 and R_1 are not in $CSp(n)$. One should replace QR by the appropriate

Iwasawa factorization. For $CSp(n)$, this has $Q \in OSp(n)$, the orthosymplectic group. This was realized by the numerical linear algebra community long ago, who developed the *symplectic QR* method for finding the eigenvalues of symplectic matrices [4]. For the pure symplectic case, a corresponding symplectic Lyapunov exponent algorithm was developed in [15].

However, we have discovered an extremely convenient shortcut which allows one to still use the ordinary QR factorization. Namely, if we take

$$Q_0 = \begin{pmatrix} I & 0 \\ 0 & I^* \end{pmatrix}, \quad I_{ij}^* = \delta_{i,n+1-i}$$

then one can show that the factors Q_1 and R_1 are related to the (conformal) symplectic factors of the Iwasawa decomposition and that R_1 (conformally) preserves the modified symplectic structure $Q_0^* \omega$. (Not surprisingly, in this structure q_i is conjugate to p_{n+1-i} , which is consistent with QR producing exponents in descending order.) This remains true for all k . Thus, merely by choosing Q_0 appropriately, the computed exponents have exactly the correct symmetry for all time steps k . In practice, the sums $\sigma_i + \sigma_{n+1-i}$ remain constant and equal to $-c$ to within 10^{-15} for all k .

Finally, we can note that since the first $n/2$ columns of Q_0 coincide with those of the identity, the first $n/2$ exponents will be identical to those computed with $Q_0 = I$. Thus, it suffices to compute the first $n/2$ using the standard QR method, since we know they are the first half of a “correct” (conformal) symplectic set.

The numerical results are less dramatic than for the Lorenz attractor, but still significant. The geometric method takes 0.57 of the CPU time per time step and captures the attractor with 14 time steps per period (2π), whereas the nongeometric method requires 20. (For larger time steps, spurious stable periodic orbits are created, while for still larger time steps, the methods are unstable.) The Lyapunov exponents are $\sigma_1 = 0.1740$, $\sigma_2 = -0.1011$, $\sigma_3 = -0.1489$, and $\sigma_4 = -0.4240$, with a sampling error of about 8×10^{-4} . (Note that they sum in pairs to $-0.25 = -c$.) These are computed by the geometric method with a maximum error of 0.0063, and by the nongeometric method with a maximum error of 0.0423, at a time step of $2\pi/24$.

4.2 Symmetries

Let the Lie group G act on M . As we discussed above, a G -invariant vector field X will in general merely leave the foliation defined by the group orbits invariant, but in the Hamiltonian case there is another foliation, the level sets of the momentum map, which is actually fixed by X . We now show that when X is conformal Hamiltonian and G acts by cotangent lifts, this second foliation is still invariant, although no longer fixed. This extra structure is not shared by general dissipative systems.

We use notation and details of the momentum map which may be found in [17]. Further results, and a generalization to conformal Poisson systems, can be found in [19].

Proposition 1 *Let $M = T^*Q$ be a cotangent bundle with its canonical symplectic 1-form θ and 2-form $\omega = -d\theta$. Let the Lie group G act by cotangent lifts Φ_g ($g \in G$) on T^*Q , and let $H = H \circ \Phi_g$ be G -invariant. Let $J_\xi : T^*Q \rightarrow \mathbb{R}$ be the components of the momentum map for $\xi \in \mathfrak{g}$, the Lie algebra of G . Then the conformal Hamiltonian*

vector field X defined by $i_X\omega = dH + c\theta$ is G -invariant, and J_ξ obeys the differential equation $\dot{J}_\xi = -cJ_\xi$ for all $\xi \in \mathfrak{g}$.

Proof Using that the cotangent lift symmetry Φ_g^* preserves θ , we have

$$\Phi_g^* i_X \omega = i_{\Phi_g^* X} \Phi_g^* \omega = i_{\Phi_g^* X} \omega = \Phi_g^* (dH + c\theta) = dH + c\theta = i_X \omega$$

and by nondegeneracy of ω we have $\Phi_g^* X = X$, showing that X is invariant.

