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An introduction to Lie group integrators – basics, new developments and applications

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ABSTRACT

We give a short and elementary introduction to Lie group methods. A selection of applications of Lie group integrators are discussed. Finally, a family of symplectic integrators on cotangent bundles of Lie groups is presented and the notion of discrete gradient methods is generalised to Lie groups.

1. Introduction

The significance of the geometry of differential equations was well understood already in the nineteenth century, and in the last few decades such aspects have played an increasing role in numerical methods for differential equations. Nowadays, there is a rich selection of integrators which preserve properties like symplecticity, reversibility, phase volume and first integrals, either exactly or approximately over long times [30]. Differential equations are inherently connected to Lie groups, and in fact one often sees applications in which the phase space is a Lie group or a manifold with a Lie group action. In the early nineties, two important papers appeared which used the Lie group structure directly as a building block in the numerical methods. Crouch and Grossman [22] suggested to advance the numerical solution by computing flows of vector fields in some Lie algebra. Lewis and Simo [45] wrote an influential paper on Lie group based integrators for Hamiltonian problems, considering the preservation of symplecticity, momentum and energy. These ideas were developed in a systematic way throughout the nineties by several authors. In a series of three papers, Munthe-Kaas [54–56] presented what are now known as the Runge–Kutta–Munthe-Kaas methods. By the turn of the millennium, a survey paper [35] summarised most of what was known by then about Lie group integrators. More recently a survey paper on structure preservation appeared with part of it dedicated to Lie group integrators [20].

The purpose of the present paper is three-fold. First, in Section 2 we give an elementary, geometric introduction to the ideas behind Lie group integrators. Secondly, we present some examples of applications of Lie group integrators in sections 3 and 4. There are many such examples to choose from, and we give here only a few teasers. These first four sections should be read as a survey. But in the last two sections, new material is presented. Symplectic Lie group integrators have been known for some time, derived by Marsden and coauthors [49] by means of variational principles. In Section 5 we consider a group structure on the cotangent bundle of a Lie group and derive symplectic Lie group integrators using the model for vector fields on manifolds defined by Munthe-Kaas in [56]. In Section 6 we extend the notion of discrete gradient methods as proposed by Gonzalez [29] to Lie groups, and thereby we obtain a general method for preserving first integrals in differential equations on Lie groups.

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We would also like to briefly mention some of the issues we are *not* pursuing in this article. One is the important family of Lie group integrators for problems of linear type, including methods based on the Magnus and Fer expansions. An excellent review of the history, theory and applications of such integrators can be found in [2]. We will also skip all discussions of order analysis of Lie group integrators. This is a large area by itself which involves technical tools and mathematical theory which we do not wish to include in this relatively elementary exposition. There have been several new developments in this area recently, in particular by Lundervold and Munthe-Kaas, see e.g. [47].

2. Lie group integrators

The simplest consistent method for solving ordinary differential equations is the Euler method. For an initial value problem of the form

$$\dot{y} = F(y), \quad y(0) = y_0,$$

one takes a small time increment h, and approximates $y(h)$ by the simple formula

$$y_1 = y_0 + hF(y_0),$$

advancing along the straight line coinciding with the tangent at y_0. Another way of thinking about the Euler method is to consider the constant vector field $F_{y_0}(y) := F(y_0)$ obtained by parallel translating the vector $F(y_0)$ to all points of phase space. A step of the Euler method is nothing else than computing the exact h-flow of this simple vector field starting at y_0. In Lie group integrators, the same principle is used, but allowing for more advanced vector fields than the constant ones. A Lie group generalisation of the Euler method is called the Lie–Euler method, and we shall illustrate its use through an example [22].

Example, the Duffing equation. Consider the system in $\mathbf{R}^2$

$$\begin{aligned} \dot{x} &= y, \\ \dot{y} &= -ax - bx^3, \end{aligned} \quad a \geqslant 0, b \geqslant 0, \tag{1}$$

a model used to describe the buckling of an elastic beam. Locally, near a point (x_0, y_0) we could use the approximate system

$$\begin{aligned} \dot{x} &= y, \quad x(0) = x_0, \\ \dot{y} &= -(a + bx_0^2)x, \quad y(0) = y_0, \end{aligned} \tag{2}$$

which has the exact solution

$$\bar{x}(t) = x_0 \cos \omega t + \frac{y_0}{\omega} \sin \omega t, \quad \bar{y}(t) = y_0 \cos \omega t - \omega x_0 \sin \omega t, \quad \omega = \sqrt{a + bx_0^2}. \tag{3}$$

Alternatively, we may consider the local problem

$$\begin{aligned} \dot{x} &= y, \\ \dot{y} &= -ax - bx_0^3, \end{aligned}$$

having exact solution

$$\begin{aligned} \bar{x}(t) &= x_0 \cos \alpha t + \tfrac{y_0}{\alpha} \sin \alpha t + bx_0^3 \frac{\cos \alpha t - 1}{\alpha^2}, \\ \bar{y}(t) &= y_0 \cos \alpha t - \alpha x_0 \sin \alpha t - bx_0^3 \frac{\sin \alpha t}{\alpha}, \end{aligned} \quad \alpha = \sqrt{a}.$$

In each of the two cases, one may take $x_1 = \bar{x}(h), y_1 = \bar{y}(h)$ as the numerical approximation at time $t = h$. The same procedure is repeated in subsequent steps. A common framework for discussing these two cases is provided by the use of frames, i.e. a set of vector fields which at each point is spanning the tangent space. In the first case, the numerical method applies the frame

$$X = \begin{bmatrix} y \\ 0 \end{bmatrix} =: y\,\partial x, \quad Y = \begin{bmatrix} 0 \\ x \end{bmatrix} =: x\,\partial y. \tag{4}$$

Taking the negative Jacobi–Lie bracket (also called the commutator) between X and Y yields the third element of the standard basis for the Lie algebra $\mathfrak{sl}(2)$, i.e.

$$H = -[X, Y] = x\,\partial x - y\,\partial y, \tag{5}$$

so that the frame may be augmented to consist of $\{X, Y, H\}$. In the second case, the vector fields $E_1 = y\,\partial x - ax\,\partial y$ and $E_2 = \partial y$ can be used as a frame, but again we choose to augment these two fields with the commutator $E_3 = -[E_1, E_2] = \partial x$ to obtain the Lie algebra of the special Euclidean group SE(2) consisting of translations and rotations in the plane. The situation is illustrated in Fig. 1. In the left part, we have considered the constant vector field corresponding to the Duffing vector field evaluated at $(x_0, y_0) = (0.75, 0.75)$, and the exact flow of this constant field is just the usual Euler method, a straight line. In the right part, we have plotted the vector field defined in (2) with the same (x_0, y_0) along with its flow (3). The exact flow of (1) is shown in both plots (thick curve).