Preserving algebraic invariants with Runge–Kutta methods

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Abstract

We study Runge–Kutta methods for the integration of ordinary differential equations and their retention of algebraic invariants. As a general rule, we derive two conditions for the retention of such invariants. The first is a condition on the coefficients of the methods, the second is a pair of partial differential equations that otherwise must be obeyed by the invariant. The cases related to the retention of quadratic and cubic invariant, perhaps of greatest relevance in applications, are thoroughly discussed. We conclude recommending a generalized class of Runge–Kutta schemes, namely Lie-group-type Runge–Kutta methods. These are schemes for the solution of ODEs on Lie groups but can be employed, together with group actions, to preserve a larger class of algebraic invariants without restrictions on the coefficients.

1 Background and notation

In this paper we study the numerical solution by Runge–Kutta methods of the ordinary differential system

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0, \tag{1}$$

for $t \geq 0$, where $\boldsymbol{y} \in \mathbb{R}^d$ and $\boldsymbol{f} : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ is a Lipschitz function. We assume that the exact solution $\boldsymbol{y}(t)$ of (1) is known to obey the condition that there exists a nontrivial function $\rho : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ (or a family of such functions) such that

$$\rho(\boldsymbol{y}(t), \boldsymbol{y}_0) \equiv 0, \quad t \geq 0 \tag{2}$$

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We say, in this case, that the solution $\boldsymbol{y}$ is *ρ-invariant.* [1] Sometimes we say that ρ is a first integral of (1) or that it is a conservation law or that it defines a manifold $\mathcal{M}$ on which the solution $\boldsymbol{y}$ evolves. All these terms will be used interchangeably in the course of the paper. The degree of smoothness of ρ is related to the degree of smoothness of the function $\boldsymbol{f}$ defining the differential equation (1). Moreover, we say that ρ is a *strong invariant* if there exists a nonempty neighbourhood $\mathcal{U}$ of $\boldsymbol{y}_0$ such that $\rho(\boldsymbol{z}, \boldsymbol{y}_0) \equiv 0$ for all $\boldsymbol{z} \in \mathcal{U}$. In the present paper, we restrict our attention to the case when ρ is a strong invariant.

There exist numerous problems in applied mathematics that can be paraphrased in the above formalism. Just to mention a few, many physical systems evolve in time and yet their total energy or the phase-space volume or angular momentum stay put. In particular, the Hamiltonian energy of *Hamiltonian systems* is preserved. See [7,19,20,14] for further examples and applications.

Given the differential equation (1) in tandem with the invariance condition (2) and having introduced a subdivision $t_0 = 0 < t_1 < \cdots < t_n < \cdots$ of the integration interval, we say that a one-step numerical method

$$\boldsymbol{y}_{n+1} = \boldsymbol{\phi}_h(\boldsymbol{y}_n), \qquad h = t_{n+1} - t_n, \tag{3}$$

is *ρ-invariant* (or equivalently *$\mathcal{M}$-invariant*) if

$$\rho(\boldsymbol{y}_n, \boldsymbol{y}_0) = 0, \quad \forall n \geq 0, \tag{4}$$

or, equivalently,

$$\boldsymbol{y}_0 \in \mathcal{M} \quad \Rightarrow \quad \boldsymbol{y}_n \in \mathcal{M} \text{ for all } n \geq 0, \tag{5}$$

$\mathcal{M}$ being the manifold defined by the function ρ [5].

The condition for invariance of Runge–Kutta methods has been already considered in a number of papers. Let us mention first the work of Cooper [3] who proved that there exists a subclass of Runge–Kutta methods that preserve quadratic invariants. The same schemes that preserve quadratic invariants do also preserve the canonical symplectic structure, a result independently discovered by Lasagni, Sanz-Serna and Suris [19]. Later, in their investigation on numerical methods and isospectral flows, Calvo, Iserles and Zanna proved that there is no subclass of such schemes that preserves also cubic laws: in

[1] Note that in this paper we discuss algebraic invariance. Therefore ρ is not to be confused with a symmetry invariant. We refer the reader to [11] and to the references therein for a treatment of symmetry invariants.

other words, given a method that preserves quadratic manifolds, it is always possible to construct a differential equation with a cubic invariant ρ for which (4) does not hold for $n = 1, 2, \ldots$ (see [2,20]).

