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# Partitioned Runge–Kutta methods as phase volume preserving integrators

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**Abstract**

We analyse the property of phase volume preservation for the partitioned Runge–Kutta methods. A family of explicit methods known to be symplectic is demonstrated to possess the volume preservation property as well. Runge–Kutta–Nyström methods are also considered.

## 1. Introduction

In the last decade the idea of preservation of integral invariants by the numerical solution on nonlinear differential equations has enjoyed great popularity. While the preservation of the *symplectic structure* by numerical integrators has become already a well-established part of numerical analysis, and even the first monograph on this subject has recently appeared [1], investigations of this property for other integral invariants are only beginning now.

In particular, the preservation of such an invariant as the *phase volume* is receiving growing attention [2–6]. It is well known that invariance of the symplectic structure or of the phase volume has an important influence on the long-term behaviour of dynamical systems [7]. Groups of diffeomorphisms having these properties play an important role in mathematical physics (cf., e.g., Refs. [7,8], and references therein). From the dynamical point of view symplectic maps and those preserving phase volume have many common features (for example, certain variants of KAM theory hold for both classes of maps, cf. Ref. [9]). However, these two classes of maps are also known to occur in many issues of a different nature (cf. the Eliashberg–Gromov theorem on the rigidity property of symplectic maps, stating that a general volume preserving map cannot be approximated by simplectic ones in $C^0$ topology, see Ref. [10]). Hence it is important to distinguish between these two classes of dynamical systems also by their numerical investigations.

In Refs. [3–6] were presented several new algorithms specially designed for source-free systems and resulting in phase volume preserving maps when integrating such systems.

Our aim in this paper is different. Rather than to invent new algorithms, we analyse under which conditions the *general purpose* integrators of the Runge–Kutta type preserve the phase volume. We also compare this property with symplecticity. We demonstrate that certain methods, previously known to be symplectic, are also phase volume preserving. However, it turns out that in general the relation between these two

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properties is rather delicate: neither of them implies, generally speaking, the other.

## 2. Some differential equations with phase volume invariant

In the present paper we will be concerned with systems of ordinary differential equations of the following type,

$$\dot{x} = g(y), \quad \dot{y} = f(x), \quad x \in \mathbb{R}^p, \quad y \in \mathbb{R}^q. \tag{1}$$

Such systems trivially possess an important qualitative feature: the phase flow in $\mathbb{R}^{p+q}\{x, y\}$ preserves the phase volume $(p+q)$-form $dx_1 \wedge \ldots \wedge dx_p \wedge dy_1 \wedge \ldots \wedge dy_q$. An equivalent expression for this fact: if $(x(0), y(0)) \mapsto (x(t), y(t))$ is the time $t$ shift along the trajectories of the system (1), then

$$\det \frac{\partial(x(t), y(t))}{\partial(x(0), y(0))} = 1$$

for all $t$ and in the whole phase space.

An important particular case of (1) constitute conservative second-order systems corresponding to $p = q$, $g(y) = y$, so that

$$\ddot{x} = \dot{y} = f(x), \quad x \in \mathbb{R}^p. \tag{2}$$

Another important particular case with $p = q$ constitute Hamiltonian systems with separable Hamiltonians $H(x, y) = T(y) + U(x)$,

$$\dot{x} = \operatorname{grad} T(y), \quad \dot{y} = -\operatorname{grad} U(x), \quad x, y \in \mathbb{R}^p. \tag{3}$$

For such equations not only the $(2p)$-form of the phase volume is preserved, but also the symplectic two-form $dx_1 \wedge dy_1 + \ldots + dx_p \wedge dy_p$. Note that, generally speaking, this two-form is not preserved by the flows described by equations of type (1) or (2).

*Remark.* Note that Eqs. (1) constitute, in turn, a particular case of more general source-free systems,

$$\dot{x}_s = f_s(x_1, \ldots, x_{s-1}, x_{s+1}, \ldots, x_n), \quad x_s \in \mathbb{R}^{p_s}, \quad 1 \leqslant s \leqslant n,$$

so that $\partial f_s / \partial x_s = 0$. The construction of partitioned Runge–Kutta methods can be generalised for such systems, along with an analysis below, but we will not develop this point in the present paper. See Refs. [3–6] for some other integrators applicable to such systems.

