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Topics in structure-preserving discretization*

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In the last few decades the concepts of structure-preserving discretization, geometric integration and compatible discretizations have emerged as subfields in the numerical approximation of ordinary and partial differential equations. The article discusses certain selected topics within these areas; discretization techniques both in space and time are considered. Lie group integrators are discussed with particular focus on the application to partial differential equations, followed by a discussion of how time integrators can be designed to preserve first integrals in the differential equation using discrete gradients and discrete variational derivatives.

Lie group integrators depend crucially on fast and structure-preserving algorithms for computing matrix exponentials. Preservation of domain symmetries is of particular interest in the application of Lie group integrators to PDEs. The equivariance of linear operators and Fourier transforms on non-commutative groups is used to construct fast structure-preserving algorithms for computing exponentials. The theory of Weyl groups is employed in the construction of high-order spectral element discretizations, based on multivariate Chebyshev polynomials on triangles, simplexes and simplicial complexes.

The theory of mixed finite elements is developed in terms of special inverse systems of complexes of differential forms, where the inclusion of cells corresponds to pullback of forms. The theory covers, for instance, composite

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piecewise polynomial finite elements of variable order over polyhedral grids. Under natural algebraic and metric conditions, interpolators and smoothers are constructed, which commute with the exterior derivative and whose product is uniformly stable in Lebesgue spaces. As a consequence we obtain not only eigenpair approximation for the Hodge–Laplacian in mixed form, but also variants of Sobolev injections and translation estimates adapted to variational discretizations.

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1. Introduction

The solution of partial differential equations (PDEs) is a core topic of research within pure, applied and computational mathematics. Both measured in the volume of published work[1] and also in terms of its practical influence on application areas such as computational science and engineering, PDEs rank above all other mathematical subjects. Historically, the field of numerical solutions of PDEs has its roots in seminal papers by Richard Courant and his students Kurt Friedrichs and Hans Lewy, in the early twentieth century. Among the nearly 4000 academic descendants of Courant we find a large fraction of the key contributors to the field, such as Friedrichs' student Peter Lax, who received the Abel Prize in 2005 for his ground-breaking contributions to the theory and application of PDEs.

Fundamental properties of PDE discretizations, which have been recognized as crucial ever since the days of the Old Masters, include accuracy, stability, good convergence properties and the existence of efficient computational algorithms. In more recent years various aspects of structure preservation have emerged as important in addition to these fundamental properties.

[1] A count of all mathematical publications from 2001 to 2010, sorted according to the AMS Mathematics Subject Classification, reveals that number **35 PDEs** ranks highest of all primary topics with 46 138 entries; in second place is **62 Statistics**, with 39 176.

Within the topics of ordinary differential equations and time integration, a systematic study of structure-preserving discretizations was undertaken by Feng Kang in Beijing, starting in the 1980s. During the past decade a systematic study of the preservation of various geometric structures[2] has evolved into a mature branch of numerical analysis, termed the *geometric integration* of differential equations (Hairer, Lubich and Wanner 2006, Leimkuhler and Reich 2004, Sanz-Serna and Calvo 1994). Experience has shown that the preservation of geometric properties can have a crucial influence on the quality of the simulations. In long-term simulations, structure preservation can have a dramatic effect on stability and global error growth. Examples of such structures are symplecticity, volume, symmetry, reversibility and first integrals. In short-term simulations it is frequently seen that discretization schemes designed with structure preservation in mind enjoy small errors per step, and hence become efficient for shorter time simulations too. An important class of problems is that of partial differential equations whose solutions may be subject to blow-up in finite time. We have seen that schemes which are designed to inherit certain symmetries of the continuous problem tend to perform well in capturing such finite-time singularities in the solution.

