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SOLVING ODE's NUMERICALLY WHILE PRESERVING SYMMETRIES, HAMILTONIAN STRUCTURE, PHASE SPACE VOLUME, OR FIRST INTEGRALS

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ABSTRACT

We give recipes for solving ODE's numerically while preserving symmetries, time-reversing symmetries, Hamiltonian structure, phase space volume, or first integrals (i.e. constants of the motion).

1. INTRODUCTION AND PRELIMINARIES

In recent years, interest has grown in special-purpose methods, designed to preserve certain **qualitative** features of various special classes of ODE's *exactly.*[1] This has led to symplectic integrators for Hamiltonian ODE's [3], volume-preserving integrators for divergence-free ODE's [4-5], integrators that preserve both symmetries and time-reversing symmetries [6,7], and integral-preserving integrators for ODE's possessing first integrals (i.e. constants of the motion) [8-12]. Preservation of these features is particularly important for the long-term stability of dynamical systems because they ensure the existence of stabilizing KAM-tori (in the case of systems that are Hamiltonian, divergence-free, or possess time-reversal symmetry) and/or integral surfaces (in the case of systems with first integrals). For long integration times the small errors of all-purpose methods generally accumulate, which can lead to qualitatively completely wrong results (e.g. bounded orbits becoming unbounded, or spurious dissipation being introduced). It then becomes crucial to use special-purpose methods in which as many qualitative properties as possible are exactly preserved.

The following table gives a broad classification of the above properties as simple or hard to preserve. The "simple" properties can (except for phase space volume) be preserved by some Runge-Kutta methods. Two of the "hard" properties (nonlinear symmetries, and non-canonical symplectic structure) are so hard that no general method preserving them seems to be known at present. The numbers in the table indicate the subsections where the various properties are discussed in this paper:

	Simple	Hard
Symmetries and time-reversing symmetries	linear[2] (2.1)	nonlinear (2.2)
Symplectic structure	canonical (3.1)	non-canonical (3.2)
First integrals	quadratic[3] (4.1)	non-quadratic (4.2)
Other integral invariants	volume (5.1)	invariant measure (5.2)

We use the following notation throughout the paper. We approximate the solution of an autonomous ODE

$$\frac{dx}{dt} = f(x), \qquad x \in \mathbb{R}^n, \tag{1a}$$

by the solution of an (implicit or explicit) mapping

$$x' = \varphi_\tau(x), \qquad x \in \mathbb{R}^n. \tag{1b}$$

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[1] Recent overviews of this area are given in refs. 1,2.

[2] More precisely: affine.

[3] More precisely: linear or quadratic.

In eq.(1b) $x := x(n\tau)$ and $x' := x((n+1)\tau)$ and τ denotes the timestep. In this paper we are interested in mappings φ that preserve some of the (qualitative) mathematical properties of f.

2. SYMMETRIES AND TIME-REVERSING SYMMETRIES

A (continuous resp. discrete) dynamical system possesses the symmetry S if its equation of motion (1a) resp. (1b) is invariant under

$$x \longrightarrow S(x). \tag{2}$$

A continuous dynamical system possesses the time-reversing symmetry R if its equation of motion (1a) is invariant under

$$\begin{cases} x \longrightarrow R(x) \\ t \longrightarrow -t. \end{cases} \tag{3}$$

A discrete dynamical system possesses the time-reversing symmetry R if its equation of motion (1b) is invariant under

$$\begin{cases} x \longrightarrow R(x) \\ \varphi_\tau \longrightarrow \varphi_\tau^{-1}. \end{cases} \tag{4}$$

(Of course, a system may possess more than one symmetry or time-reversing symmetry. The combined set of all symmetries and reversing symmetries of a system is called its reversing symmetry group.)

For reviews of dynamical systems with symmetries or time-reversing symmetries see [13-15].

2.1. Preserving linear symmetries and time-reversing symmetries.

The linear or affine symmetries of an ODE (i.e. those symmetries for which the function S in (2) is linear or affine) are preserved by all Runge-Kutta (RK) methods [16,17]:

$$\begin{aligned} x' &= x + \tau \sum_{j=1}^{s} b_j f(x_i) \\ x_i &= x + \tau \sum_{j=1}^{s} a_{ij} f(x_j), \qquad i = 1, \ldots, s \end{aligned} \tag{5}$$

(here $\sum b_j = 1$).

