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Volume-preserving integrators

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Abstract

We obtain a novel family of general n-dimensional volume-preserving integrators which can be used to numerically integrate divergence free vector fields. The ABC map and the method of Thyagaraja and Haas [Phys. Fluids 28 (1985) 1005] occur as special cases.

1. Introduction

In recent years there has been a great interest in constructing numerical integration schemes for ordinary differential equations (ODEs) in such a way that some *qualitative* geometrical property of the solution of the ODE is *exactly* preserved. This has resulted in a lot of work on integration schemes that preserve the Hamiltonian structure of the ODEs (the so-called symplectic integrators) [1–3], integrals such as momentum [4], symmetries and time-reversing symmetries [5], or energy [4].

In this Letter we are interested in preserving the source free structure of divergence free ODEs, through the construction of volume-preserving integrators (VPIs). Volume preservation is a key feature of large classes of physical systems, and to capture this feature in a numerical scheme is a difficult problem. Among other things, it is important to preserve this source free structure as it gives rise to the existence of invariant tori [6]. This has applications, e.g., in hydrodynamics [7].

Some of the first people to study VPIs were Thyagaraja and Haas [8]. They constructed VPIs for source free vector fields in three dimensions (cf. also Ref. [9]). Very recently, Feng and Wang developed another method, which works in any dimension and reduces the n-dimensional integration to the integration of two-dimensional (Hamiltonian) vector fields, using the so-called splitting method [10].

The contents of this Letter are as follows. In Section 2 we derive a new three-dimensional VPI, as an example of our method. In Section 3 we derive the main result, a family of general n-dimensional VPIs, which provide an alternative to Feng and Wang's method. The ABC map [11] and the method of Thyagaraja and Haas occur as special cases. An extended paper on this topic will be published elsewhere [12].

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2. A three-dimensional volume-preserving integrator

Consider a map $\mathbb{R}^3 \to \mathbb{R}^3$ represented implicitly by the equations

$$x_1 = f_1(x_1', x_2, x_3), \tag{1a}$$

$$x_2' = f_2(x_1', x_2, x_3), \tag{1b}$$

$$x_3' = f_3(x_1', x_2', x_3). \tag{1c}$$

It is easy to show that (1) is volume-preserving iff

$$\frac{\partial x_1}{\partial x_1'} = \frac{\partial x_2'}{\partial x_2} \frac{x_3'}{x_3}. \tag{2}$$

(For the interpretation of the notation used here, see below.)

This determines f_1 as a function of the generating functions f_2 and f_3 (up to an integration constant), and can be used to construct VPIs by projecting any integration method onto the space of VPIs (care must be taken to preserve the order of integration in this projection). As an example we here derive a first-order VPI from the explicit Euler method. Consider the ODE in $\mathbb{R}^3$,

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{v}(\boldsymbol{x}). \tag{3}$$

We assume that (3) is divergence free, i.e.

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = 0. \tag{4}$$

The explicit Euler method for integrating (3) is given by

$$x_1' = x_1 + \tau v_1(x_1, x_2, x_3), \tag{5a}$$

$$x_2' = x_2 + \tau v_2(x_1, x_2, x_3), \tag{5b}$$

$$x_3' = x_3 + \tau v_3(x_1, x_2, x_3), \tag{5c}$$

where τ denotes the time step. The integrator (5), however, is not volume-preserving. This can be remedied in the following way.