For spatial PDEs, a parallel investigation of *compatible discretizations* has been undertaken (Arnold, Bochev, Lehoucq, Nicolaides and Shashkov 2006*a*). The equations of mathematical physics (describing fluids, electromagnetic waves or elastic bodies, for instance) have been presented in geometric language, easing the construction of discretizations which preserve important geometric features, such as topology, conservation laws, symmetries and positivity structures. When well-posedness of the continuous PDE depends on the conservation or monotonicity of certain quantities, such as energy, it seems equally important for the stability of numerical schemes that they enjoy similar properties. Rather than approximately satisfying the exact conservation law, as – it could be argued – any consistent scheme would do, it seems preferable, in order to obtain stable methods, to exactly satisfy a discrete conservation law. For PDEs written in terms of grad, curl and div acting on scalar and vector fields, one is led to construct operators acting on certain finite-dimensional spaces of scalar and vector fields, forming a complex which, in spatial domains with trivial topology, is an exact sequence. More generally, various discretizations of the de Rham sequence of differential forms have been introduced, and the successful ones are related to constructs of combinatorial topology such as simplicial cochain complexes (Arnold, Falk and Winther 2010).

[2] A geometric structure is understood as a structural property which can be defined independently of particular coordinate representations of the differential equations.

This survey paper takes a view of PDEs analogous to looking at the moon through a telescope with very high magnification. In the vast lunar landscape we will focus on a small number of craters with particularly beautiful properties, and leave the rest of the lunar surface out of our main focus.

One goal of the paper has been to tie together recent time integration techniques, in particular Lie group techniques and integral-preserving integration, and combine these with recent developments in structure-preserving spatial discretizations.

The paper consists of four main parts: Sections 2–5. Section 2 covers *integration methods based on Lie group techniques*. We provide an introduction to the theory of Lie group integrators and describe how computational algorithms can be devised, given a group action on a manifold and coordinates on the acting group. Various choices of coordinates are discussed. Another type of Lie group integrator consists of those based on compositions of flows, and we discuss some applications of these methods to the time integration of PDEs. We focus in particular on applications outside the class of exponential integrators for semilinear problems.

In Section 3 we discuss *integral-preserving schemes*. These methods apply to any PDE which has a known first integral, for instance an energy functional. We demonstrate how the method of discrete variational derivatives can be used to devise integral-preserving time integration schemes for PDEs. We consider, in particular, schemes that are linearly implicit, and therefore need the solution of only one linear system per time step. We also discuss methods which apply discrete variational derivatives, or discrete gradients, to conserve an arbitrary number of first integrals.

In Section 4 we cover *spatial symmetries*, *high-order discretizations* and *fast group-theoretic algorithms*. The topic of this section is the exploitation of spatial symmetries. A recurring theme is that of linear differential operators commuting with groups of isometries acting on the domain. We investigate high-order spectral element discretization techniques based on simplicial subdivisions (into triangles, tetrahedra and simplexes in general) using high-order multivariate Chebyshev bases on the triangles. The efficient computation of matrix (and operator) exponentials is crucial for time integrators based on Lie group actions. We survey recent work on high-order discretization techniques, fast Fourier algorithms based on group-theoretic concepts and fundamental results from representation theory.

In Section 5 we discuss *finite element systems for differential forms*. A framework for mixed finite elements is developed, general enough to allow for non-polynomial basis functions and a decomposition of space into non-canonical polytopes, but restrictive enough to yield spaces with local bases, interpolators commuting with the exterior derivative, and exact sequences where desirable. A smoothing technique gives L^q-stable commuting quasi-interpolation operators, from which various error estimates can be derived.

2. Integration methods based on Lie group techniques

The use of Lie group techniques for obtaining solutions to differential equations dates back to the Norwegian mathematician Sophus Lie in the second half of the nineteenth century. In Lie's time these were used exclusively as analytical tools; however, more recently it has become increasingly popular to include Lie groups as an ingredient in numerical methods. The use of Lie groups in the numerical approximation of differential equations can be divided into two categories: one in which the aim is to preserve symmetries or invariance of the continuous model, and another in which Lie groups are used as building blocks for a time-stepping procedure. In this section we shall give a brief introduction to the mathematical machinery we use, and we will focus on the second category, that of using Lie groups as a fundamental component when designing numerical time integrators. We shall give a short introduction to the basics of Lie group integrators; for more details consult Iserles, Munthe-Kaas, Nørsett and Zanna (2000) and Hairer *et al.* (2006). The variety of studies related to Lie group integrators is now too large to cover in an exposition of this type. For this reason we shall focus on a selected part of the theory, and mostly consider integrators designed for nonlinear problems. Important classes of schemes that we shall *not* discuss here are methods based on the Magnus expansions and Fer expansions, usually applied to linear differential equations. This work developed in the 1990s, in large part due to Iserles and Nørsett: see, *e.g.*, Iserles and Nørsett (1999). There are several excellent sources for a summary of these methods and their analysis, for instance the *Acta Numerica* article by Iserles *et al.* (2000), the monograph by Hairer *et al.* (2006) and the more recent survey by Blanes, Casas, Oteo and Ros (2009), which also contains many applications of these integrators.