The components J_ξ of the momentum map are defined by $i_{\xi_x} \omega = dJ_\xi$ and obey $J_\xi = i_{\xi_x} \theta$ for cotangent lifts. (Here ξ_x is the vector field which generates the symmetry). Then the momentum equation is

$$\begin{aligned} \frac{d}{dt} J_\xi \circ \exp(tX) &= X(J_\xi) \\ &= i_X dJ_\xi \\ &= i_X i_{\xi_x} \omega \\ &= -i_{\xi_x} i_X \omega \\ &= -i_{\xi_x} (dH + c\theta) \\ &= 0 - cJ_\xi \end{aligned}$$

•

The momentum obeys $J_\xi(t) = e^{-ct} J_\xi(0)$, which allows a reduction to a smaller, nonautonomous system. Note that the proof relies crucially on Φ_g preserving θ , which is only true for cotangent lift symmetries.

Example 8 Consider a particle in \mathbb{R}^3 , with rotationally invariant Hamiltonian $H = \frac{1}{2}\|p\|^2 + V(\frac{1}{2}\|q\|^2)$. The equations of motion are

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -V'(\frac{1}{2}\|q\|^2)q - cp \end{aligned}$$

and one can check that the angular momentum $J = q \times p$ indeed obeys $\dot{J} = -cJ$.

A similar result, and hence reduction, holds true in the discrete case, i.e., for a symmetric \mathfrak{G} -integrator. In practice it is quite easy to preserve cotangent lift symmetries in the integrator, e.g., p - q splitting does this. The next proposition shows that such an integrator usually gets the values of the momentum exactly right.

Proposition 2 *Let the conformal symplectic map φ be equivariant with respect to the cotangent lift action Φ_g and obey $\varphi^* \omega = C\omega$. Then the foliations defined by the momentum map are invariant under φ . The momenta obey $J_\xi \circ \varphi = CJ_\xi + d$, where d is a constant.*

Proof We are given $\varphi \circ \Phi_g = \Phi_g \circ \varphi$, which implies $\varphi^* \xi_x = \xi_x$. With notation as in

the preceding proposition, we compute

$$\begin{aligned}
\mathcal{L}_{\xi_x} \varphi^* \theta &= di_{\xi_x}(\varphi^* \theta) + i_{\xi_x} d(\varphi^* \theta) \\
&= d\varphi^* i_{\xi_x} \theta - i_{\xi_x} \varphi^* \omega \\
&= d\varphi^* J_\xi - i_{\xi_x} C\omega \\
&= d(\varphi^* J_\xi - C J_\xi) \\
&= \mathcal{L}_{\varphi^* \xi_x} \varphi^* \theta \\
&= \varphi^* \mathcal{L}_{\xi_x} \theta \\
&= \varphi^* 0 \\
&= 0.
\end{aligned}$$

Therefore,

$$\varphi^* J_\xi = J_\xi \circ \varphi = C J_\xi + d.$$

•

The constant d is usually zero. For example, if φ is an integrator preserving the fixed points of the vector field X , then $J_\xi = 0$ at any fixed points (since $\dot{J}_\xi = -cJ_\xi$), implying $d = 0$. If φ is constructed by splitting off the dissipative part of X and solving it exactly, then $C = \exp(-\tau c)$ and the integrator achieves exactly the correct evolution of the momentum. In any event, if $d \neq 0$ then there is a nearby function $\tilde{J}_\xi = J_\xi + d/C$ which does obey $\tilde{J}_\xi \circ \varphi = C\tilde{J}_\xi$.

Another way to view conformal Hamiltonian systems, at least in the canonical case (2), is to make a time-dependent change of variables. Eq. (2) is Hamiltonian in the variables (q, \tilde{p}) where $\tilde{p} = e^{ct}p$ with respect to the nonautonomous Hamiltonian $\tilde{H}(q, \tilde{p}) = e^{ct}H(q, e^{-ct}\tilde{p})$.

5 Some nonprimitive pseudogroups

The largest nonprimitive Lie pseudogroup is one that just leaves a foliation invariant. If the codimension- k foliation is given by the level sets of the function $x : M \rightarrow \mathbb{R}^k$, then we can take local coordinates $x_1, \dots, x_k, y_1, \dots, y_{n-k}$ and write the diffeomorphisms in the form

$$\begin{aligned}
x &\mapsto f(x), \\
y &\mapsto g(x, y).
\end{aligned} \tag{4}$$

Each leaf is given by $L_x = \{x = \text{const}\}$. The foliate systems are precisely those that can be reduced to the space of leaves. This is a case when it is much easier to construct a \mathfrak{G} -integrator when the structure is in its local canonical form! This pseudogroup has a large variety of subpseudogroups which have not been classified. We consider some examples.

