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Explicit volume-preserving and symplectic integrators for trigonometric polynomial flows

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Abstract

We introduce explicit volume-preserving and symplectic integrators for the case of generalized trigonometric polynomial flows. The method is demonstrated using the Arter flow, and computational trials are conducted using a 4-dimensional vector field.

Keywords: Geometric integration; Symplectic integration; Volume-preserving integration

1. Introduction

The growing interest in structure-preserving numerical integrators for systems of ordinary differential equations has recently been espoused by many authors, including McLachlan and Quispel [1] and Hairer et al. [23]. The need for exact preservation of features such as first integrals [2–6], symmetries [7,9], phase-space volume [11,12] and other structural features is well understood, and integrators preserving them are collectively called "geometric integrators". Many types of geometric integrators have been shown to have superior error-growth behaviour, with linear error growth for (certain) periodic and quasi-periodic problems, rather than the quadratic growth given by most standard, non-geometric integrators (see [18], for example).

A feature common to most of these geometric integrators is that they result in a system of implicit difference equations. There are some exceptions to this, for example many splitting methods [10,26], the explicit partitioned Runge–Kutta methods, and Runge–Kutta–Nyström methods discussed by Sanz-Serna and Calvo [13]. Explicit methods offer the possibility of faster execution, along with the absence of

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the need to ensure convergence of the implicit loop needed at each step of an implicit method. In a calculation where extremely long run-times are required, such as in the case of astronomical models, a method that offers desirable geometric features plus higher speed and accuracy is clearly worth considering.

Our principal interest here relates to the construction of volume-preserving integrators for source-free vector fields, of particular importance in fluid dynamics [14]. Although two general methods for this problem are known, they are both *implicit* [8,11,12,15,17]. In this paper, we construct *explicit* integrators for a large subclass of source-free vector fields.

In this paper, we are concerned with source-free vector fields that are polynomial functions of trigonometric functions of the field variables, cf. also [24]. In this case we show that a unique splitting can be constructed in which the individual vector fields are source free and explicitly exactly integrable. The exact solution for each field is given by the explicit Euler method, from which higher order integrators can be constructed, e.g., via the generalized Yoshida method [19,20].

2. An example: the Arter flow

Before we present our method in full generality, we first demonstrate it on an example, the 3-dimensional *Arter flow* of fluid dynamics

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \mathbf{v}(x,y,z), \tag{1}$$

where the vector field $\mathbf{v}(x,y,z)$ is given by

$$\mathbf{v}(x,y,z) = \begin{pmatrix} -\sin x\cos y\cos z + b\sin 2x\cos 2z \\ -\cos x\sin y\cos z + b\sin 2y\cos 2z \\ 2\cos x\cos y\sin z - b(\cos 2x + \cos 2y)\sin 2z \end{pmatrix} \tag{2}$$

and b is a parameter. It is easy to check that $\mathbf{v}(x,y,z)$ is divergence free.

Using repeated applications of the product formulae

$$\begin{aligned} \sin\alpha\cos\beta &= \frac{1}{2}\sin(\alpha+\beta) + \frac{1}{2}\sin(\alpha-\beta), \\ \sin\alpha\sin\beta &= -\frac{1}{2}\cos(\alpha+\beta) + \frac{1}{2}\cos(\alpha-\beta), \\ \cos\alpha\cos\beta &= \frac{1}{2}\cos(\alpha+\beta) + \frac{1}{2}\cos(\alpha-\beta) \end{aligned} \tag{3}$$

the vector field $\mathbf{v}$ can be split as follows:

$$\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2 + \cdots + \mathbf{v}_7 + \mathbf{v}_8, \tag{4}$$