2.1. Background and notation

Let M be some differentiable manifold and let $\mathcal{X}(M)$ be the set of smooth vector fields on M. We consider every $X \in \mathcal{X}(M)$ as a differential operator on the set of smooth functions $\mathcal{F}(M)$ on M. Thus, in local coordinates $(x_1, \ldots, x_m)$ in which X has components $X_1, \ldots, X_m$, we write $X = \sum_i X_i(x) \frac{\partial}{\partial x_i}$, so $X[f] = \mathrm{d}f(X)$, $f \in \mathcal{F}(M)$ is the directional derivative of f along the vector field X. The flow of a vector field $X \in \mathcal{X}(M)$ is a one-parameter family of maps $\exp(tX) : \mathcal{D}_t \to M$, where $\mathcal{D}_t \subset M$. For any $x \in \mathcal{D}_t$ we have $\exp(tX)x = \gamma(t)$, where

$$\dot{\gamma}(t) = X|_{\gamma(t)}, \quad \gamma(0) = x, \quad t \in (a(x), b(x)), \ a(x) < 0 < b(x).$$

The domain for $\exp(tX)$ is the set $\mathcal{D}_t = \{x \in M : t \in (a(x), b(x))\}$; for further details see, *e.g.*, Warner (1983, 1.48).

The chain rule for the derivative of compositions of maps between manifolds is

$$(\psi \circ \phi)' = \psi' \circ \phi', \quad \phi : M \to N,\ \psi : N \to P.$$

From this, we easily obtain the useful formula

$$X[f \circ \phi](x) = \phi'(X|_x)[f](y), \quad \phi : M \to N,\ X \in \mathcal{X}(M),\ f \in \mathcal{F}(N), \quad \text{for } x \in M,\ y = \phi(x). \tag{2.1}$$

The Lie–Jacobi bracket on $\mathcal{X}(M)$ is defined simply as the commutator of vector fields $Z = [X, Y] = XY - YX$. With respect to coordinates $(x_1, \ldots, x_m)$ it has the form

$$Z_i = [X, Y]_i = \sum_{j=1}^{m} X_j \frac{\partial Y_i}{\partial x_j} - Y_j \frac{\partial X_i}{\partial x_j}.$$

This bracket makes $\mathcal{X}(M)$ a Lie algebra; the important properties of the bracket is that it is bilinear, skew-symmetric and satisfies the Jacobi identity

$$[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0, \quad \forall X, Y, Z \in \mathcal{X}(M).$$

It is an easy consequence of (2.1) that

$$\phi'([X, Y]) = [\phi'(X), \phi'(Y)], \quad X, Y \in \mathcal{X}(M),\ \phi : M \to N. \tag{2.2}$$

We say that Y is ϕ-related to $X \in \mathcal{X}(M)$ if $Y|_{\phi(x)} = \phi'(X|_x)$ for each $x \in M$. Note that Y is not generally a vector field on N: since ϕ does not have to be either injective or surjective, we must treat Y as a pullback section of $\phi^* TN$ over M. In the particular case when ϕ is a diffeomorphism, there is a unique $Y \in \mathcal{X}(N)$ which is ϕ-related to X; this vector field is then called the pushforward of X with respect to ϕ:

$$Y = \phi_* X = \phi'(X) \circ \phi^{-1}.$$

A Lie group G is a differentiable manifold which is furnished with a group structure such that the multiplication is a smooth map from $G \times G$ to G, and the map $g \mapsto g^{-1}$, $g \in G$ is smooth as well. We briefly review some important concepts related to Lie groups. Every Lie group G has a Lie algebra associated to it, which can be defined as the linear subspace $\mathfrak{g} \subset \mathcal{X}(G)$, of right-invariant vector fields on G equipped with the Lie–Jacobi bracket. By right-invariance we mean invariance under right translation. Consider the diffeomorphism $R_g : G \to G$ defined as $R_g(h) = h \cdot g$. A vector field $X \in \mathcal{X}(G)$ is right-invariant if it is R_g-related to itself, *i.e.*, $R_{g*} X = X$. By (2.2) it follows that the Lie–Jacobi bracket between two right-invariant vector fields is again right-invariant. For every $v \in T_{\mathrm{e}} G$, where e is the identity element, there is a unique $X_v \in \mathfrak{g}$ such that $X_v|_g = R'_g(v)$, and for $X \in \mathcal{X}(G)$ there is an element $v_X \in T_{\mathrm{e}} G$ given as $v_X = X|_{\mathrm{e}}$. This shows that $\mathfrak{g}$ is isomorphic to $T_{\mathrm{e}} G$, and it may often be convenient to represent

$\mathfrak{g}$ as T_eG rather than as right-invariant vector fields on G. We next let the group act locally on a manifold. A left group action on a differentiable manifold M by a Lie group G is a map $G \times M \to M$, which we denote as $y = g \cdot x \in M$ or simply $y = gx$ for $g \in G$ and $x \in M$. The group action must satisfy the conditions

$$\mathrm{e} \cdot x = x, \ \forall x \in M, \quad g \cdot (h \cdot x) = (g \cdot h) \cdot x.$$

The group action is said to be *free* if $g \cdot x = x \Rightarrow g = \mathrm{e}$, so that the only group element which leaves $x \in M$ fixed is the identity element. If it is true that for every pair of points $x \in M, y \in M$ there exists a group element g such that $y = g \cdot x$, the action is called transitive. We usually just need a local version of transitivity, requiring that for every $x \in M$, $G \cdot x$ contains some open neighbourhood of x. The *orbit* of the group action containing x is the set $\mathcal{O}_x = \{g \cdot x \,|\, g \in G\}$. It is sometimes useful to restrict the action to an orbit when transitivity is a desired property. Similarly, if one needs the group action to be free, it may be useful to extend the action to multispace $M \times^r M$ (r copies of M) or to a suitable jet space whenever M takes the form of a fibred space.

Let G be a Lie group with Lie algebra $\mathfrak{g}$. Assume that G acts locally on the manifold M, and set $\Lambda_x(g) = g \cdot x$ for $g \in U \subseteq G$, $x \in M$ where U is some open neighbourhood of the identity element. For every fixed $v \in \mathfrak{g}$ there is a vector field $X_v \in \mathcal{X}(\mathcal{M})$ defined by

$$X_v|_x = \lambda_*(v)|_x = \Lambda'_x(v) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \gamma(t) \cdot x,$$

where $\gamma(t)$ is any smooth curve on G such that $\gamma(0) = \mathrm{e}$, $\dot\gamma(0) = v$. So λ_* is a Lie algebra homomorphism of $\mathfrak{g}$ into its image in $\mathcal{X}(M)$. For Lie group integrators, it is important that the action is locally transitive; in this case it is true that for every $x \in X$

$$\lambda_*(\mathfrak{g})|_x = T_xM.$$

This property means, in particular, that for any smooth vector field $F \in \mathcal{X}(M)$ there exists a map $f : M \to \mathfrak{g}$ such that

$$F|_x = \lambda_*(f(x))|_x, \tag{2.3}$$

a formulation called the *generic presentation of ODEs on manifolds* by Munthe-Kaas (1999). If the action is free then the map $f(x)$ is unique for a given vector field F. Suppose further that the Lie algebra $\mathfrak{g}$ is of dimension d and let $e_1, \ldots, e_d$ be a basis for $\mathfrak{g}$. Let $E_i = \lambda_*(e_i)$, $i = 1, \ldots, d$. We call the set $\{E_1, \ldots, E_d\}$ a *frame*,[3] and let $\bar{\mathfrak{g}} = \mathrm{span}\{E_1, \ldots, E_m\}$, that is,

[3] In the literature, a 'frame' is often used as a local object requiring that $E_1|_x, \ldots, E_d|_x$ is a basis for T_xM. We do not impose this condition here *per se*, as we find it useful to have a global representation of vector fields on M.