The linear or affine reversing symmetries of an ODE (i.e. those reversing symmetries for which the function R in (3) is linear or affine) are preserved by those RK methods that possess time symmetry:

$$\varphi_\tau = \varphi_{-\tau}^{-1}, \tag{6}$$

i.e. if the following constraint on the coefficients in (5) holds:

$$a_{s+1-i,\ s+1-j} + a_{ij} = b_{s+1-j} = b_j, \qquad i, j = 1, \ldots, s. \tag{7}$$

2.2. Preserving nonlinear symmetries and time-reversing symmetries.

No general method seems to be known for preserving nonlinear symmetries and time-reversing symmetries.

If the reversing symmetry group of a system is generated by one nonlinear reversing symmetry R and only linear symmetries, then an integrator ψ preserving this group is given by

$$\psi_\tau = \varphi_{\tau/2} \circ R \circ \varphi_{\tau/2}^{-1} \circ R^{-1} \tag{8}$$

where φ_τ is a time-symmetric RK method given by (5) with (7).

More results about symmetry-preserving integrators are given in [7].

3. SYMPLECTIC STRUCTURE

A symplectic structure on $\mathbb{R}^n$ is a skew-symmetric matrix $\Omega(x)$ that satisfies the Jacobi identity:

$$\sum_{\ell=1}^{n}\{\Omega_{i\ell}\frac{\partial}{\partial x_\ell}\Omega_{jk}+\Omega_{j\ell}\frac{\partial}{\partial x_\ell}\Omega_{ki}+\Omega_{k\ell}\frac{\partial}{\partial x_\ell}\Omega_{ij}\}\equiv 0, \qquad i,j,k=1,\dots,n. \tag{9}$$

An ODE is Hamiltonian if there exists a function H (the Hamiltonian) and a symplectic structure Ω such that

$$\frac{dx_i}{dt}=\sum_{j=1}^{n}\Omega_{ij}(x)\frac{\partial H(x)}{\partial x_j}. \tag{10}$$

A map φ is symplectic if there is a symplectic structure Ω such that

$$\sum_{j,k=1}^{n}\frac{\partial\varphi_i(x)}{\partial x_j}\Omega_{jk}(x)\frac{\partial\varphi_\ell}{\partial x_k}(x)=\Omega_{i\ell}(x'). \tag{11}$$

The standard or canonical symplectic structure (for even dimension n) is

$$\Omega=\begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}. \tag{12}$$

3.1. Preserving the canonical symplectic structure.

A Hamiltonian ODE (10) with the standard symplectic structure (12) can be integrated using symplectic RK methods given by (5) with

$$b_i a_{ij}+b_j a_{ji}-b_i b_j=0, \qquad i,j=1,\dots,s. \tag{13}$$

These symplectic RK methods all preserve the symplectic structure of the ODE [3].

3.2. Preserving non-canonical symplectic structure.

No method is known for preserving general non-canonical symplectic structures (or Poisson structures). For a wide class of special symplectic structures that are linear in x, however, (the so-called Lie-Poisson structures) symplectic integrators have been constructed [18].

4. FIRST INTEGRALS

The dynamical system (1a) resp. (1b) possesses the first integral (or constant of the motion) $I(x)$ if there is a function I such that

$$I(x(t))=I(x(0)), \tag{14}$$

for all $t\in\mathbb{R}$ in the continuous case (1a) resp. for all $t=n\tau$, $n\in\mathbb{Z}$, in the discrete case (1b).

4.1. Preserving quadratic first integrals.

The linear and quadratic first integrals of an ODE are all preserved by symplectic RK methods, given by (5) with (13).

4.2. Preserving non-quadratic first integrals.

If the ODE (1a) has the first integral $I(x)$, then it can be written as a skew-gradient system:

$$\frac{dx_i}{dt}=\sum_{j=1}^{n}S_{ij}(x)\frac{\partial I}{\partial x_j}. \tag{15}$$

Here the skew-symmetric matrix S can be taken to be e.g.

$$S_{ij}(x) := \frac{f_i(x)\frac{\partial I(x)}{\partial x_j} - f_j(x)\frac{\partial I(x)}{\partial x_i}}{\sum_{k=1}^{n}(\frac{\partial I}{\partial x_k})^2}. \tag{16}$$

An integral-preserving discretization of (15), and hence of (1a), is given by the discrete gradient method[4] [11,12]:

$$\frac{x_i' - x_i}{\tau} = \sum_{j=1}^{n} S_{ij}(x)(\frac{\Delta I}{\Delta x})_j, \tag{17}$$

where the discrete gradient $\Delta I/\Delta x$ is any (consistent) solution of

$$\sum_j (\frac{\Delta I}{\Delta x})_j (x_j' - x_j) \equiv I(x') - I(x). \tag{18}$$