With regard to other class of methods and their preservation of conservation laws, we mention that results along similar lines have been derived by Iserles also for *multistep methods* and for *Taylor-type* methods [10] and independently by Hairer and Leone in the context of symplecticity [6]. We will follow here the approach of [2,20,10] and show that cubic invariance is equivalent to requiring very strong condition on the invariant, namely that it has to be the solution of a partial differential equation called the Bateman equation. Although the Bateman-equation condition arises also in the case of multistep and Taylor-type methods [10], Runge–Kutta methods are a case apart since their error term is not a constant times a derivative of the function but as a linear combination of mixtures of derivatives of various orders (elementary differentials [8]), a feature that makes RK schemes different from many other numerical schemes for integration of ODEs.

The paper is organised as follows. In Section 2 we discuss classical RK methods and their condition for invariance, deriving the Bateman equation, a second-order partial differential equation, and a third-order partial differential equation, for the algebraic invariant ρ. Section 3 is devoted to the analysis of the third-order counterpart of the Bateman equation. In Section 4 we discuss RK methods in the class of Lie-group schemes, of which classical RK schemes are but one representative. We argue that Lie-group formalism for RK schemes allows us to preserve a larger class of algebraic invariants and other qualitative features of the problem in question without restriction on the coefficients of the underlying scheme.

2 Necessary condition for invariance: the Bateman equation and its third-order counterpart

Without loss of generality, let us assume that the differential equation (1) is *autonomous*, namely that $\boldsymbol{f} \equiv \boldsymbol{f}(\boldsymbol{y})$ does not depend explicitely on time. The exact solution of (1) is numerically approximated by means of a ν-stage Runge–Kutta method,

$$
\begin{aligned}
\boldsymbol{Y}_i &= \boldsymbol{y}_n + h \sum_{j=1}^{\nu} a_{i,j} \boldsymbol{K}_j, \\
\boldsymbol{K}_i &= \boldsymbol{f}(\boldsymbol{Y}_i), \quad i = 1, 2, \ldots, \nu, \\
\boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + h \sum_{i=1}^{\nu} b_i \boldsymbol{K}_i,
\end{aligned}
\tag{6}
$$

defined in terms of the *RK matrix* $A = (a_{i,k})$ and the *RK weights* $\boldsymbol{b} = (b_i)$ [8,9].

Recall that any system (1) that is ρ-invariant and autonomous can be written in the *skew-gradient* form

$$\boldsymbol{y}' = S(\boldsymbol{y})\nabla\rho(\boldsymbol{y}), \tag{7}$$

whereby $S(\cdot)$ is a $d \times d$ skew-symmetric matrix [13,18], and in particular, we will restrict our attention to the case of two variables, i.e. $d = 2$, in which case (7) yields

$$\begin{aligned} y_1' &= \psi(\boldsymbol{y})\frac{\partial\rho(\boldsymbol{y})}{\partial y_2}, \\ y_2' &= -\psi(\boldsymbol{y})\frac{\partial\rho(\boldsymbol{y})}{\partial y_1}, \end{aligned} \tag{8}$$

for some arbitrary smooth function $\psi : \mathbb{R}^2 \to \mathbb{R}$. Since we wish to derive necessary conditions for invariance, we may assume without loss of of generality that $\psi \equiv 1$.

Proposition 1 *Assume that the function ρ is not a solution of the* Bateman equation

$$\mathcal{B}(u) = \left(\frac{\partial u}{\partial y_2}\right)^2 \frac{\partial^2 u}{\partial y_1^2} - 2\frac{\partial u}{\partial y_1}\frac{\partial u}{\partial y_2}\frac{\partial^2 u}{\partial y_1 \partial y_2} + \left(\frac{\partial u}{\partial y_1}\right)^2 \frac{\partial^2 u}{\partial y_2^2} = 0 \tag{9}$$

[4], where $u \equiv u(y_1, y_2)$. Then for the RK method (6) *to preserve ρ it is necessary that*

$$b_i a_{i,j} + b_j a_{j,i} = b_i b_j, \quad i, j = 1, 2, \ldots, \nu. \tag{10}$$

