DISCRETE GRADIENT METHODS FOR SOLVING ODE's NUMERICALLY WHILE PRESERVING A FIRST INTEGRAL

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Abstract

We show that all direct methods for preserving a first integral during the numerical integration of an ordinary differential equation fit into the unified framework of Discrete Gradient Methods. Using this framework we construct several new integral-preserving schemes.

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1. Introduction

In the numerical analysis of dynamical systems there has been an increased emphasis in recent years on qualitative aspects [1, 2]. This has come about for two reasons. Firstly, the ever increasing power of computers that is making feasible the implementation of sophisticated algorithms, hitherto computationally too costly. Secondly, the discovery that certain *qualitative* features of ODE's can be preserved **exactly** in numerical integration schemes (while simultaneously quantitative features are not neglected)[2]. Examples of such qualitative features that can be preserved are: Hamiltonian structure [4], the presence of symmetries [5,6], conservation of phase space volume in source-free systems [7,8], the presence of attractors and other ω-limit sets [1], and conservation of first integrals [9]-[19].

In this Letter we will concentrate on the preservation of a single first integral[3]. More precisely, we will study a system of coupled autonomous first-order ODE's

$$\frac{dx}{dt} = f(x), \tag{1}$$

where the vectorfield $f : \mathbf{R}^n \to \mathbf{R}^n$ is such that there exists a scalar integral I, i.e.

$$\frac{dI(x)}{dt} = 0. \tag{2}$$

We want to find a discrete approximation to (1):

$$\frac{x' - x}{\tau} = \varphi(x, x', \tau), \tag{3}$$

such that the integral I is preserved exactly, i.e.

$$I(x') = I(x). \tag{4}$$

(In (3) and (4) and below, by a slight abuse of notation, $x = x(n\tau)$ and $x' = x((n+1)\tau)$, where τ is the timestep).

Preserving first integrals is important because of their physical relevance, e.g. in mechanics and astronomy, but also because they can ensure long-term stabilising effects. They also play a significant role in determining which bifurcations generically occur. It is particularly important that a first integral be preserved if the dimension of the system is low, if the integration time is very long, and if the integral-surface is compact.

To date, direct methods for preserving a first integral have mostly fallen into three categories[4]:

[2]These two points are exemplified by the recent 100 million year integration of the equations of motion of the entire solar system, using a symplectic integrator [3].

[3]The case of more than 1 first integral will be treated in [17].

[4]Some indirect methods are also given in [15,20].

1. *Integrators that preserve quadratic integrals.*

Cooper [9] showed that the implicit midpoint rule

$$\frac{x' - x}{\tau} = f\Big(\frac{x' + x}{2}\Big), \tag{5}$$

preserves quadratic integrals (actually, so do all symplectic Runge-Kutta methods).

2. *Hamiltonian-preserving methods.*

Consider a system of Hamiltonian ODE's,

$$\frac{dx}{dt} = \omega \cdot \frac{DH(x)}{Dx}, \tag{6}$$

where ω is the standard symplectic structure

$$\omega := \begin{pmatrix} 0 & Id \\ -Id & 0 \end{pmatrix}, \tag{7}$$

(with Id the $n/2$-dimensional unit matrix), and the gradient is denoted by

$$\frac{DH(x)}{Dx} := \begin{pmatrix} \frac{\partial H(x)}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial H(x)}{\partial x_n} \end{pmatrix}. \tag{8}$$

Some Hamiltonian-preserving methods for (6) are given in [10-14, 19].

3. *Splitting methods that preserve general integrals.*

Quispel and Capel [16] found a direct method for preserving general integrals. It consisted of 4 steps:

- Write the ODE in skew-gradient form

$$\frac{dx}{dt} = S(x) \cdot \frac{DI(x)}{Dx}, \tag{9}$$

where S is some skew-symmetric matrix (i.e. $S^t = -S$).

- Split the r.h.s. of (9) into 2D vectorfields, each possessing the integral I.
- Integrate these 2D vectorfields using an essentially 2D integral-preserving integrator.
- Construct an n-dimensional integral-preserving integrator from the 2D integrators obtained in the previous step.