Of the infinitely many solutions of (18) we give the one due to Itoh and Abe [8]:

$$\left(\frac{\Delta I}{\Delta x}\right)_j := \frac{I(x_1', \ldots, x_j', x_{j+1}, \ldots x_n) - I(x_1', \ldots, x_{j-1}', x_j, \ldots, x_n)}{x_j' - x_j} \tag{19}$$

If the ODE (1a) has 2 first integrals $I_1(x)$ and $I_2(x)$, then it can again be written as a skew-gradient system[5]:

$$\frac{dx_i}{dt} = \sum_{j,k=1}^{n} S_{ijk}(x)\frac{\partial I_1}{\partial x_j}\frac{\partial I_2}{\partial x_k}. \tag{20}$$

Here the skew-symmetric 3-tensor S can be taken to be e.g.

$$S_{ijk}(x) := \frac{\begin{vmatrix} f_i(x) & \partial I_1/\partial x_i & \partial I_2/\partial x_i \\ f_j(x) & \partial I_1/\partial x_j & \partial I_2/\partial x_j \\ f_k(x) & \partial I_1/\partial x_k & \partial I_2/\partial x_k \end{vmatrix}}{\sum_{m,n=1}^{n} (\partial I_1/\partial x_m \partial I_2/\partial x_n - \partial I_1/\partial x_n \partial I_2/\partial x_m)^2} \tag{21}$$

Again, an integral-preserving discretization of (20) is given by the discrete-gradient method.

$$\frac{x_i' - x_i}{\tau} = \sum_{j,k=1}^{n} S_{ijk}(x)\left(\frac{\Delta I_1}{\Delta x}\right)_j \left(\frac{\Delta I_2}{\Delta x}\right)_k \tag{22}$$

where the discrete gradients $\Delta I_1/\Delta x$ resp. $\Delta I_2/\Delta x$ are given by (19) (with I replaced by I_1 resp. I_2), or any other (consistent) solution of (18).

Example.

As an example of a system with 2 first integrals consider the Kepler problem in polar coordinates:

$$\begin{aligned} \frac{dp_r}{dt} &= \frac{\mu^2}{r^3} - \frac{1}{r^2} \\ \frac{dr}{dt} &= p_r \\ \frac{d\theta}{dt} &= \frac{\mu}{r^2}, \end{aligned} \tag{23}$$

---

[4] For an alternative method see ref. 19.

[5] Actually the skew-gradient method can be extended to the case of an arbitrary number of first integrals [12]

where the parameter μ represents the constant angular momentum.
Eq. (23) has the 2 first integrals

$$
\begin{aligned}
I_1 &= \frac{1}{2}p_r^2 + \frac{1}{2}\mu^2/r^2 - 1/r, \\
I_2 &= \operatorname{arctg}\left(\frac{\mu r p_r}{\mu^2 - r}\right) - \theta,
\end{aligned}
\tag{24}
$$

and can be rewritten as a skew gradient system[6]

$$
\frac{dx_i}{dt} = \sum_{j,k=1}^{3} \varepsilon_{ijk} \frac{\partial I_1}{\partial x_j} \frac{\partial I_2}{\partial x_k},
\tag{25}
$$

where $x_1 := p_r, x_2 := r, x_3 := \theta$, and the skew-symmetric tensor S reduces to the Levi-Civita tensor ε (determined by $\varepsilon_{123} = 1$ and skew-symmetry). A numerical integration of the Kepler problem (23) is given in Fig.1.