where

$$\begin{aligned}
\mathbf{v}_1 &= \sin(x+y+z)\begin{pmatrix}-1/4\\-1/4\\1/2\end{pmatrix}, \quad \mathbf{v}_2 = \sin(x+y-z)\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix},\\
\mathbf{v}_3 &= \sin(x-y+z)\begin{pmatrix}-1/4\\1/4\\1/2\end{pmatrix}, \quad \mathbf{v}_4 = \sin(x-y-z)\begin{pmatrix}-1/4\\1/4\\-1/2\end{pmatrix},\\
\mathbf{v}_5 &= \sin(2y+2z)\begin{pmatrix}0\\b/2\\-b/2\end{pmatrix}, \quad \mathbf{v}_6 = \sin(2y-2z)\begin{pmatrix}0\\b/2\\b/2\end{pmatrix},\\
\mathbf{v}_7 &= \sin(2x+2z)\begin{pmatrix}b/2\\0\\-b/2\end{pmatrix}, \quad \mathbf{v}_8 = \sin(2x-2z)\begin{pmatrix}b/2\\0\\b/2\end{pmatrix}.
\end{aligned} \tag{5}$$

The first thing to notice about the vector fields $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_8$ is that each of them is divergence free (as can be easily checked). That is not a big deal, however, since there are much simpler ways to split the Arter flow into divergence-free vector fields [15,18]. The truly miraculous thing about the splitting (5) is that each vector field $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_8$ is explicitly exactly integrable! Let us demonstrate this on $\mathbf{v}_2$.

The vector field $\mathbf{v}_2$ corresponds to the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}x\\y\\z\end{pmatrix} = \sin(x+y-z)\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix}. \tag{6}$$

To solve (6), we note that this ODE has the integral (i.e., conserved quantity) $I_2 = x+y-z$, because

$$\frac{\mathrm{d}}{\mathrm{d}t}(x+y-z) = \left(-\frac{1}{4}-\frac{1}{4}+\frac{1}{2}\right)\sin(x+y-z) = 0.$$

This means that the vector field is constant on orbits and the exact solution of (6) is given by

$$\begin{pmatrix}x(\tau)\\y(\tau)\\z(\tau)\end{pmatrix} = \varphi_{2,\tau}\begin{pmatrix}x(0)\\y(0)\\z(0)\end{pmatrix}, \tag{7}$$

where the map $\varphi_{2,\tau}$ is given by

$$\varphi_{2,\tau}\begin{pmatrix}x(0)\\y(0)\\z(0)\end{pmatrix} = \begin{pmatrix}x(0)\\y(0)\\z(0)\end{pmatrix} + \tau\sin(x(0)+y(0)-z(0))\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix}, \tag{8}$$

i.e., Euler's method applied to $\mathbf{v}_2$!

The integration of $\mathbf{v}_1, \mathbf{v}_3, \ldots, \mathbf{v}_8$ proceeds completely analogously, using their respective integrals

$$\begin{aligned}
&I_1 = x+y+z, \quad I_3 = x-y+z, \quad I_4 = x-y-z, \quad I_5 = 2y+2z,\\
&I_6 = 2y-2z, \quad I_7 = 2x+2z, \quad I_8 = 2x-2z.
\end{aligned} \tag{9}$$

With these integrals, it is easily shown that the exact flows $\varphi_{i,\tau}$ of the vector fields $\mathbf{v}_i$ are given by Euler's method, i.e.,

$$\varphi_{i,\tau}\begin{pmatrix} x(0) \\ y(0) \\ z(0) \end{pmatrix} = \begin{pmatrix} x(0) \\ y(0) \\ z(0) \end{pmatrix} + \tau \mathbf{v}_i(x(0), y(0), z(0)). \tag{10}$$

An explicit first-order volume-preserving integrator for the Arter flow (1) and (2) is then given by

$$\psi_\tau = \varphi_{1,\tau} \circ \varphi_{2,\tau} \circ \varphi_{3,\tau} \circ \varphi_{4,\tau} \circ \varphi_{5,\tau} \circ \varphi_{6,\tau} \circ \varphi_{7,\tau} \circ \varphi_{8,\tau} \tag{11}$$

and explicit volume-preserving integrators of any order are obtained using composition methods [10,19], see below.