## 3. Runge–Kutta type methods

The well-known Runge–Kutta methods are applicable to an arbitrary system of ordinary differential equations. However, it is well known (cf., e.g., Refs. [1,2]) that restricting to some special classes of differential equations allows one to construct special methods of the Runge–Kutta type often being more effective than general ones.

We will consider in the present paper two such classes of special Runge–Kutta type methods: partitioned Runge–Kutta methods (PRK) applicable to systems of type (1), and Runge–Kutta–Nyström methods (RKN) applicable to systems of type (2).

The formulas of a general $m$-stage PRK method with time step $h$ applied to system (1) read

$$\xi_i = x_n + h \sum_{j=1}^{m} d_{ij} g(\eta_j), \quad \eta_i = y_n + h \sum_{j=1}^{m} c_{ij} f(\xi_j), \quad 1 \leqslant i \leqslant m \tag{4}$$

$$x_{n+1} = x_n + h \sum_{j=1}^{m} \delta_j g(\eta_j),$$

$$y_{n+1} = y_n + h \sum_{j=1}^{m} \gamma_j f(\xi_j). \tag{5}$$

Here $\xi_i \in \mathbb{R}^p$, $\eta_i \in \mathbb{R}^q$ $(1 \leqslant i \leqslant m)$ are auxiliary vectors used to compute the updates $(x_{n+1}, y_{n+1})$.

In such a general setting it might well occur that the method is *reducible* to a method with a smaller number of auxiliary stages (for example, some of the vectors $\xi_i$, $\eta_i$ could be redundant, i.e. not used really in the computation of $x_{n+1}$, $y_{n+1}$, or some of the stages with different numbers could coincide identically). In what follows we consider only *irreducible* methods.

The method is completely characterized by its parameters: matrices $D = (d_{ij})_{i,j=1}^{m}$, $C = (c_{ij})_{i,j=1}^{m}$, and vectors $\delta = (\delta_1, \ldots, \delta_m)^{\mathrm{T}}$, $\gamma = (\gamma_1, \ldots, \gamma_m)^{\mathrm{T}}$. A method is called explicit, if its application does not require the solution of algebraic equations. Formulas (4), (5) define an explicit method if, for example, both the matrices $D$ and $C$ are lower triangular, and

$d_{ii}c_{ii} = 0$ for all $1 \leqslant i \leqslant m$, so that the product matrix $DC$ is strictly lower triangular.

An important role in the theory of Runge–Kutta type methods is played by the so-called adjoint methods. For example, it is easy to see that the procedure allowing one to compute $(x_n, y_n)$ starting from $(x_{n+1}, y_{n+1})$, is also a PRK method with time step $-h$ and parameters

$$D^- = e\delta^{\mathrm{T}} - D, \quad C^- = e\gamma^{\mathrm{T}} - C,$$

$$\delta^- = \delta, \quad \gamma^- = \gamma$$

(here and below $e$ stands for the $m$-dimensional vector $e = (1, \ldots, 1)^{\mathrm{T}}$).

The formulas of a general $m$-stage RKN method with time step $h$ applied to system (2) read

$$\xi_i = x_n + h\alpha_i y_n + h^2 \sum_{j=1}^{m} a_{ij} f(\xi_j), \quad 1 \leqslant i \leqslant m, \tag{6}$$

$$x_{n+1} = x_n + hy_n + h^2 \sum_{j=1}^{m} \beta_j f(\xi_j),$$

$$y_{n+1} = y_n + h \sum_{j=1}^{m} \gamma_j f(\xi_j). \tag{7}$$

It is characterized by the matrix $A = (a_{ij})_{i,j=1}^{m}$ and vectors $\alpha = (\alpha_1, \ldots, \alpha_m)^{\mathrm{T}}$, $\beta = (\beta_1, \ldots, \beta_m)^{\mathrm{T}}$, and $\gamma = (\gamma_1, \ldots, \gamma_m)^{\mathrm{T}}$.

An RKN method is explicit if, for example, the matrix $A$ is strictly lower triangular.