To obtain (5b) into the required form (1b) we first invert (5a) to first order in τ, i.e.

$$x_1 = x_1' - \tau v_1(x_1', x_2, x_3). \tag{6}$$

To obtain (5c) into the required form (1c) we invert (5a) and (5b) to zeroth order in τ, i.e.

$$x_1 = x_1', \quad x_2 = x_2'. \tag{7}$$

We now use (6) and (7) to obtain (1b) and (1c) to first order in τ (for this we only need the zeroth order from (6)),

$$x_2' = x_2 + \tau v_2(x_1', x_2, x_3), \tag{8a}$$

$$x_3' = x_3 + \tau v_3(x_1', x_2', x_3). \tag{8b}$$

Finally, x_1 is obtained from (8) by integration in accordance with (2),

$$\begin{aligned} x_1(x_1', x_2, x_3) &= \int^{x_1'} \frac{\partial x_2'}{\partial x_2} \frac{\partial x_3'}{\partial x_3} \, \mathrm{d}x_1' \\ &= \int^{x_1'} \left(1 + \tau \frac{\partial v_2}{\partial x_2}\right)\left(1 + \tau \frac{\partial v_3}{\partial x_3}\right) \mathrm{d}x_1'. \end{aligned} \tag{9}$$

At this point the reader should beware. Since (2) is an identity, the integrand in (9) should be expressed as a function of x_1', x_2 and x_3, i.e. (9) should be interpreted as

$$\begin{aligned} x_1(x_1', x_3, x_3) = \int^{x_1'} &[1 + \tau v_{2,2}(x_1', x_2, x_3)] \\ &\times [1 + \tau v_{3,3}(x_1', x_2 \\ &+ \tau v_2(x_1', x_3, x_3), x_3)] \, \mathrm{d}x_1', \end{aligned} \tag{10}$$

where e.g.

$$v_{3,3}(d, e, f) := \left.\frac{\partial v_3(a, b, c)}{\partial c}\right|_{a=d, b=e, c=f}.$$

The integration constant in (10) should be adjusted such that (10) agrees with (6) to first order in τ. To this end we use the fact that $\boldsymbol{v}$ is divergence free (cf. Eq. (4)) to rewrite (10), yielding

$$\begin{aligned} x_1 = x_1' &- \tau v_1(x_1', x_2, x_3) \\ &+ \int^{x_1'} [\tau v_{3,3}(x_1', x_2 + \tau v_2(x_1', x_2, x_3), x_3) \\ &- \tau v_{3,3}(x_1', x_2, x_3) \\ &+ \tau^2 v_{2,2}(x_1', x_2, x_3) v_{3,3}(x_1, x_2 \\ &+ \tau v_2(x_1', x_2, x_3), x_3)] \, \mathrm{d}x_1', \end{aligned} \tag{11a}$$

$$x_2' = x_2 + \tau v_2(x_1', x_2, x_3), \tag{11b}$$

$$x_3' = x_3 + \tau v_3(x_1', x_2', x_3). \tag{11c}$$

Note that the integrand is $O(\tau^2)$, and that (11a) agrees with (6) to first order in τ provided we also take the integration constant $O(\tau^2)$.

We point out that standard methods use only the vector field. Then there are multiderivative methods, etc. In this sense our method is slightly unusual, as it uses an integral. (There are no known VPIs, however, using only the vector field.)

3. The general n-dimensional method

Define a partition I of the set of integers

$$\{1,\dots,n\} \tag{12}$$

into k subsets

$$\{1,\dots,i_1\},\ \{i_1+1,\dots,i_2\},\dots,\{i_{k-1}+1,\dots,n\} \tag{13}$$

(with $1 \leqslant i_1 < i_2 < i < n$). Define also the correspondingly partition of the vector

$$\boldsymbol{x} = (x_1,\dots,x_n) \tag{14}$$

into k vectors

$$\boldsymbol{x} = (z_1,\dots,z_k), \tag{15a}$$

with

$$z_{j+1} := (x_{i_j+1},\dots,x_{i_{j+1}}), \quad j = 0,\dots,k-1 \tag{15b}$$

(where $i_0 := 0$, $i_k := n$). Note that the dimension of z_j may be different for different values of j.