3. The general case

We now describe our method for a general trigonometric divergence-free vector field

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n, \tag{12}$$

where the vector field $\mathbf{v}$ is a polynomial in *sines and cosines* of multiples of the variables $x_1, \ldots, x_n$:

$$v_i(\mathbf{x}) = P_i(\{\sin(ax)\}, \{\cos(ax)\}), \tag{13}$$

where $\{\sin(ax)\}$ denotes the list

$$\sin(a_{11}x_1), \sin(a_{21}x_1), \ldots, \sin(a_{m1}x_1), \sin(a_{12}x_2), \ldots, \sin(a_{1n}x_n), \ldots,$$

and similarly for $\{\cos(ax)\}$, and where $\mathbf{v}$ is divergence free, i.e.,

$$\sum_{i=1}^{n} \frac{\partial v_i}{\partial x_i} = 0. \tag{14}$$

A typical term in such a polynomial will have the form

$$\prod_{i,j} \sin^{m_{ij}}(a_{ij}x_j)\cos^{m'_{ij}}(b_{ij}x_j). \tag{15}$$

As noted (for example) by Hardy [21], this can be expressed as the sum of a finite number of terms of the form

$$\alpha\cos\left(\sum_{i=1}^{m}\sum_{j=1}^{n}(p_{ij}a_{ij} + q_{ij}b_{ij})x_j\right) + \beta\sin\left(\sum_{i=1}^{m}\sum_{j=1}^{n}(p_{ij}a_{ij} + q_{ij}b_{ij})x_j\right),$$

using identities such as the product formulae (3) above. (Here p_{ij} and q_{ij} are integers satisfying $-m_{ij} \leqslant p_{ij} \leqslant m_{ij}$, $-m'_{ij} \leqslant q_{ij} \leqslant m'_{ij}$.)

Hence $\mathbf{v}$ can be expressed in the following simpler form:

$$\mathbf{v}(\mathbf{x}) = \sum_{k_1,k_2,\ldots,k_n} \mathbf{v}_{k_1,k_2,\ldots,k_n}(\mathbf{x}), \tag{16}$$

where

$$\mathbf{v}_{k_1,k_2,\ldots,k_n}(\mathbf{x}) = \sin(k_1x_1 + k_2x_2 + \cdots + k_nx_n)\mathbf{c}_{k_1,k_2,\ldots,k_n} + \cos(k_1x_1 + k_2x_2 + \cdots + k_nx_n)\mathbf{d}_{k_1,k_2,\ldots,k_n}. \tag{17}$$

Here, **c** and **d** are constant vectors. Note (i) that the vectors **d** are zero in the expansion (5) of the Arter flow, because the Arter flow is an *odd* vector field; (ii) the coefficients in the expansion $z^m = \sum_{i=0}^{m} r_{m,i} T_i(z)$, where T_i is the ith Chebyshev polynomial of the first kind, are known explicitly (cf. for example [25]). Therefore $\cos^m(x) = \sum_{i=0}^{m} r_{m,i}\cos(ix)$. Similarly for sine functions and Chebyshev polynomials of the second kind. Hence, the first constructive step in going from (15) to (16) could be to express the product (15) in terms of T_is and U_js, followed by an application of standard trigonometric identities; (iii) that the process above can also be implemented in the case where the vectors **k** are incommensurate, leading to the class of functions known as generalized trigonometric polynomials, which in turn belong to the set of almost periodic functions (in the sense of Bohr) (see [22]).

From the fact that **v** is source free it follows that

$$\nabla \cdot \mathbf{v} = \sum_{\mathbf{k}} \mathbf{k} \cdot \mathbf{c}_{\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{x}) - \mathbf{k} \cdot \mathbf{d}_{\mathbf{k}} \sin(\mathbf{k} \cdot \mathbf{x}) = 0 \tag{18}$$

and hence (since all sines and cosines appearing in the sum are linearly independent)

$$\mathbf{k} \cdot \mathbf{c}_{\mathbf{k}} = 0 \text{ and } \mathbf{k} \cdot \mathbf{d}_{\mathbf{k}} = 0 \quad \text{for all } \mathbf{k}. \tag{19}$$

Thus it follows readily that each vector field $\mathbf{v}_{\mathbf{k}}$ given by (17) is nilpotent [16], and is again integrable with integral $I_{\mathbf{k}} = \mathbf{k} \cdot \mathbf{x}$ and can hence be integrated exactly using Euler's method

$$\varphi_{\mathbf{k},\tau}(\mathbf{x}(0)) = \mathbf{x}(0) + \tau \mathbf{v}_{\mathbf{k}}(\mathbf{x}(0)). \tag{20}$$

An explicit first-order volume-preserving integrator for the vector field (12) is then given by

$$\psi_\tau = \prod_{\mathbf{k}} \varphi_{\mathbf{k},\tau}, \tag{21}$$

where the product $\prod$ denotes composition of maps.