the linear span of the frame fields over $\mathbb{R}$ or $\mathbb{C}$. Now we can represent any smooth vector field $X \in \mathcal{X}(M)$ by means of d functions $f_i : M \to \mathbb{R}$:

$$F|_x = \sum_{i=1}^{d} f_i(x)\, E_i|_x. \tag{2.4}$$

The set of functions f_i is uniquely given only if the action is free. There are two alternative ways to proceed, following either the terminology introduced by Crouch and Grossman (1993) or that of Munthe-Kaas (1995, 1998, 1999). In the former case, one introduces a freeze operator $\mathrm{Fr} : M \times \mathcal{X}(M) \to \bar{\mathfrak{g}}$ relative to the frame. It is defined by

$$X_p|_x := \mathrm{Fr}(p, X)|_x = \sum_i f_i(p) E_i|_x. \tag{2.5}$$

The frozen vector field X_p has the property that it coincides with the unfrozen field X at the point $x = p$, *i.e.*, $X_p|_x = X|_x$. A main assumption underlying many Lie group integrators is that flows of frozen vector fields can be calculated, or in some cases approximated with acceptable computational cost.

2.2. Integrators based on coordinates on the Lie group

In what follows, we shall take $\mathfrak{g}$ to be $T_{\mathrm{e}}G$. Consider a diffeomorphism defined from some open subset of $U \subseteq \mathfrak{g}$ containing 0, *i.e.*, $\Psi : U \to G$ and we require that $\Psi(0) = \mathrm{e}$, $\Psi_0'(v) = v$, $\forall v \in \mathfrak{g}$. For convenience, we shall work with a right-trivialized version of Ψ_u', setting

$$\Psi_u' = R'_{\Psi(u)} \circ \mathrm{d}\Psi_u, \quad \mathrm{d}\Psi_u : \mathfrak{g} \to \mathfrak{g}.$$

Let the group act locally on the manifold M; suppose that the action is defined on a subset $G_p \subseteq G$, where $\Psi(U) \subset G_p$ for every $p \in M$. For any $p \in M$ and $u \in U$, set $\lambda_p(u) = \Psi(u) \cdot p$, and let $f : \mathcal{M} \to \mathfrak{g}$ represent the vector field $F \in \mathcal{X}(M)$ through the form (2.3). We define the vector field $\tilde{F}_p$ on $\mathcal{X}(U)$ by

$$\tilde{F}_p\big|_u = \mathrm{d}\Psi_u^{-1} f(\lambda_p(u)). \tag{2.6}$$

A simple calculation (Munthe-Kaas 1999, Owren and Marthinsen 2001) shows that F is λ_p-related to $\tilde{F}$ such that, for any $u \in U$, we have $F|_{\lambda_p(u)} = \lambda_p'\big|_u(\tilde{F}_p|_u)$. This local relatedness between vector fields F of the form (2.3) whose flows are to be approximated, and vector fields on the algebra of the acting group serves as the key underlying principle of many Lie group integrators. The idea is that near any point $p \in M$ one may represent curves in the form $y(t) = \lambda_p(\sigma(t))$, and if the differential equation for $y(t)$ is given by F, then a differential equation for $\sigma(t)$ is that of $\tilde{F}$. Most of the known integrators for ODEs have the property that when the solution belongs to

some linear space, the numerical method will provide approximations for the solution belonging to the same linear space. So one may now approximate solutions to the ODE given by $\tilde{F}$, and obtain numerical approximations in the linear space $\mathfrak{g}$. The map λ_p will then map these approximations onto M by definition. One may typically choose the initial value in each step to be p, so that when solving for σ in $\mathfrak{g}$ one sets $\sigma(t_n) = 0$. Suppose that a one-step method map which preserves linear structure is denoted $\Phi_{h,\tilde{F}_p}$, where h is the time step.

Algorithm 2.1.

for $n = 0, 1, \ldots$ **do**
  $p \leftarrow y_n$
  $\sigma_{n+1} \leftarrow \Phi_{h,\tilde{F}_p}(0)$
  $y_{n+1} \leftarrow \lambda_p(\sigma_{n+1})$
end for

We may be more specific and for instance insist that the scheme $\Phi_{h,\tilde{F}}$ to be used in the Lie algebra is an explicit Runge–Kutta method, with weights b^i and coupling coefficients a_i^j, $1 \le j < i \le s$. In this case we can phrase the scheme as follows for integrating a system in the form (2.3) from t_0 to $t_0 + h$, with initial value $y(t_0) = y_0 \in M$.