As before, to obtain $(x_n, y_n)$ starting from $(x_{n+1}, y_{n+1})$, one has simply to use the RKN procedure with time step $-h$ and parameters

$$A^- = A - e\beta^{\mathrm{T}} + (e - \alpha)\gamma^{\mathrm{T}},$$

$$\alpha^- = e - \alpha, \quad \beta^- = \gamma - \beta, \quad \gamma^- = \gamma.$$

Recall that systems of type (2) constitute a subclass of systems of type (1). It turns out that every PRK method (4), (5) with $\sum_{j=1}^{m} \delta_j = 1$, when applied to a system of type (2), may be rewritten in the form of the RKN method (6), (7) with

$$a_{ij} = \sum_{k=1}^{m} d_{ik}c_{kj}, \quad \alpha_i = \sum_{j=1}^{m} d_{ij}, \quad \beta_j = \sum_{k=1}^{m} \delta_k c_{kj}.$$

In other words, the parameters of the RKN method (6), (7) derived from a PRK method (4), (5) are given by

$$A = DC, \quad \alpha = De, \quad \beta = C^{\mathrm{T}}\delta, \quad \gamma = \gamma. \tag{8}$$

## 4. The formulas for the rate of phase volume change

To formulate the result concerning the rate of the phase volume change for PRK methods, we will need the following compact notations,

$$\boldsymbol{D} = D \otimes E_p, \quad \boldsymbol{C} = C \otimes E_q,$$

$$\boldsymbol{\delta} = \delta \otimes E_p, \quad \boldsymbol{\gamma} = \gamma \otimes E_q,$$

$$\boldsymbol{D}^- = D^- \otimes E_p, \quad \boldsymbol{C}^- = C^- \otimes E_q$$

(here and below $\otimes$ denotes the Kronecker product, and $E_p$ stands for the $p \times p$ identity matrix),

$$\mathcal{F} = \mathrm{diag}(f'(\xi_1), \ldots, f'(\xi_m)),$$

$$\mathcal{G} = \mathrm{diag}(g'(\eta_1), \ldots, g'(\eta_m)).$$

(Obviously, the last two matrices are $mq \times mp$ and $mp \times mq$ block diagonal matrices, respectively.)

We will need also the following well-known fact from the linear algebra.

*Lemma.* Let $a$ and $d$ be non-degenerate $M \times M$ and $N \times N$ matrices, respectively, $b$ an $M \times N$ matrix, and $c$ an $N \times M$ matrix. Then

$$\det(a)\det(d + ca^{-1}b) = \det(d)\det(a + bd^{-1}c).$$

Now we are in a position to formulate and prove the first of our main results.

*Proposition 1.* For an arbitrary PRK method:

$$\det \frac{\partial(x_{n+1}, y_{n+1})}{\partial(x_n, y_n)} = \frac{\det(E_{mp} - h^2\boldsymbol{D}^-\mathcal{G}\boldsymbol{C}^-\mathcal{F})}{\det(E_{mp} - h^2\boldsymbol{D}\mathcal{G}\boldsymbol{C}\mathcal{F})} = \frac{\det(E_{mq} - h^2\boldsymbol{C}^-\mathcal{F}\boldsymbol{D}^-\mathcal{G})}{\det(E_{mq} - h^2\boldsymbol{C}\mathcal{F}\boldsymbol{D}\mathcal{G})}. \tag{9}$$

*Proof.* In order to have a more compact notation we set additionally

$$\boldsymbol{\xi} = (\xi_1, \ldots, \xi_m)^{\mathrm{T}}, \quad \boldsymbol{\eta} = (\eta_1, \ldots, \eta_m)^{\mathrm{T}},$$

$$f(\xi) = (f(\xi_1), \dots, f(\xi_m))^{\mathrm{T}},$$

$$g(\eta) = (g(\eta_1), \dots, g(\eta_m))^{\mathrm{T}},$$

$$e_p = e \otimes E_p, \quad e_q = e \otimes E_q.$$

Then formulas (4), (5) take the form

$$\xi = e_p x_n + h\boldsymbol{D}g(\eta), \quad \eta = e_q y_n + h\boldsymbol{C}f(\xi),$$

$$x_{n+1} = x_n + h\boldsymbol{\delta}^{\mathrm{T}} g(\eta), \quad y_{n+1} = y_n + h\boldsymbol{\gamma}^{\mathrm{T}} f(\xi).$$