An explicit second-order integrator (hereafter referred to as RQ2) is given by the composition $\psi_{\tau/2} \circ \psi^{-1}_{-\tau/2}$, where ψ is given by (21), and explicit volume-preserving integrators of any order are obtained using composition methods [1] [10,19].

We get the Hamiltonian case as a bonus! If **v** above had a Hamiltonian H, then H must have the form

$$H = \sum_{\mathbf{k}} a_{\mathbf{k}} \sin(\mathbf{k} \cdot \mathbf{x}) + b_{\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{x}) \tag{22}$$

hence

$$\mathbf{v} = \sum_{\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{x}) a_{\mathbf{k}} \Omega \cdot \mathbf{k} - \sin(\mathbf{k} \cdot \mathbf{x}) b_{\mathbf{k}} \Omega \cdot \mathbf{k}, \tag{23}$$

where Ω is the symplectic matrix. The volume-preserving splitting before gives

$$\mathbf{v} = \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}}, \tag{24}$$

where

$$\mathbf{v}_{\mathbf{k}} = \cos(\mathbf{k} \cdot \mathbf{x}) a_{\mathbf{k}} \Omega \cdot \mathbf{k} - \sin(\mathbf{k} \cdot \mathbf{x}) b_{\mathbf{k}} \Omega \cdot \mathbf{k}. \tag{25}$$

[1] Since ψ_τ is the product of exact flows, its adjoint $\psi^{-1}_{-\tau}$ is also explicit.

But in this case $\mathbf{v_k}$ is a Hamiltonian vectorfield:

$$\mathbf{v_k} = \Omega \nabla H_{\mathbf{k}}(\mathbf{k} \cdot \mathbf{x}), \tag{26}$$

where

$$H_{\mathbf{k}}(\mathbf{k} \cdot \mathbf{x}) = a_{\mathbf{k}} \sin(\mathbf{k} \cdot \mathbf{x}) + b_{\mathbf{k}} \cos(\mathbf{k} \cdot \mathbf{x}) \tag{27}$$

and since the integrator $\varphi_{\mathbf{k},\tau}$ gives the exact flow of $\mathbf{v_k}$, it follows that $\varphi_{\mathbf{k},\tau}$ in this case is symplectic!

4. Numerical experiments

The Robust Quadrature method (RQ2) discussed above will be compared to results obtained using another second-order volume-preserving integrator employing Feng's splitting, referred to as FK2. (For evidence that volume-preserving integrators give superior results, see [18].)

The following 4-dimensional vector field is used: [2]

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \mathbf{v}(\mathbf{x}) = \sum_{i=1}^{7} \mathbf{v}_i(\mathbf{x}), \tag{28}$$

where

$$\begin{aligned} &\mathbf{v}_1 = c_1 \sin(y+z)\begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \quad \mathbf{v}_2 = c_2 \sin(x+y)\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \\ &\mathbf{v}_3 = c_3 \sin(x-w)\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{v}_4 = c_4 \cos(z+w)\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \\ &\mathbf{v}_5 = c_5 \sin(x-z)\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{v}_6 = c_6 \cos(x+y)\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \\ &\mathbf{v}_7 = c_7 \sin(y+z)\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \end{aligned} \tag{29}$$

Each of these vector fields has an integral and is ready to be treated as summarized in Eqs. (20) and (21) above.

[2] It can be shown [27] that a large class of 4-dimensional trigonometric vector fields can be written in a similar normal form, using at most seven split vector fields.