PROOF. For clarity's sake we suppress the dependence of ρ on the initial condition $\boldsymbol{y}_0$ and assume that it is a smooth function. Expanding in powers of h and using (6), we have

$$\begin{aligned} \rho(\boldsymbol{y}_{n+1}) &= \rho\left(\boldsymbol{y}_n + h\sum_{i=1}^{\nu} b_i \boldsymbol{K}_i\right) \\ &= \rho(\boldsymbol{y}_n) + \sum_{k=1}^{\infty}\frac{h^k}{k!}\sum_{i_1,\ldots,i_k=1}^{\nu} b_{i_1}\cdots b_{i_k} \\ &\quad \times \sum_{l=1}^{k}\binom{k}{l}\frac{\partial^k\rho(\boldsymbol{y}_n)}{\partial^{k-l}y_1\partial^l y_2} f_1(\boldsymbol{Y}_{i_1})\cdots f_1(\boldsymbol{Y}_{i_{k-l}})f_2(\boldsymbol{Y}_{i_{k-l+1}})\cdots f_2(\boldsymbol{Y}_{i_k}), \end{aligned} \tag{11}$$

whereby the index of $\boldsymbol{f}$ denotes either its first or its second component, namely,

$$f_1(\boldsymbol{Y}_i) = \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_2}, \quad f_2(\boldsymbol{Y}_i) = -\frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_1}, \qquad i = 1, 2, \ldots, \nu.$$

Let us assume that $\rho(\boldsymbol{y}_n) = 0$ and let us focus on the terms up to order two in h. Using the identity

$$\boldsymbol{y}_n = \boldsymbol{Y}_i - h \sum_{j=1}^{\nu} a_{i,j} \boldsymbol{K}_j,$$

and expanding the functions $\partial\rho/\partial y_l$, $l = 1, 2$, we obtain

$$\begin{aligned}
&\frac{\partial \rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_2}(\boldsymbol{Y}_i) - \frac{\partial \rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_1}(\boldsymbol{Y}_i) \\
&= -h \sum_{j=1}^{\nu} a_{i,j} \left[\frac{\partial^2 \rho(\boldsymbol{Y}_i)}{\partial y_1^2} \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_2} \frac{\partial \rho(\boldsymbol{Y}_j)}{\partial y_2} - \frac{\partial^2 \rho(\boldsymbol{Y}_i)}{\partial y_1 \partial y_2} \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_2} \frac{\partial \rho(\boldsymbol{Y}_j)}{\partial y_1} \right. \\
&\quad \left. - \frac{\partial^2 \rho(\boldsymbol{Y}_i)}{\partial y_1 \partial y_2} \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_1} \frac{\partial \rho(\boldsymbol{Y}_j)}{\partial y_2} + \frac{\partial^2 \rho(\boldsymbol{Y}_i)}{\partial y_2^2} \frac{\partial \rho(\boldsymbol{Y}_i)}{\partial y_1} \frac{\partial \rho(\boldsymbol{Y}_j)}{\partial y_1} \right].
\end{aligned}$$

Taking into account that $\boldsymbol{Y}_j = \boldsymbol{Y}_i + \mathcal{O}(h)$, we expand the above expression at $\boldsymbol{Y}_i$ to obtain

$$\frac{\partial \rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_2}(\boldsymbol{Y}_i) - \frac{\partial \rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial \rho}{\partial y_1}(\boldsymbol{Y}_i) = -h \sum_{j=1}^{\nu} a_{i,j} \mathcal{B}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^3\right).$$

By the same token,

$$\begin{aligned}
&\frac{h^2}{2} \sum_{i,j=1}^{\nu} b_i b_j \sum_{l=1}^{2} \binom{2}{l} \frac{\partial^2 \rho(\boldsymbol{y}_n)}{\partial^{2-l} y_1 \partial^l y_2} f_1(\boldsymbol{Y}_{i_1}) \cdots f_1(\boldsymbol{Y}_{i_{2-l}}) f_2(\boldsymbol{Y}_{i_{2-l+1}}) \cdots f_2(\boldsymbol{Y}_{i_2}) \\
&\quad = \frac{h^2}{2} \sum_{i,j=1}^{\nu} b_i b_j \mathcal{B}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^3\right).
\end{aligned}$$

Hence, reordering indices, we obtain

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2} h^2 \sum_{i,j=1}^{\nu} (b_i b_j - b_i a_{i,j} - b_j a_{j,i}) \mathcal{B}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^3\right).$$

Thus, unless ρ is a solution of the Bateman equation (9), annihilation of the $\mathcal{O}(h^2)$ term requires the relations (10). $\square$

The Bateman equation (9) plays a very important role also in the context of linear multistep methods and retention of conservation laws. As a matter of facts, Iserles proves that a necessary condition for ρ-invariance of a multistep method is that ρ obeys the Bateman equation [10].

The following result characterises the level sets of the solutions of the Bateman equation (9), which are essentially linear functions.

Proposition 2 (Iserles [10]) *Solutions $\rho(x, y)$ of the Bateman equation* (9) *such that $\rho(x, y) = const$ have the form*

$$\rho(x, y) = \omega(\alpha x + \beta y + \gamma),$$

where α, β and γ are arbitrary constants and $\omega \equiv \omega(z)$ is an arbitrary analytic function.