Example 9 The Lie pseudogroup

$$\{x \mapsto f(x), y \mapsto g(y)\} \cup \{x \mapsto f(y), y \mapsto g(x)\}$$

shows that \mathfrak{G} need not be connected. In fact, if M is orientable then $\text{Diff}(M)$ itself is not connected. Its identity component consists of the orientation-preserving maps, but this is not of Lie type.

\mathfrak{G} can be restricted to the space of leaves of the foliation (giving the map $x \mapsto f(x)$ in Eq. (4)). This restriction may be one of the primitive Lie pseudogroups or may itself preserve a foliation. Continuing in this way, we get a recursive decomposition of \mathfrak{G} . One limiting case is the pseudogroup on \mathbb{R}^n ,

$$x_i \mapsto f_i(x_1, \dots, x_i), \quad i = 1, \dots, n,$$

the (local) diffeomorphisms whose derivative lies in the Lie algebra of lower triangular matrices. However, descending to sub-foliations is only part of the story, because the maps *on* the leaves ($y \mapsto g(x, y)$ in Eq. 4) may have structure of their own. Part of it can be studied by freezing x (the leaf) and looking at the structure of the diffeomorphisms $\varphi_x : L_x \rightarrow L_{f(x)}$.

Example 10 The pseudogroup of diffeomorphisms of the form

$$x \mapsto f(x), \quad y \mapsto g(x, y), \quad z \mapsto h(x, y)z$$

leaves the foliation $x = \text{const.}$ invariant. Freezing x , the leaf maps themselves leave the second foliation $(x, y) = \text{const.}$ invariant. The leaf maps on the second foliation, namely $z \mapsto h(x, y)z$, have additional structure: freezing (x, y) , they are linear in z , i.e., they belong to the 1-dimensional Lie pseudogroup $GL(1)$.

Apart from the maps on the space of leaves, and the maps on the leaves themselves, the maps on the whole space can have further structure, describing how the maps on the leaves vary from leaf to leaf.

Example 11 The pseudogroup of diffeomorphisms of the form

$$x \mapsto f(x), \quad y \mapsto g(y)$$

leaves the foliation $x = \text{const.}$ invariant, while the maps on the leaves $x = \text{const.}$, namely $y \mapsto g(y)$, are independent of the leaf. In the pseudogroup of diffeomorphisms of the form

$$x \mapsto f(x), \quad y \mapsto \frac{\partial f}{\partial x}(x)y,$$

not only are the maps on the leaves linear, they are related to the maps on the space of leaves.

Although there is no complete classification, identifying any pseudogroup \mathfrak{G} to which a flow belongs does provide important information. The nonprimitive Lie pseudogroups can be organised by

- (i) the primitive Lie pseudogroup of which \mathfrak{G} is a subset;
- (ii) the Lie pseudogroup of \mathfrak{G} restricted to the space of leaves;
- (iii) the Lie pseudogroup of \mathfrak{G} restricted to each leaf; and
- (iv) their structure transverse to the leaves.

We describe three classes of nonprimitive Lie pseudogroups which arise frequently in dynamical systems.

1. Systems leaving a foliation invariant.
2. Systems with a continuous symmetry. Let the Lie group G act on M . Then the G -equivariant maps leave the foliation defined by the group orbits of G invariant. The maps between the leaves are called the *reduced* dynamics, while the maps on the leaves are called the *reconstruction*. If the action is free then each leaf is isomorphic to G and the maps on the leaves are G -equivariant. At the Lie algebra level, we have ODEs of the form

$$\begin{aligned} \dot{x} &= f(x), \quad x \in M/G && \text{(the reduced dynamics)} \\ \dot{y} &= g(x)y, \quad y \in G, g \in \mathfrak{g} && \text{(the reconstruction equations)} \end{aligned} \tag{5}$$

If we can integrate on M/G , the reduced dynamics can be integrated by any appropriate \mathfrak{G} -integrator, and the reconstruction equations by a Lie group integrator.