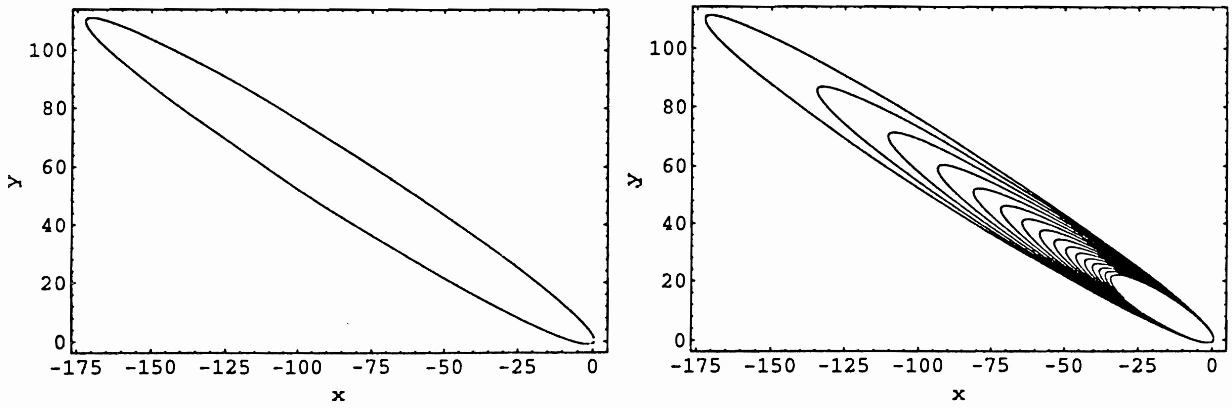

Fig 1a *Fig. 1b*

Figure 1. This figure illustrates that conventional integration methods do not preserve first integrals. It shows an orbit in configuration space ($x := r\cos\theta,\ y := r\sin\theta$) for the Kepler 2-body problem (Eq (23), with $p_r(0) = 0.99511,\ r(0) = 1,\ \theta(0) = 1,\ \mu = 1$), as calculated by the first-order integral preserving method (22) (Figure 1a), and the standard fourth-order RK method (Figure 1b). In both calculations the time step used is $\tau = 0.15$. Note that the Runge-Kutta method violates Kepler's first law.

5. OTHER INTEGRAL INVARIANTS

The ODE (1a) has the invariant measure

$$
\int m(x)dx
\tag{26}
$$

iff

$$
\operatorname{div}(mf) = 0.
\tag{27}
$$

A map φ has the invariant measure (26) if

$$
\det\left(\frac{\partial \varphi_i}{\partial x_j}\right) = \frac{m(x')}{m(x)}.
\tag{28}
$$

The standard invariant measure is volume, given by $m(x) \equiv 1$.

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[6] Equation (25) is an example of a so-called Nambu system [20].

5.1. Preserving volume.

If the ODE (1a) preserves volume, i.e. if

$$\mathrm{div}(f) = 0, \tag{29}$$

then the vectorfield (1a) can be split into $n-1$ quasi-twodimensional volume preserving vectorfields

$$\begin{aligned} \frac{dx_i}{dt} &= 0, & i \neq j, n, \\ \frac{dx_j}{dt} &= f_j(x) \\ \frac{dx_n}{dt} &= -\frac{\partial}{\partial x_j}\int_0^{x_n} f_j(x)dx_n. \end{aligned} \tag{30}$$

A volume-preserving integrator φ is then given by

$$\varphi = \varphi_1 \circ \varphi_2 \circ \cdots \circ \varphi_{n-1} \tag{31}$$

where for each $j \in \{1, \ldots, n-1\}, \varphi_j$ is obtained by applying any symplectic integrator (see section 3.1) to the ODE (30).

5.2. Preserving an invariant measure.

If our ODE (1a) is measure-preserving, i.e. satisfies eq. (27), then an (implicit) measure-preserving integrator is given by

$$x_i' = F_i, \qquad i = 1, \ldots, n-1, \tag{32a}$$

$$\int_0^{x_n} m(x_1, \ldots, x_n)dx_n = \int_0^{x_n'} m(F_1, \ldots, F_{n-1}, x_n')J(x_1, \ldots, x_{n-1}, x_n')dx_n' \tag{32b}$$

where

$$F_i := F_i(x_1, \ldots, x_{n-1}, x_n') \tag{33}$$

is any function that is consistent, i.e. satisfies

$$F_i(x_1, \ldots, x_{n-1}, x_n') = x_i + \tau f_i(x_1, \ldots, x_n) + \mathcal{O}(\tau^2), \tag{34}$$

and

$$J := \det\left(\frac{\partial F_i}{\partial x_j}\right) \qquad i, j = 1, \ldots, n-1. \tag{35}$$

In general the integrator (32) is not suitable for application to periodic vectorfields f, as in many cases (32b) does not preserve periodicity.

6. CONCLUDING REMARKS

Many of the numerical recipes given above yield first-order integrators. If desired, these can be used as building blocks to construct higher-order integrators[7]. If φ is any integrator, then

$$\psi_\tau := \varphi_{\tau/2} \circ \varphi^{-1}_{-\tau/2} \tag{36}$$

is second-order and possesses time-symmetry (i.e. satisfies (6)). Higher-order integrators can be constructed from ψ using the (generalized) Yoshida method [22]. For example, writing $\gamma := (2 - 2^{\frac{1}{3}})^{-1}$, a fourth order integrator is obtained as follows:

$$\chi_\tau := \psi_{\gamma\tau} \circ \psi_{(1-2\gamma)\tau} \circ \psi_{\gamma\tau}. \tag{37}$$

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[7] The procedure for systems with time-reversal symmetry is more subtle [7].

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