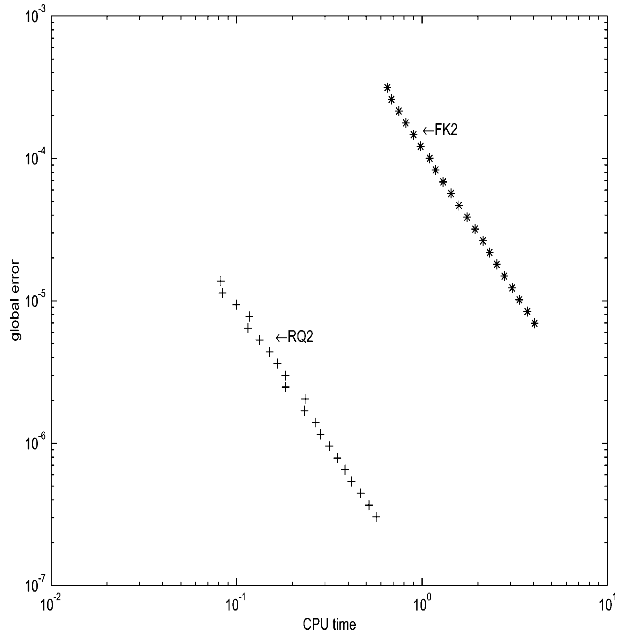

Fig. 1. Global error vs CPU time for the two integrators RQ2 and FK2, for 21 step sizes—starting at $\tau = 0.005$ and reducing exponentially by a factor of 1.1. The system was integrated up to $t_{\max} = 200$ in each case.

For FK2 the vector field $\mathbf{v}$ is split into the sum of three 2-dimensional volume-preserving parts, A, B and C, as follows:

$$A : \begin{cases} \dot{x} = f_1, \\ \dot{y} = -f_1, \\ \dot{z} = 0, \\ \dot{w} = 0, \end{cases} \quad B : \begin{cases} \dot{x} = 0, \\ \dot{y} = f_2, \\ \dot{z} = f_3, \\ \dot{w} = 0, \end{cases} \quad C : \begin{cases} \dot{x} = f_4, \\ \dot{y} = 0, \\ \dot{z} = 0, \\ \dot{w} = f_5, \end{cases} \tag{30}$$

where

$$\begin{aligned} f_1 &= c_2 \sin(x+y), \\ f_2 &= c_1 \sin(y+z) - c_3 \sin(x-w) + c_5 \sin(x-z), \\ f_3 &= -c_1 \sin(y+z) + c_2 \sin(x+y) - c_3 \sin(x-w) + c_6 \cos(x+y), \\ f_4 &= c_1 \sin(y+z) + c_3 \sin(x-w) + c_4 \cos(z+w), \\ f_5 &= -c_1 \sin(y+z) - c_2 \sin(x+y) + c_3 \sin(x-w) + c_7 \sin(y+z). \end{aligned} \tag{31}$$

The integrator FK2 is given by the composition

$$\Psi = A_{\tau/2} \circ B_{\tau/2} \circ C_{\tau} \circ B_{\tau/2} \circ A_{\tau/2} \tag{32}$$

and the five stages $A_{\tau/2}$, $B_{\tau/2}$ (both twice) and C_τ are integrated using the implicit midpoint method, [3] which is volume-preserving for 2-dimensional systems.

[3] Solved using fixed-point iteration.

The initial point for the calculated orbit is $(x, y, z, w) = (0.1, 0.1, 0.1, 0.1)$, and the parameter values are $c_1 = c_2 = -0.1$ and $c_3 = c_4 = c_5 = c_6 = c_7 = 0.1$.

The comparison of interest is maximum global error vs elapsed CPU time, for a range of step sizes, calculating up to the final t-value $t_{\max} = 200$. The code was executed using double precision on a 400 MHz Macintosh G4.

Beginning with step size $\tau_0 = 0.005$, the maximum global error and CPU times were computed, and the step size reduced by a factor of 1.1 (20 times), each reduction followed by a repeat of the computations. The "exact" solution for the error calculations was provided by a fourth-order Runge–Kutta integrator using a smaller step size (by a factor of 10). The results are summarized in Fig. 1 and indicate that RQ2 performs better for this problem.

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