3. Systems leaving a foliation fixed, i.e. systems with integrals. (The functions whose level sets define the foliation are first integrals.) \mathfrak{G} -integrators, those that preserve a given set of first integrals, are studied in [23, 31]. Another example is provided by Poisson systems, whose flow fixes the symplectic leaves and is symplectic on them. \mathfrak{G} -integrators are only known in the special cases of constant or Lie-Poisson structure.

Hamiltonian systems with symmetry provide examples of all of these cases. The symmetry alone lets one reduce to equations of the form (5). The symplectic structure then guarantees that the reduced dynamics are Poisson, and have first integrals given by the Casimirs of the reduced Poisson bracket and by the energy. The symplectic structure also provides the reconstruction equations with further integrals. Alternatively, one can introduce the momentum map $J : M \rightarrow \mathfrak{g}^*$ and split the system into three parts,

$$\begin{aligned} \dot{J} &= 0 && \text{(the first integrals)} \\ \dot{x} &= f(J, x), \quad x \in J^{-1}(\mu)/G_\mu && \text{(the reduced, Hamiltonian dynamics)} \\ \dot{y} &= g(J, x)y, \quad y \in G_\mu, g \in \mathfrak{g}_\mu && \text{(the reconstruction equations)} \end{aligned}$$

where G_μ is the isotropy subgroup of $\mu \in M$ and \mathfrak{g}_μ its Lie algebra.

We know no way of telling when a given system preserves some (unknown) foliation. However, the systems foliate with respect to a Lie group action do have an elegant structure, which is used to construct \mathfrak{G} -integrators in [20].

Once the pseudogroup structure of equations such as these is known, one can determine the best approach for constructing \mathfrak{G} -integrators in each case. This is not necessarily by carrying out the reductions analytically: in [24], for example, integrators for the case $M = T^*G$ are applied to the simpler, unreduced equations, which do however stay in the appropriate pseudogroup.

Finally, all of the above Lie pseudogroups have infinite-dimensional subpseudogroups which are not of Lie type, i.e. are not defined by PDEs. For, let \mathfrak{G} be a Lie pseudogroup, G a discrete group acting on M , and consider the G -equivariant maps, $\mathfrak{G}_G := \{\varphi \in \mathfrak{G} : \varphi \circ g = g \circ \varphi \ \forall g \in G\}$. \mathfrak{G}_G is primitive if \mathfrak{G} is. It can be transitive unless there are points in M fixed under all of G , for the set of such points must be

invariant under \mathfrak{G}_G . One can consider classifying the pseudogroups of G -equivariant diffeomorphisms on M by passing to the quotient M/G , an orbifold, although this is not in general a manifold so the preceding classification does not apply directly.

6 Remarks

Let us review the kinds of dynamics—i.e., the pseudogroups of local diffeomorphisms—for which geometric integrators are known. In all cases, this depends on whether the manifold is simple (e.g. \mathbb{R}^n) and the geometric structure (e.g. symplectic structure, foliation, etc.) is presented in its local canonical form. If it is not, then in most cases geometric integrators are not known. For example, it is not known how to preserve an arbitrary symplectic structure, or canonical symplectic structure together with an arbitrary symmetry.

On the other hand, \mathfrak{G} -integrators are known for each of the 14 primitive Lie pseudogroups listed in Section 2 when presented in their canonical form. In Sections 3 and 4 we have given \mathfrak{G} -integrators for $\mathfrak{G} = \text{Diff}_{\text{CVol}}$ and $\mathfrak{G} = \text{Diff}_{\text{CSp}}$, respectively, based on splitting off the dissipative part; a similar method works for cases 13 and 14, $\text{CDiff}_{\text{CVol}}$ and $\text{CDiff}_{\text{CSp}}$. \mathfrak{G} -integrators for the complex cases are provided simply by expressing the integrators in complex variables.

Developing geometric integrators for the nonprimitive pseudogroups, on more general manifolds, with possibly non-canonical structures, remains a problem for the future. Even the dynamics of systems in many of these groups has not yet begun to be studied.

We close with some further remarks.