An important consequence of the above result is that linear multistep methods (and in general Taylor-type methods) can be invariant solely in linear manifolds.

We have seen that

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2}h^2 \sum_{i,j=1}^{\nu} (b_i b_j - b_i a_{i,j} - b_j a_{j,i}) \mathcal{B}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^3\right),$$

whereby the $\mathcal{O}(h^3)$ term contains partial derivatives of ρ of order greater than two. Hence, if ρ is a quadratic manifold, all these derivatives are zero and we are left with the condition

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2}h^2 \sum_{i,j=1}^{\nu} (b_i b_j - b_i a_{i,j} - b_j a_{j,i}) \mathcal{B}(\rho)(\boldsymbol{Y}_i),$$

which implies that the condition (10) is necessary and sufficient for the retention of quadratic conservation laws, a result well known and understood in the literature of Runge–Kutta methods [3,2,20].

Theorem 3 *A necessary condition for preserving a non-quadratic algebraic invariant ρ is that ρ is a solution of the partial differential equation*

$$\begin{aligned}\mathcal{L}(u) = &\left(\frac{\partial u}{\partial y_2}\right)^3 \frac{\partial^3 u}{\partial y_1^3} - 3\left(\frac{\partial u}{\partial y_2}\right)^2 \frac{\partial u}{\partial y_1} \frac{\partial^3 u}{\partial y_1^2 \partial y_2} \\ &+ 3\frac{\partial u}{\partial y_2}\left(\frac{\partial u}{\partial y_1}\right)^2 \frac{\partial^3 u}{\partial y_1 \partial y_2^2} - \left(\frac{\partial u}{\partial y_1}\right)^3 \frac{\partial^3 u}{\partial y_2^3} = 0.\end{aligned} \tag{12}$$

PROOF. Proceeding as in Proposition 1 but carrying the expansions a step further, we obtain, as a first contribution, the term

$$\frac{1}{3}h^3 \sum_{i,j,l=1}^{\nu} b_i b_j b_l \mathcal{L}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^4\right)$$

when $k = 3$ in (11). The second contribution, is obtained from the term for $k = 2$ in (11): substituting $\boldsymbol{y}_n = \boldsymbol{Y}_i - h\sum_{l=1}^{\nu} a_{i,l}\boldsymbol{K}_l$ and collecting similar terms, we obtain

$$\begin{aligned}
&\frac{1}{2}h^2 \sum_{i,j=1}^{\nu} b_i b_j \left[\frac{\partial^2\rho(\boldsymbol{y}_n)}{\partial y_1^2} f_1^2 + 2\frac{\partial^2\rho(\boldsymbol{y}_n)}{\partial y_1 \partial y_2} f_1 f_2 + \frac{\partial^2\rho(\boldsymbol{y}_n)}{\partial y_2^2} f_2^2\right] \\
&= \frac{1}{2}h^2 \sum_{i,j=1}^{\nu} b_i b_j \mathcal{B}(\rho)(\boldsymbol{Y}_i) - \frac{1}{2}h^3 \sum_{i,j,l=1}^{\nu} b_i b_j a_{i,l} \mathcal{L}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\left(h^4\right),
\end{aligned}$$

whereby $f_1 \equiv f_1(\boldsymbol{Y}_i)$ and $f_2 \equiv f_2(\boldsymbol{Y}_i)$. Finally, the last contribution arises from the series expansion of the $\mathcal{O}(h)$ term. We have