Algorithm 2.2. (Runge–Kutta–Munthe-Kaas)

for $i = 1 \to s$ **do**
  $u_i \leftarrow h \sum_{j=1}^{i-1} a_i^j k_j$
  $k_i' \leftarrow f(\Psi(u_i) \cdot y_0)$
  $k_i \leftarrow \mathrm{d}\Psi_{u_i}^{-1}(k_i')$
end for
$v \leftarrow h \sum_{j=1}^{s} b^j k_j$
$y_1 = \Psi(v) \cdot y_0$

An obvious benefit of schemes of this form is that they will preserve the manifold structure, a feature which cannot be expected when M is modelled as some embedded submanifold of Euclidean space. If the manifold happens to belong to a level set of one or more first integrals, then the Lie group integrators will automatically preserve these integrals. There are, however, other interesting situations, when the group action is used as a building block for obtaining a more accurate representation of the exact solution than is possible with other methods. The idea behind Lie group integrators can also be seen as a form of preconditioning.

Coordinate maps. The computational cost of the Lie group integrators is an important issue, and the freedom one has in choosing the coordinate map Ψ may be used to optimize the computational cost. The generic choice for $\Psi(u)$ is of course the exponential map $\Psi(u) = \exp u$. This choice is called

canonical coordinates of the first kind. If the Lie group and its Lie algebra are realized as matrices, we have

$$\exp u = \sum_{k=0}^{\infty} \frac{u^k}{k!}.$$

Issues related to computing the matrix exponential have been thoroughly debated in the literature, going back to the seminal paper of Moler and Van Loan (1978), and its follow-up, Moler and van Loan (2003). For dense $n \times n$ matrices one would normally expect a computational complexity of approximately $C\,n^3$, where C will depend on several factors, as the tolerance for the accuracy, the size of the matrix elements and the conditioning of the matrix. The methods presented in these papers, however, do not usually respect the Lie group structure, such that an approximation $\tilde{g} \approx \exp u,\ u \in \mathfrak{g}$ will not belong to the group, *i.e.*, $\tilde{g} \notin G$; this is a crucial issue as far as exact conservation is concerned. In practice, one is left with two alternatives.

(1) Apply a standard method which yields $g = \exp u$ to machine accuracy. For relevant examples with Lie group integrators, the factor C typically lies in the range 20–30 (Owren and Marthinsen 2001).

(2) Apply some approximation which is not exact, but which respects the Lie group structure, *i.e.*, $\tilde{g} \approx \exp u$ with $\tilde{g} \in G$. This approach has been pursued by Celledoni and Iserles (2000, 2001) for approximation by low-rank decomposition, as well as Zanna and Munthe-Kaas (2001/02) and Iserles and Zanna (2005) by means of the generalized polar decomposition. These approaches still have a computational cost of $C\,n^3$ for Lie algebras whose matrix representation yields dense matrices, but the constant C may be smaller than for the general algorithms.

It is interesting to explore other possible choices of analytic matrix functions than the exponential. One then replaces the exponential map with some local diffeomorphism from a neighbourhood of $0 \in \mathfrak{g}$ to G, usually required to map $0 \mapsto \mathrm{e}$. But it turns out that the exponential map is the only possible choice of analytic map that works for all Lie groups: this is asserted, for instance, using a result by Kang and Shang (1995).

Lemma 2.3. Let $\mathfrak{sl}(d)$ denote the set of all $d \times d$ real matrices with trace equal to zero and let $\mathrm{SL}(d)$ be the set of all $d \times d$ real matrices with determinant equal to one. Then, for any real analytic function $R(z)$ defined in a neighbourhood of $z = 0$ in $\mathbb{C}$ satisfying the conditions: $R(1) = 1$ and $R'(0) = 1$, we have that $R(\mathfrak{sl}(d)) \subseteq \mathrm{SL}(d)$ for some $d \geq 3$ if and only if $R(z) = \exp(z)$.

They prove this result by taking the Lie group $\mathrm{SL}(d)$ of unit determinant $d \times d$ matrices, $d \geq 3$, whose Lie algebra $\mathfrak{sl}(d)$ consists of $d \times d$ matrices with