1. We expect the use of geometric integrators for the conformal cases to be particularly useful when the dissipation rate c is small; in particular, for studying the limit $c \rightarrow 0$.
2. If the dissipation rate depends on time, the flow still lies in the conformal pseudogroup. If the dissipation rate is periodic with mean zero, then the one-period map is symplectic or volume preserving, but may be best computed with a conformal geometric integrator.
3. What is the difference between the dynamics of systems in $\text{Diff}_{\text{CVol}}$ (resp. Diff_{CSp}) and nearby systems? One topological invariant of conformal volume preserving systems is that they cannot contain both sources and sinks, for a source implies that the conformal constant c is positive, while a sink implies that it is negative.
4. A theory of conformal symplectic reduction is developed in [19], the system dropping to a Poisson manifold whose leaves are permuted by the reduced flow. The local flows of these conformal Poisson systems form a natural example of a nonprimitive pseudogroup.
5. Instead of continuous groups (both in the finite-dimensional case and in the infinite-dimensional case), one can study *symmetric spaces*, sets of diffeomorphisms closed under the symmetric product $\varphi\psi^{-1}\varphi$, systems with a reversing

symmetry being the main example. Their classification is an extension of the classification of Lie groups [27].

6. What are the applications of the complex pseudogroups?
7. Integrators for systems on Lie groups and homogeneous spaces provide \mathfrak{G} -integrators in two different cases, in both of which M is a homogeneous space: (i) in the nonlinear case, for $\mathfrak{G} = \text{Diff}(M)$ [28]; and (ii) in the nonautonomous linear case, for $\mathfrak{G} = G$, a finite-dimensional Lie group [13]. The latter is particularly important from the point of view of reproducing qualitatively correct dynamics, since \mathfrak{G} is so small. It remains to be seen whether these integrators can be extended to other infinite-dimensional pseudogroups.

Acknowledgements

We thank Hans Munthe-Kaas for alerting us to the Cartan classification, and thank Stig Faltinsen, Victor Guillemin, Arieh Iserles, Per Christian Moan, Matthew Perlmutter, and Olle Stormark for their useful comments. Proposition 1 is due to Matthew Perlmutter. We thank the MSRI (Berkeley, 1998) and the NZMRI (Kaikoura, 2000) for providing a stimulating environment, and the Australian Research Council and the Marsden Fund of the Royal Society of New Zealand for financial support. MSRI wishes to acknowledge the support of the NSF through grant no. DMS-9701755.

References

- [1] A. Banyaga, *The structure of classical diffeomorphism groups*, Mathematics and its Applications 400, Kluwer, Dordrecht, 1997.
- [2] P. Bochev and C. Scovel, On quadratic invariants and symplectic structure, *BIT* **34** (1994), pp. 337-345.
- [3] C. J. Budd and A. Iserles, eds., Geometric integration: numerical solution of differential equations on manifolds, *R. Soc. Lond. Philos. Trans. A* **357**(1754) (1999), 943-1133.
- [4] A. Bunse-Gerstner, Matrix factorizations for symplectic QR-like methods, *Lin. Alg. Appl.* **83** (1986), 49-77.
- [5] E. Cartan, Les groupes de transformation continus, infinis, simples, *Ann. Sci. Ecole Norm. Sup.* **26** (1909), 93-161; *Œuvres Complète d'Elie Cartan*, Springer-Verlag 1984.
- [6] U. Dessler, Symmetry property of the Lyapunov spectra of a class of dissipative dynamical systems with viscous damping, *Phys. Rev. A* **38** (1988), 2103.
- [7] L. Dieci, R. D. Russell, and E. S. van Vleck, On the computation of Lyapunov exponents for continuous dynamical systems, *SIAM J. Numer. Anal.* **34** (1997), 402-423.
- [8] K. Feng, Contact algorithms for contact dynamical systems, *J. Comput. Math.* **16** (1998), 1-14.
- [9] K. Feng and D.-L. Wang, Dynamical systems and geometric construction of algorithms, in *Contemporary Mathematics* 163, pp. 1-32, AMS, Providence, 1994.
- [10] Ge, Z., and J. Marsden, Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators, *Phys. Lett. A* **133** (1988), 135-139.
- [11] V. Guillemin, D. Quillen, and S. Sternberg, The classification of the complex primitive infinite pseudogroups, *Proc. Nat. Acad. Sci.* **55** (1966) 687-690;
- [12] E. Hairer, S.P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations I*, Springer-Verlag, 1993.