For a given partition I, consider a map $\mathbb{R}^n \to \mathbb{R}^n$, represented implicitly by the equations

$$\begin{aligned} z_1 &= f_1(z_1', z_2,\dots,z_k),\\ z_j' &= f_j(z_1',\dots,z_{j-1}', z_j,\dots,z_k), \quad j = 2,\dots,k. \end{aligned} \tag{16}$$

It is not difficult to show that (16) is volume-preserving iff

$$\mathrm{D\tilde{e}t} = \prod_{j=2}^{k} (\mathrm{Det}_j), \tag{17}$$

where

$$\mathrm{D\tilde{e}t} := \mathrm{Det}\left(\frac{\partial z_{1,l}}{\partial z_{1,m}'}\right), \quad 1 \leqslant l,\ m \leqslant i_1, \tag{18a}$$

$$\mathrm{Det}_j := \mathrm{Det}\left(\frac{\partial z_{j,l}'}{\partial z_{j,m}}\right),$$

$$1 \leqslant l,\ m \leqslant i_j - i_{j-1}, \quad j = 2,\dots,k. \tag{18b}$$

As an example, let us indicate how (16) can be used to obtain VPIs in the case $i_1 = i$, starting from the explicit Euler method.

Consider the ODE

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{v}(\boldsymbol{x}). \tag{19}$$

We assume (19) is divergence free, i.e.

$$\nabla \cdot \boldsymbol{v} = 0. \tag{20}$$

We now use the above general partition, with $i_1 = 1$, to rewrite the ODE (19) in terms of the vectors z_j

$$\frac{\mathrm{d}z_j}{\mathrm{d}t} = \boldsymbol{v}_j(z_1,\dots,z_k), \quad j = 1,\dots,k \tag{21}$$

(where it is understood that $z_1 := z_1 = x_1$, and that $\boldsymbol{v}$ is partitioned in the same way as $\boldsymbol{x}$).

The Euler method for integrating (21) is given by

$$z_j' = z_j + \tau \boldsymbol{v}_j(z_1,\dots,z_k), \quad j = 1,\dots,k. \tag{22}$$

To make this into a VPI, we invert the first component equation of (22) (i.e. $j = 1$) to first order in τ, as an intermediate step, i.e.

$$z_1 = z_1' - \tau v_1(z_1', z_2,\dots,z_k). \tag{23}$$

Analogously to Section 2, we obtain

$$z_1(z_1', z_2,\dots,z_k) = \int^{z_1'} \left(\prod_{j=2}^{k} (\mathrm{Det}_j)\right) \mathrm{d}z_1', \tag{24a}$$

$$z_j' = z_j + \tau \boldsymbol{v}_j(z_1', z_2',\dots,z_{j-1}', z_j,\dots,z_k),$$
$$j = 2,\dots,k, \tag{24b}$$

where Det_j is defined by (18b), and it should be remembered that the integrand in (24a) must be expressed in terms of $z_1', z_2,\dots,z_k$, and the integration constant should be taken such that (24a) agrees to first order with (23).

For $i_2 = 2$ and $n = 3$, Eq. (24) reduces to the method described in Section 2. For $i_2 = n = 3$ Eq. (24) reduces to the method of Thyagaraja and Haas [8], (cf. also Ref. [9]).

Note that (24) becomes particularly simple if the integrand reduces to a constant. An example for which this special case occurs is the ODE

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = a_1 x_1 + f_1(x_2,\dots,x_n), \quad \dots,$$
$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = a_n x_n + f_n(x_1,\dots,x_{n-1}), \tag{25}$$

where the constants $a_1, \dots, a_n$ satisfy

$$\sum_{i=1}^{n} a_i = 0, \tag{26a}$$

and the functions $f_1, \dots, f_n$ satisfy

$$\frac{\partial f_i}{\partial x_i} = 0 \tag{26b}$$

(no summation is implied in (26b)). We choose the partition $i_j = j$ $(j = 1, \dots, n-1)$ to obtain

$$x_1' = \frac{x_1 + \tau f_1(x_2, \dots, x_n)}{\prod_{i=2}^{n} (1 + \tau a_i)},$$

$$x_j' = (1 + \tau a_j) x_j + \tau f_j(x_1', \dots, x_{j-1}', x_{j+1}, \dots, x_n),$$
$$j = 2, \dots, n \tag{27}$$

(the x_j and z_j are identical in this case). The ABC flow of hydrodynamics [13] is an example of the very special case $n = 3$, $a_1 = a_2 = a_3 \equiv 0$ and (27) then reduces to the so-called ABC map [11].