$$\begin{aligned}
&\frac{\partial\rho}{\partial y_1}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_2}(\boldsymbol{Y}_i) - \frac{\partial\rho}{\partial y_2}(\boldsymbol{y}_n)\frac{\partial\rho}{\partial y_1}(\boldsymbol{Y}_i) \\
&= \frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2}\left\{\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1} - h\sum_{j=1}^{\nu} a_{i,j}[\rho_{y_1y_1}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j) + \rho_{y_1y_2}(\boldsymbol{Y}_i) f_2(\boldsymbol{Y}_j)]\right. \\
&\quad + \frac{1}{2}h^2 \sum_{j,l=1}^{\nu} a_{i,j} a_{i,l}[\rho_{y_1y_1y_1}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j) f_1(\boldsymbol{Y}_l) + 2\rho_{y_1y_1y_2} f_1(\boldsymbol{Y}_j)\boldsymbol{f}_2(\boldsymbol{Y}_2) \\
&\quad \left. + \rho_{y_1y_2y_2} f_2(\boldsymbol{Y}_j) f_2(\boldsymbol{Y}_l)]\right\} \\
&+ \frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_1}\left\{\frac{\partial\rho(\boldsymbol{Y}_i)}{\partial y_2} - h\sum_{j=1}^{\nu} a_{i,j}[\rho_{y_1y_2}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j) + \rho_{y_2y_2}(\boldsymbol{Y}_i) f_2(\boldsymbol{Y}_j)]\right. \\
&\quad + \frac{1}{2}h^2 \sum_{j,l=1}^{\nu} a_{i,j} a_{i,l}[\rho_{y_1y_1y_2}(\boldsymbol{Y}_i) f_1^2(\boldsymbol{Y}_j) + 2\rho_{y_1y_2y_2} f_1(\boldsymbol{Y}_j)\boldsymbol{f}_2(\boldsymbol{Y}_j) \\
&\qquad \left. + \rho_{y_2y_2y_2} f_2^2(\boldsymbol{Y}_j)]\right\} + \mathcal{O}\left(h^3\right).
\end{aligned}$$

Let us focus on the term

$$\sum_{i,j=1}^{\nu} b_i a_{i,j} \rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j)$$

and similar expressions. We write this term in the form

$$\frac{1}{2}\sum_{i,j=1}^{\nu} b_i a_{i,j} \rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i) f_1(\boldsymbol{Y}_j) + \frac{1}{2}\sum_{i,j=1}^{\nu} b_j a_{j,i} \rho_{y_2}(\boldsymbol{Y}_j)\rho_{y_1y_1}(\boldsymbol{Y}_j) f_1(\boldsymbol{Y}_i),$$

and expand in series whilst exploiting the relation

$$\boldsymbol{Y}_j = \boldsymbol{Y}_i + h\sum_{l=1}^{\nu}(a_{j,l} - a_{i,l})\boldsymbol{K}_l.$$

We have

$$\begin{aligned}
&\frac{1}{2}\sum_{i,j=1}^{\nu} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)f_1(\boldsymbol{Y}_j)\\
=&\frac{1}{2}\sum_{i,j=1}^{\nu} b_i a_{i,j}\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)\rho_{y_2}(\boldsymbol{Y}_i)\\
&-h\sum_{i,j,l=1}^{\nu} b_i a_{i,j}(a_{i,l} - a_{j,l})\rho_{y_2}(\boldsymbol{Y}_i)\rho_{y_1y_1}(\boldsymbol{Y}_i)[\rho_{y_1y_2}f_1(\boldsymbol{Y}_l) + \rho_{y_2y_2}f_2(\boldsymbol{Y}_l)]\\
&+\mathcal{O}\Big(h^2\Big)
\end{aligned}$$

and

$$\begin{aligned}
&\frac{1}{2}\sum_{i,j=1}^{\nu} b_j a_{j,i}\rho_{y_2}(\boldsymbol{Y}_j)\rho_{y_1y_1}(\boldsymbol{Y}_j)\rho_{y_2}(\boldsymbol{Y}_i)\\
=&\frac{1}{2}\sum_{i,j=1}^{\nu} b_j a_{j,i}(\rho_{y_2}(\boldsymbol{Y}_i) - h\sum_{l=1}^{\nu}(a_{j,l} - a_{i,l})(\rho_{y_1y_2}f_1 + \rho_{y_2y_2}f_2)\rho_{y_1y_1}(\boldsymbol{Y}_j)\rho_{y_2}(\boldsymbol{Y}_i)\\
&-\frac{1}{2}h\sum_{i,j,l=1}^{\nu} b_j a_{j,i}(a_{j,l} - a_{i,l})\rho_{y_2}(\boldsymbol{Y}_i)[\rho_{y_1y_1y_1}(\boldsymbol{Y}_i)f_1 + \rho_{y_1y_1y_2}(\boldsymbol{Y}_i)f_2]\rho_{y_2}(\boldsymbol{Y}_i)\\
&+\mathcal{O}\Big(h^2\Big).
\end{aligned}$$

Expanding in an identical manner all similar terms, we observe that the terms containing two second derivatives of ρ sum up to zero, hence we are left with terms containing just one second derivative and one third derivative of the function ρ. After some tedious algebra along the lines of [2,20], the contribution of the $k = 1$ term in (11) reduces to

$$-\frac{1}{2}h^2\sum_{i,j=1}^{\nu}(b_i a_{i_j} + b_j a_{j,i})\mathcal{B}(\rho)(\boldsymbol{Y}_i) + \frac{1}{2}h^3\sum_{i,j,l=1}^{\nu} b_j a_{j,i}a_{i,l}\mathcal{L}(\rho)(\boldsymbol{Y}_i) + \mathcal{O}\Big(h^4\Big).$$