- [13] A. Iserles and S. P. Nørsett, On the solution of linear differential equations in Lie groups, *Phil. Trans. Roy. Soc. A* **357** (1999), 983–1020.
- [14] S. Kobayashi, *Transformation Groups in Differential Geometry*, Springer, 1972.
- [15] B. J. Leimkuhler and E. S. van Vleck, Orthosymplectic integration of linear Hamiltonian systems. *Numer. Math.* **77** (1997), no. 2, 269–282.
- [16] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion*, Springer-Verlag, New York, 1983.
- [17] J. E. Marsden and T. S. Ratiu, *Introduction to mechanics and symmetry*, 2nd ed., Springer, New York, 1999.
- [18] R. I. McLachlan, On the numerical integration of ordinary differential equations by symmetric composition methods, *SIAM J. Sci. Comput.* **16** (1995), pp. 151–168.
- [19] R. I. McLachlan and M. Perlmutter, Conformal Hamiltonian Systems, *J. Geom. Phys.*, to appear.
- [20] R. I. McLachlan, M. Perlmutter, and G. R. W. Quispel, Lie group foliate integrators, in preparation.
- [21] R. I. McLachlan and G. R. W. Quispel, Six Lectures on Geometric Integration, *Foundations of Computational Mathematics* pages 155–210, R. DeVore, A. Iserles, and E. Süli, eds., Cambridge University Press, Cambridge, 2001.
- [22] R. I. McLachlan and G. R. W. Quispel, Numerical integrators that contract volume, *Appl. Numer. Math.* **34** (2000), 253–260.
- [23] R. I. McLachlan, G. R. W. Quispel, and N. Robidoux, Geometric integration using discrete gradients, *Phil. Trans. Roy. Soc. A* **357** (1999), 1021–1046.
- [24] R. I. McLachlan and C. Scovel, Equivariant constrained symplectic integration, *J. Non-linear Sci.* **5** (1995), 233–256.
- [25] J. Moser, On the volume elements on a manifold, *Trans. Amer. Math. Soc.* **120** (1965), 286–294.
- [26] J. Moser, On quadratic symplectic mappings, *Math. Z.* **216** (1994), 417–430.
- [27] H. Z. Munthe-Kaas, Yu. Nikolayevsky, G. R. W. Quispel, and A. Zanna, Applications of symmetric spaces and Lie triple systems in numerical analysis, in preparation.
- [28] H. Munthe-Kaas and A. Zanna, Numerical integration of differential equations on homogeneous manifolds, *Foundations of Computational Mathematics (Rio de Janeiro, 1997)*, 305–315, F. Cucker and M. Shub, eds., Springer, Berlin, 1997.
- [29] H. Omori, *Infinite-dimensional Lie groups*, Translations of Mathematical Monographs 158, AMS, Providence, 1997.
- [30] G. R. W. Quispel, Volume-preserving integrators, *Phys. Lett. A* **206** (1995), 26–30.
- [31] G. R. W. Quispel and H. W. Capel, Solving ODE’s numerically while preserving a first integral, *Phys. Lett. A* **218** (1996), 223–228.
- [32] S. Shnider, Classification of the real infinite simple and real infinite primitive Lie algebras, *J. Diff. Geom.* **4** (1970), 81–89;
- [33] I. M. Singer and S. Sternberg, On the infinite groups of Lie and Cartan, I, *J. Analyse Math.* **15** (1965) 1–114.
- [34] J. C. Sprott, Lyapunov exponent and dimension of the Lorenz attractor, <http://sprott.physics.wisc.edu/chaos/lorenzle.htm>
- [35] Olle Stormark, *Lie’s Structural Approach to PDE Systems*, Cambridge University Press, Cambridge, 2000.
- [36] A.M. Stuart and A.R. Humphries, *Dynamical systems and numerical analysis*, Cambridge University Press, Cambridge, 1996.
- [37] Y. B. Suris, On the complex separatrices of some standard-like maps, *Nonlinearity* **7** (1994), 1225–1236.
- [38] H. Yoshida, Construction of higher order symplectic integrators, *Phys. Lett. A* **150** (1990), 262–268.