The choice of integrator, i.e. the choice of partition, may be adjusted to the ODE we wish to integrate. For instance, consider the ODE

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = v_1(x_{i+1}, \dots, x_n), \quad \dots,$$
$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i(x_{i+1}, \dots, x_n),$$
$$\frac{\mathrm{d}x_{i+1}}{\mathrm{d}t} = v_{i+1}(x_1, \dots, x_i), \quad \dots,$$
$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = v_n(x_1, \dots, x_i), \tag{28}$$

for some i, with $1 \leqslant i < n$. It is easy to see that (28) is divergence free. Choosing the partition $k = 2$ and $i_1 = i$, i.e.

$$z_1 = (x_1, \dots, x_i), \quad z_2 = (x_{i+1}, \dots, x_n), \tag{29}$$

the ODE (28) can be rewritten as

$$\frac{\mathrm{d}z_1}{\mathrm{d}t} = \boldsymbol{v}_1(z_2), \quad \frac{\mathrm{d}z_2}{\mathrm{d}t} = \boldsymbol{v}_2(z_1), \tag{30}$$

and we obtain the VPI

$$z_1' = z_1 + \tau \boldsymbol{v}_1(z_2), \quad z_2' = z_2 + \tau \boldsymbol{v}_2(z_1'). \tag{31}$$

Eq. (31) is equivalent to the so-called first-order splitting method. In the special case that (28) is Hamiltonian, (31) corresponds to a generating function of the second or third kind.

4. Discussion

In this section we compare our method with that of Feng and Wang [10]. Their method relies on the decomposition of a source-free vectorfield into a sum of essentially 2-D source-free fields, for which essentially area-preserving algorithms can be constructed. For example, a 3-D source-free ODE can always be written as follows,

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = -\frac{\partial b_3}{\partial x_3} - \frac{\partial b_2}{\partial x_2},$$
$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = \frac{\partial b_2}{\partial x_1}, \quad \frac{\mathrm{d}x_3}{\mathrm{d}t} = \frac{\partial b_3}{\partial x_1}, \tag{32}$$

where

$$b_3 := \int^{x_1} v_3 \,\mathrm{d}x_1, \quad b_2 := \int^{x_1} v_2 \,\mathrm{d}x_1.$$

In this example, the vector field can thus be split into two 2-D source-free vectorfields as follows,

$$\sum_{i=1}^{3} v_i \frac{\partial}{\partial x_i} = \left(\frac{\partial b_3}{\partial x_1} \frac{\partial}{\partial x_3} - \frac{\partial b_3}{\partial x_3} \frac{\partial}{\partial x_1} \right) + \left(\frac{\partial b_2}{\partial x_1} \frac{\partial}{\partial x_2} - \frac{\partial b_2}{\partial x_2} \frac{\partial}{\partial x_1} \right). \tag{33}$$

Each of the two vector fields on the r.h.s. of (33) is then integrated, e.g., by the implicit midpoint-rule.

Comparing Feng and Wang's method to our own, we see that:

(i) Both methods require the evaluation of integrals.

(ii) Both methods are implicit.

In some cases (see e.g. Eqs. (27) and (31)) the integral(s) can be evaluated analytically *and* inverted explicitly. Of course this will not be true in general. For vector fields consisting for example only of polynomials, trigonometric functions and/or exponentials, however, the integral(s) can *always* be evaluated analytically (although the resulting map will in general be implicit), thus removing the major drawback. The comparative usefulness of VPIs whose integrals cannot be evaluated analytically awaits future analysis.

We do not claim that our method is better than that of Feng and Wang, it is just different. With the view to future applications (e.g. integrators that preserve both volume *and* symmetries), it would seem that the larger our arsenal of methods the better.

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