Collecting all the relevant terms, we obtain

$$\rho(\boldsymbol{y}_{n+1}) = \frac{1}{2}h^2\sum_{i,j=1}^{\nu}(b_i b_j - b_i a_{i,j} - b_j a_{j,i})\mathcal{B}(\rho)(\boldsymbol{Y}_i)$$

$$+\frac{1}{6}h^3\sum_{i,j,l=1}^{\nu}(b_ib_jb_l-3b_ib_ja_{i,l}+3b_ia_{i,j}a_{j,l})\mathcal{L}(\rho)(\boldsymbol{Y}_i)+\mathcal{O}\left(h^4\right),$$

whereby the coefficients of $\mathcal{B}$ and $\mathcal{L}$ are exactly those derived in [2,20].

Assume now that ρ does not obey the Bateman equation (see above), whose level sets are lines. Hence, in order to annihilate the $\mathcal{O}(h^2)$ term, the condition (10) must be satisfied by the coefficients of the RK scheme in question.

In order to annihilate the $\mathcal{O}(h^3)$ term, we have two possibilities: either the coefficients of the scheme obey $\Upsilon = O$, where

$$\begin{aligned}\Upsilon_{i,j,l} = {} & b_ib_jb_l-(b_ib_ja_{i,l}+b_jb_la_{j,i}+b_lb_ia_{lj})\\ & +(b_ia_{i,j}a_{j,l}+b_ja_{j,l}a_{l,i}+b_la_{l,i}a_{i,j})=0, \quad \forall i,j,l=1,\ldots,\nu\end{aligned} \tag{13}$$

(which has been already encountered in [2,20] in a discussion of cubic invariants) or ρ obeys the differential equation (12). However, it is well known that the condition (10) and the $\Upsilon = O$ condition (13) are contradictory [2,20], therefore the only possibility is that the differential condition (13) is satisfied. $\square$

3 On the solutions of the equation $\mathcal{L}(u) = 0$

In this section we wish to analyse some properties of the solutions of the partial differential equation (12). Following the same approach as [10], we distinguish two cases: first, we note that when $\partial\rho/\partial y_2 = 0$ identically, then ρ does not depend on the second variable, hence the system (8) can be reduced to the 1-variable case which is trivial to integrate: from $\rho(y_1, y_2) = f(y_1)$, we have

$$\begin{aligned}y_1' &= 0,\\ y_2' &= -f(y_1),\end{aligned}$$

hence $y_1 = c$ is constant and $y_2 = -f(c)t + y_2(0)$.

Let us assume hence $\partial\rho/\partial y_2 \neq 0$ at some point, hence, as a consequence of the analyticity of ρ, the same is true in a proper neighbourhood $\mathcal{U}$. Because of the implicit function theorem, there exists then a function η, such that

$$\rho(y_1, y_2) = 0 \quad \Leftrightarrow \quad y_2 = \eta(y_1), \quad \forall \boldsymbol{y} \in \mathcal{U},$$

hence $\rho(y_1, \eta(y_1)) = 0$. In order to avoid confusion, let us denote such independent variable as x; thus,

$$\rho(x, \eta(x)) = 0. \tag{14}$$

Differentiating $\rho(x, \eta(x)) = 0$ with regards to x, we have

$$\frac{\partial \rho(x, \eta(x))}{\partial y_1} + \frac{\partial \rho(x, \eta(x))}{\partial y_2} \eta'(x) = 0,$$

from which we deduce that

$$\eta' = -\frac{\partial \rho(x, \eta(x))}{\partial y_1} \left[\frac{\partial \rho(x, \eta(x))}{\partial y_2} \right]^{-1}.$$

Further differentiation of (14) implies that

$$\mathcal{B}(\rho(x, \eta(x))) + \left[\frac{\partial \rho(x, \eta)}{\partial y_2} \right]^3 \eta'' = 0,$$

as in [10]. In particular, we deduce that

$$\eta'' = -\mathcal{B}(\rho(x, \eta(x))) \left[\frac{\partial \rho(x, \eta)}{\partial y_2} \right]^{-3}. \tag{15}$$

From a third differentiation of (14), we obtain

$$\mathcal{L}(\rho(x, \eta)) - 3\mathcal{B}(\rho(x, \eta)) \left[\frac{\partial^2 \rho(x, \eta)}{\partial y_1 \partial y_2} + \frac{\partial^2 \rho(x, \eta)}{\partial y_2^2} \eta' \right] + \left[\frac{\partial \rho(x, \eta)}{\partial y_2} \right]^4 \eta''' = 0. \tag{16}$$