This implies straightforwardly the following expression for the Jacobi matrix of the map generated by PRK,

$$\frac{\partial(x_{n+1}, y_{n+1})}{\partial(x_n, y_n)} = \begin{pmatrix} E_p & 0 \\ 0 & E_q \end{pmatrix} + h \begin{pmatrix} 0 & \boldsymbol{\delta}^{\mathrm{T}}\mathcal{G} \\ \boldsymbol{\gamma}^{\mathrm{T}}\mathcal{F} & 0 \end{pmatrix} \times \left[ E_{m(p+q)} - h \begin{pmatrix} 0 & \boldsymbol{D}\mathcal{G} \\ \boldsymbol{C}\mathcal{F} & 0 \end{pmatrix} \right]^{-1} \begin{pmatrix} e_p & 0 \\ 0 & e_q \end{pmatrix}.$$

According to the lemma above, we obtain

$$\det \frac{\partial(x_{n+1}, y_{n+1})}{\partial(x_n, y_n)} = \frac{\det \left[ E_{m(p+q)} + h \begin{pmatrix} 0 & \boldsymbol{D}^{-}\mathcal{G} \\ \boldsymbol{C}^{-}\mathcal{F} & 0 \end{pmatrix} \right]}{\det \left[ E_{m(p+q)} - h \begin{pmatrix} 0 & \boldsymbol{D}\mathcal{G} \\ \boldsymbol{C}\mathcal{F} & 0 \end{pmatrix} \right]}.$$

This implies immediately the statement of Proposition 1.

To formulate a corresponding result for RKN methods, we will need the following additional notations,

$$\boldsymbol{A} = A \otimes E_p, \quad \boldsymbol{A}^{-} = A^{-} \otimes E_p.$$

*Proposition 2.* For an arbitrary RKN method

$$\det \frac{\partial(x_{n+1}, y_{n+1})}{\partial(x_n, y_n)} = \frac{\det(E_{mp} - h^2 \boldsymbol{A}^{-}\mathcal{F})}{\det(E_{mp} - h^2 \boldsymbol{A}\mathcal{F})}. \tag{10}$$

*Proof.* In our compact notations, supplied by

$$\boldsymbol{\alpha} = \alpha \otimes E_p, \quad \boldsymbol{\beta} = \beta \otimes E_p,$$

formulas (6), (7) take the form

$$\xi = e_p x_n + h\boldsymbol{\alpha} y_n + h^2 \boldsymbol{A} f(\xi),$$

$$x_{n+1} = x_n + h y_n + h^2 \boldsymbol{\beta}^{\mathrm{T}} f(\xi),$$

$$y_{n+1} = y_n + h\boldsymbol{\gamma}^{\mathrm{T}} f(\xi).$$

This implies

$$\frac{\partial(x_{n+1}, y_{n+1})}{\partial(x_n, y_n)} = \begin{pmatrix} E_p & hE_p \\ 0 & E_p \end{pmatrix} + \begin{pmatrix} h^2\boldsymbol{\beta}^{\mathrm{T}} \\ h\boldsymbol{\gamma}^{\mathrm{T}} \end{pmatrix} \mathcal{F}(E_{mp} - h^2 \boldsymbol{A}\mathcal{F})^{-1} \begin{pmatrix} e_p & h\boldsymbol{\alpha} \end{pmatrix}.$$

Now the result follows upon application of the lemma above.

*Remark.* Note that for RKN methods derived from PRK methods, formula (10) follows directly from (9) and (8), as in the case $p = q$, $g(y) = y$ one trivially has $\mathcal{G} = E_{mp}$.

## 5. Explicit volume preserving integrators

Before we give complete criteria for PRK and RKN methods to be phase volume preserving, we give here important examples.

*Proposition 3.* Let an explicit PRK method be characterized by the following relations,

$$d_{ij} = c_{ij} = 0 \quad \text{for } i \leqslant j,$$

$$d_{ij} = \delta_j, \quad c_{ij} = \gamma_j \quad \text{for } i > j, \tag{11}$$

$$d_{ii} = \delta_i, \quad c_{ii} = 0 \quad \text{or } d_{ii} = 0, \quad c_{ii} = \gamma_j. \tag{12}$$

Then it preserves phase volume for an arbitrary system of type (1).