Assume that ρ obeys the partial differential equation (12). Substituting in (16) the expression for η'' and dividing by $(\partial \rho / \partial y_2)^2$ which we are assuming not equal identically to zero, we deduce

$$\eta''' \frac{\partial \rho(x, \eta)}{\partial y_2} + 3\eta'' \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial \rho(x, \eta)}{\partial y_2} \right) = 0. \tag{17}$$

Proposition 4 *Subject to the same assumptions as above, all solutions of the equation* (17) *obey the differential equation*

$$\mathcal{B}(\rho(x, \eta(x))) = \text{const}.$$

PROOF. We distinguish two cases. Either $\eta'' = 0$, in which case the assertion is satisfied because of (15), choosing the constant equal to zero. Otherwise, it is true that $\eta'' \neq 0$ in a certain neighbourhood of x. Hence, we can write

$$\frac{\eta'''}{\eta''} = -3\frac{\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial\rho}{\partial y_2}\right)}{\frac{\partial\rho}{\partial y_2}},$$

and, integrating both sides with respect to x, we obtain

$$\log \eta'' = -3 \log \frac{\partial\rho}{\partial y_2} + \text{ an integration constant},$$

from which we deduce that

$$\eta'' = K\left(\frac{\partial\rho}{\partial y_2}\right)^{-3},$$

K being an arbitrary constant of integration. The result follows by comparing the above expression for η'' with (15). □

Hence the problem reduces to studying solutions that render the Bateman operator $\mathcal{B}$ constant. Note that if $\rho(x, y)$ is a polynomial of degree n in x and y, then

$$\rho_{xx}\rho_y^2 - 2\rho_{xy}\rho_x\rho_y + \rho_{yy}\rho_x^2$$

is a polynomial of degree $(n-2) + 2(n-1) = 3n - 4$. In particular, it follows that $3n - 4 = n$ for $n = 2$, while $3n - 4 > n$ for all $n \geq 3$. Assume that

$$\rho(x, y) = ax^2 + bxy + cy^2 + dx + ey + f = 0.$$

Direct computation reveals that

$$\frac{1}{2}\mathcal{B}(\rho) = (4ac - b^2)[\rho(x, y) - f)] + ae^2 - bde + cd^2,$$

hence $\mathcal{B}(\rho)$ is constant, provided that so is ρ. If $n > 2$ then $\mathcal{B}(\rho)$ is a proper polynomial in x and y of degree strictly greater then n. Therefore, the system must admit a conservation law other than ρ, of order lower then n if ρ is a factor of the polynomial $\mathcal{B}(\rho)$, larger than n otherwise. This, for example, rules out the important case when ρ is the only integral of the the system.

That Runge–Kutta schemes could not preserve all arbitrary cubic algebraic invariants had been already established in [2], by constructing a cubic integral depending on a scheme which was not preserved by the method.

Assume now that ρ is not a polynomial but an analytic function ω of $q(x, y)$, namely $\rho(x, y) = \omega(q(x, y))$. Differentiating and substituting into $\mathcal{B}(\rho) =$ const, we obtain $\omega'(q(x, y))\mathcal{B}(q) = K$, hence, if q is such that $\mathcal{B}(q) =$ const, also $\omega'(q)$ is constant and we obtain a new solution. Thus, the solutions of $\mathcal{B}(\rho) =$ const are defined up to an arbitrary analytic function ω. This reflects the fact that the manifolds $\{\rho(\boldsymbol{x}) = c\}$ and $\{\omega(\rho(\boldsymbol{x})) = \omega(c)\}$ are identical for bijective ω.

Finally, we search for a solution separating variables. Assume that $\rho(x, y) = v(x)w(y)$, whereby v and w are two analytic functions of x and y respectively such that $v', w' \neq 0$, i.e. v and w are at least linear functions. Then the condition $\mathcal{L}(\rho) = 0$ is equivalent to

$$\frac{v'''v^2}{v'^3} - 3\frac{v''v}{v'^2} + 3\frac{w''w}{w'^2} - \frac{w'''w^2}{w'^3} = 0,$$

(the prime denoting differentiation with respect to the independent variable) which is equivalent two identical ordinary differential equations for v and w, namely

$$\frac{z'''z^2}{z'^3} - 3\frac{z''z}{z'^2} = K, \qquad z \equiv z(t)$$

with K arbitrary. When $K = 0$, we can reduce the above third-order differential equation into a second order one by integration,

$$z'' = cz^3,$$

whereby c is an arbitrary integration constant. The solution of the latter is given in implicit form by

$$t = \pm \int_0^{z(t)} \frac{2\mathrm{d}s}{\sqrt{2cs^4 + 4C_1}} + C_2,$$

where c, C_1 and C_2 are arbitrary integration constants.

4 Runge–Kutta methods in a Lie-group formulation

Although we have seen that the equation $\mathcal{L}(\rho)$ admits solutions that are not necessarily linear or quadratic in y_1, y_2, the sheer complexity of (17) reveals that such manifolds described by $\rho(y_1, y_2) = 0$ are by far very special. Moreover, recall that $\mathcal{L}(\rho) = 0$ is merely a necessary condition for invariance. We deduce that generic retention of conservation laws by means of classical RK integration cannot be easily achieved.

However, in the last few years, there has been a growing interest in devising Lie-group methods that somehow follow the logic of Runge–Kutta schemes. Let us present here the main ideas, referring the reader to [15,12,21] and to the review article [16] for further details.

Lie groups are smooth manifolds endowed with a multiplicative group operation, and without loss of generality we can identify them with subgroups of $\mathrm{GL}(\mathbb{R}^d)$, the set of all $d \times d$ real matrices. (Identical theory can be extended to the complex field.) An ordinary differential system on a Lie group G has a very special form,

$$y' = \gamma(t, y)y, \quad y(0) = y_0,$$

where $y \in G$ and $\gamma : \mathbb{R}^+ \times \mathfrak{g}$, where $\mathfrak{g}$ is the Lie algebra of G, and can be solved so that the numerical approximation resides in G,

$$y_n \in G \quad n = 0, 1, 2, \ldots,$$

provided that $y_0 \in G$, by using a Lie-group modification of classical Runge–Kutta schemes. In other words, at each step, the original ODE on G is translated into another ODE in $\mathfrak{g}$, thereby obtaining the so-called *dexpinv equation*,

$$\sigma' = \mathrm{dexp}_\sigma^{-1}\gamma, \quad \sigma(t_n) = 0,$$

which acts in $\mathfrak{g}$ instead of G. The function dexp^{-1} is defined as

$$\mathrm{dexp}_\sigma^{-1}(\gamma) = \sum_{k=0}^{\infty} \frac{\mathrm{B}_k}{k!} \mathrm{ad}_\sigma^k \gamma,$$

where the B_k's are Bernoulli numbers [1] and the *adjoint operators* ad^k's are k-times iterated commutators of σ and γ, namely $[\sigma, [\sigma, \cdots [\sigma, \gamma] \cdots]]$ (see [15,12,21,16]).

The redeeming feature of this transformation is that $\mathfrak{g}$ is a linear space while G is usually described by nonlinear conservation laws. Thus, arbitrary Runge–Kutta methods can be employed in $\mathfrak{g}$ to produce some numerical approximation $\sigma_{n+1} \approx \sigma(t_{n+1})$, so that

$$y_{n+1} = \exp(\sigma_{n+1}) y_n \in G$$

is a numerical approximation for $y(t_{n+1})$ which has the same order as the original RK scheme while remaining in the Lie group. Thus, if $G = \mathrm{SL}(\mathbb{R}^d)$, the set of all $d \times d$ matrices with determinant equal to one, such Lie-group based RK schemes allow us to preserve to machine accuracy the algebraic invariant $\det y = 1$, a polynomial equation of degree n, while, as we have seen in Section 2, standard RK schemes are bound to fail. Similarly, when $G = \mathrm{SO}(d)$, the set of orthogonal matrices, with Lie-groups schemes we can employ an explicit Lie-group RK method and obtain an orthogonal approximation, while with standard schemes we would require that the RK method obeys the condition (10), hence being an implicit scheme.

Such Lie-group schemes do not apply only to Lie groups, but also to a wider class of problems, evolving on *homogeneous spaces* [17], i.e. manifolds on which the dynamics is described by a Lie-group action. In this setting, one can obtain the classical Runge–Kutta schemes as a particular case of Lie-group Runge–Kutta methods for which the acting Lie-group is $\mathbb{R}^d$ with the group operation '+' and the manifold acted upon is also $\mathbb{R}^d$. In this framework, one might choose different group action and preserve different underlying geometrical features of the problem in question. The search for a good action has to take into account the 'qualitative features' preserved as well as the computational cost of the scheme, and is an open problem currently under investigation.

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