*Proposition 4.* Let an explicit RKN method be characterized by the following relations,

$$\beta_i = \gamma_i(1 - \alpha_i), \tag{13}$$

$$a_{ij} = 0 \quad \text{for } i \leqslant j,$$

$$a_{ij} = \gamma_j(\alpha_i - \alpha_j) \quad \text{for } i > j. \tag{14}$$

Then it preserves phase volume for an arbitrary system of type (2).

The proofs are based on formulas (9), (10). Indeed, under conditions (11), (12) the matrix $\boldsymbol{D}\mathcal{G}\boldsymbol{C}\mathcal{F}$ is strictly lower triangular, while the matrix $\boldsymbol{D}^{-}\mathcal{G}\boldsymbol{C}^{-}\mathcal{F}$ is strictly upper triangular, so that both the numerator and the denominator in the right-hand side of (9) are identically equal to 1. Analogously, under conditions (13), (14) the matrix $\boldsymbol{A}\mathcal{F}$ is strictly lower triangular, the matrix $\boldsymbol{A}^{-}\mathcal{F}$ is strictly upper triangular, hence both the numerator and the denominator in the right-hand side of (10) are identically equal to 1.

*Remark 1.* The PRK methods described in Proposition 3 are known also to be symplectic for an arbitrary system of type (3) [11–14], and RKN methods described in Proposition 4 are known to be symplectic for an arbitrary system of type (2) with $f(x) = -\operatorname{grad} U(x)$ [15–16]. There exist numerous publications devoted to the construction of high order integrators of these types [17–20].

*Remark 2.* The simplest possible PRK from Proposition 3 with $m = 1$, $d_{11} = 0$, $c_{11} = 1$, $\delta_1 = \gamma_1 = 1$ is nothing else but one of Quispel's integrators [5, (31)]. Hence the methods from Proposition 3 serve as its wide generalizations. Analogous generalizations for other integrators from Ref. [5] will be given in a separate publication.

## 6. Criteria for volume preservation by RK-type methods

*Proposition 5.* A PRK method preserves phase volume for an arbitrary system of type (1) in arbitrary dimensions, if and only if

$$d_{k_1l_1}c_{l_1k_2}\dots d_{k_{r-1}l_{r-1}}c_{l_{r-1}k_r}d_{k_rl_r}c_{l_rk_1} = \bar{d}_{k_1l_1}\bar{c}_{l_1k_2}\dots \bar{d}_{k_{r-1}l_{r-1}}\bar{c}_{l_{r-1}k_r}\bar{d}_{k_rl_r}\bar{c}_{l_rk_1} \qquad (15)$$

for arbitrary $1 \leqslant r \leqslant m$ and two arbitrary ordered sets $(k_1,\dots,k_r)$ and $(l_1,\dots,l_r)$ of different natural numbers from $[1,m]$.

*Proposition 6.* An RKN method preserves phase volume for an arbitrary right-hand side $f(x)$ in arbitrary dimension, if and only if

$$a_{k_1k_2}\dots a_{k_{r-1}k_r}a_{k_rk_1} = \bar{a}_{k_1k_2}\dots \bar{a}_{k_{r-1}k_r}\bar{a}_{k_rk_1} \qquad (16)$$

for arbitrary $1 \leqslant r \leqslant m$ and arbitrary ordered set $(k_1,\dots,k_r)$ of different natural numbers from $[1,m]$.

We first comment on these results.

Recall that for PRK methods

$$\bar{d}_{ij} = \delta_j - d_{ij}, \quad \bar{c}_{ij} = \gamma_j - c_{ij}.$$

Formula (15) with $r = 1$, $(k_1,l_1) = (i,j)$ reads $d_{ij}c_{ji} = \bar{d}_{ij}\bar{c}_{ji}$, which is equivalent to

$$\gamma_i d_{ij} + \delta_j c_{ji} - \gamma_i\delta_j = 0, \qquad (17)$$

i.e. to the necessary and sufficient condition for PRK to be symplectic on the class of separable Hamiltonian equations (3) [11,12,14]. Hence *volume preserving PRK methods form a subset of symplectic ones.*

The situation is different *for RKN methods: neither of these two properties implies the other.* Recall that

$$\bar{a}_{ij} = a_{ij} - \beta_j + \gamma_j(1-\alpha_i).$$

Hence (16) with $r = 1$, $k_1 = i$ is equivalent to $\beta_i = \gamma_i(1-\alpha_i)$, i.e. to (13), and under this condition (16) with $r = 2$, $(k_1,k_2) = (i,j)$ is equivalent to

$$(\alpha_i - \alpha_j)[\gamma_i a_{ij} - \gamma_j a_{ji} - \gamma_i\gamma_j(\alpha_i - \alpha_j)] = 0. \qquad (18)$$

The vanishing of the second factor in (18) is equivalent to the symplecticity of the RKN method [15,16], but, as we see, it is *not necessary* for the phase volume preservation, because the first factor in (14) might vanish as well. A simple example of the phase volume preserving RKN method, which is not symplectic,

$$m = 2, \quad A = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & 0 \end{pmatrix},$$

$$\alpha = (\tfrac{1}{2},\tfrac{1}{2})^{\mathrm{T}}, \quad \beta = (\tfrac{1}{2},\tfrac{1}{2})^{\mathrm{T}}, \quad \gamma = (\tfrac{1}{4},\tfrac{1}{4})^{\mathrm{T}}.$$

Note, however, that a symplectic RKN method also does not necessarily preserve phase volume for an arbitrary $f(x)$ (although the contrary is alleged, e.g., in Ref. [21]). As a simple counterexample serves the following implicit symplectic RKN method of order 6 with $m = 3$ stages,

$$A = \begin{pmatrix} \frac{1}{120} & \frac{1}{12} - \frac{1}{45}\sqrt{15} & \frac{13}{120} - \frac{1}{36}\sqrt{15} \\ \frac{5}{96} + \frac{1}{72}\sqrt{15} & \frac{1}{48} & \frac{5}{96} - \frac{1}{72}\sqrt{15} \\ \frac{13}{120} + \frac{1}{36}\sqrt{15} & \frac{1}{12} + \frac{1}{45}\sqrt{15} & \frac{1}{120} \end{pmatrix},$$

$\alpha = (\frac{1}{2} - \frac{1}{10}\sqrt{15}, \frac{1}{2}, \frac{1}{2} + \frac{1}{10}\sqrt{15})^{\mathrm{T}}$,

$\gamma = (\frac{5}{18}, \frac{4}{9}, \frac{5}{18})^{\mathrm{T}}$,

$\beta$ is defined by (13). It is straightforward to check that for this method $a_{ij}^{-} = a_{4-j,4-i}$, so that (16) with $r = 3$, $(k_1, k_2, k_3) = (1, 2, 3)$ would mean $a_{12}a_{23}a_{31} = a_{32}a_{21}a_{13}$, which is false.

The proofs of propositions 5, 6 are similar, so we restrict ourselves here to the simpler one, namely that of Proposition 6. We start with formula (10). In order for its left-hand side to be identically equal to 1 for an arbitrary smooth function $f(x)$ in the dimension $p$ the following two polynomials on the $mp^2$ nonvanishing elements of the matrix $\mathcal{F}$ have to coincide identically: $\det(E_{mp} + A\mathcal{F})$ and $\det(E_{mp} + A^{-}\mathcal{F})$. (Since we are concerned only with irreducible methods, these elements have to be considered as independent variables.) [2] It is easy to obtain the following expression,

$$\det(E_{mp} + A\mathcal{F}) = 1 + \sum A\begin{pmatrix} J \\ I \end{pmatrix} \mathcal{F}_{i_1 j_1} \dots \mathcal{F}_{i_n j_n}.$$

Here $I = (i_1, \dots, i_n)$, $J = (j_1, \dots, j_n)$ run over all pairs of ordered sets of $n \leqslant mp$ different natural numbers from $[1, mp]$ satisfying, due to the block-diagonal structure of the matrix $\mathcal{F}$, the following condition:

(P) For each $1 \leqslant s \leqslant n$, the elements $i_s$ and $j_s$ belong to one and the same interval of the type $[(k-1)p + 1, kp]$ $(1 \leqslant k \leqslant m)$.

We use the notation $A\binom{J}{I}$ for the minor of the matrix $A$ composed of the elements of the rows $j_1, \dots, j_n$, and the columns $i_1, \dots, i_n$.

So we obtain the following statement:

An RKN method preserves phase volume for an arbitrary right-hand side in dimension $p$ if and only if

$$A\begin{pmatrix} J \\ I \end{pmatrix} = A^{-}\begin{pmatrix} J \\ I \end{pmatrix} \tag{19}$$

for all sequences $I$, $J$ satisfying the property (P).

[2] Indeed, consider $m$ arbitrary $p \times p$ matrices $F_1, \dots, F_m$; further, take $m$ arbitrary though distinct $p$-dimensional vectors $f_1, \dots, f_m$, and construct $m$ vectors $\xi_1, \dots, \xi_m$ according to the formula $\xi_i = x + h\alpha_i y + h^2 \sum_{j=1}^{m} a_{ij} f_j$. Then there exists a smooth function $f(x) : \mathbb{R}^p \mapsto \mathbb{R}^p$ satisfying $f(\xi_i) = f_i$, $f'(\xi_i) = F_i$, $1 \leqslant i \leqslant m$.

We need now to express this criterion in terms of the matrix $A$ proper, rather than $A = A \otimes E_p$.

To see that (16) is sufficient for (19), note that $A\binom{J}{I}$ is a sum of monomials of the form $\pm A_{j_1 l_1} \dots A_{j_n l_n}$, where $(l_1, \dots, l_n)$ is a permutation of $(i_1, \dots, i_n)$. If in such a monomial $j_s \not\equiv l_s \pmod p$ for some $1 \leqslant s \leqslant n$, then the whole monomial vanishes, as well as an analogous monomial for the matrix $A^{-}$. Each nonvanishing monomial takes the form $\pm a_{u_1 v_1} \dots a_{u_n v_n}$, where all integers $u_s$, $v_s$ belong to $[1, m]$, and, according to the property (P), the sequence $(u_1, \dots, u_n)$ is a permutation of the sequence $(v_1, \dots, v_n)$. Since each substitution $\binom{u_1 \dots u_n}{v_1 \dots v_n}$ may be decomposed in a product of cycles $\binom{k_1 \dots k_{r-1}\ k_r}{k_2 \dots k_r\ \ k_1}$, the sufficiency of (16) is demonstrated.

To prove that (16) is also necessary for (19), take $p > m$, so that for every $1 \leqslant r \leqslant m$ we have also $r < p$, and consider sets $J$, $I$ consisting of following $n = r$ elements,

$$j_1 = (k_1 - 1)p + 1, \quad j_2 = (k_2 - 1)p + 2, \dots,$$
$$j_r = (k_r - 1)p + r,$$
$$i_1 = (k_1 - 1)p + r, \quad i_2 = (k_2 - 1)p + 1, \dots,$$
$$i_r = (k_r - 1)p + r - 1.$$

Due to $r < p$ they satisfy condition (P). It is easy to see that

$$A\begin{pmatrix} J \\ I \end{pmatrix} = \pm a_{k_1 k_2} \dots a_{k_{r-1} k_r} a_{k_r k_1},$$

which ends the proof.

## 7. Conclusion

We analysed in this Letter the phase volume preservation by Runge–Kutta type methods when applied to the systems

$$\dot{x} = g(y), \quad \dot{y} = f(x), \quad x \in \mathbb{R}^p, \quad y \in \mathbb{R}^q.$$

We demonstrated that large classes of *explicit* volume preserving integrators of *arbitrary high order* exist.

This analysis may be generalised for a larger class of systems, namely for

$$\dot{x}_s = f_s(x_1, \dots, x_{s-1}, x_{s+1}, \dots, x_n),$$
$$x_s \in \mathbb{R}^{p_s}, \quad 1 \leqslant s \leqslant n.$$

It turns out that there exist (multi-)partitioned Runge–Kutta methods of an arbitrary high order, which preserve phase volume when applied to such systems. The details will be presented elsewhere.

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