2. Necessary and sufficient conditions for a dynamical system to possess a first integral.

In [16] we proved the following theorem:

Theorem 1. *The autonomous ODE*

$$\frac{dx}{dt} = f(x), \tag{10}$$

has a first integral $I(x)$ if and only if (10) can (formally) be written as a skew-gradient system:

$$\frac{dx}{dt} = S(x) \cdot \frac{DI}{Dx}(x). \tag{11}$$

In (11), S is some skew-symmetric matrix

$$S^t = -S, \tag{12}$$

and the gradient is denoted by

$$\frac{DI}{Dx}(x) := \begin{pmatrix} \frac{\partial I(x)}{\partial x_1} \\ \cdot \\ \cdot \\ \cdot \\ \frac{\partial I(x)}{\partial x_n} \end{pmatrix}. \tag{13}$$

The (constructive) proof of theorem 1 is given in [16]. It uses the infinitesimal identity

$$dx \cdot \frac{DI}{Dx} = dI. \tag{14}$$

It turns out that theorem 1 carries over to the discrete case:

Theorem 2. *Let the "discrete gradient" $\Delta I/\Delta x$ be any vector satisfying the crucial discrete analog of identity (14) [10,12,19]:*

$$(x' - x) \cdot \frac{\Delta I}{\Delta x}(x, x') = I(x') - I(x). \tag{15}$$

Then the (implicit) mapping

$$\frac{x' - x}{\tau} = \varphi(x, x', \tau) \tag{16}$$

has a first integral $I(x)$ if and only if (16) can (formally) be written as a discrete skew-gradient system

$$\frac{x' - x}{\tau} = \tilde{S}(x, x', \tau) \cdot \frac{\Delta I}{\Delta x}(x, x'). \tag{17}$$

In (17), $\tilde{S}$ is some skew-symmetric matrix

$$\tilde{S}^t = -\tilde{S}. \tag{18}$$

The proof is analogous to the proof of theorem 1, and will therefore be omitted. Note, though, that for a given integral the choice of discrete gradient satisfying (15) is not unique, and that for a given discrete gradient the matrix $\tilde{S}$ is not unique (see below).

3. Discrete Gradient Methods as integral-preserving integrators.

Theorem 2 implies that the exact flow of an integral-possessing ODE is a discrete skew-gradient system. Combining theorems 1 and 2 then suggests the following 2-step method for constructing integral-preserving integrators (IPI's):

(i) Write the ODE in the skew-gradient form

$$\frac{dx}{dt} = S(x) \cdot \frac{DI(x)}{Dx} \tag{19}$$

(ii) Integrate (19), using an integral-preserving Discrete Gradient Method

$$\frac{x' - x}{\tau} = \tilde{S}(x, x', \tau) \cdot \frac{\Delta I}{\Delta x}(x, x') \tag{20}$$

STEP (i): WRITE THE ODE IN THE FORM $\frac{dx}{dt} = S \cdot \frac{DI}{Dx}$.

For a given vectorfield f and integral I, there are in general infinitely many choices for the skew matrix S (see [16]). Here we restrict ourselves to giving a family of particular solutions. For any arbitrary vectorfield $a(x)$, a skew matrix S as in Theorem 1 is given by [21]

$$S_{i,j}(x) = \frac{f_i(x)a_j(x) - a_i(x)f_j(x)}{\sum_{k=1}^{n}(a_k(x)\frac{\partial I(x)}{\partial x_k})}. \tag{21}$$

(This is easily shown using $f \cdot \frac{DI}{Dx} = 0$.) The choice of the vectorfield $a(x)$ is governed by our two conflicting wishes that we want S to be as simple as possible, but preferably free from singularities.

Example I. $\exists k$, $\forall x$, $\frac{\partial I(x)}{\partial x_k} \neq 0$.

In this case we can choose

$$a(x) = \hat{e}_k, \tag{22}$$

where $\hat{e}_k$ is a unit vector in the x_k direction.

Example II. The general case.

In this case we can choose[5]

$$a(x) = \frac{DI(x)}{Dx} \tag{23}$$

STEP (ii): INTEGRAL-PRESERVING DISCRETE GRADIENT METHODS.

[5] A sufficient condition for this to work is that $(\frac{DI}{Dx}) \neq 0$ on the integral surface we are integrating on.

Even though, formally, all discrete gradients are equivalent (cf. theorem 2), in practice (depending on the vectorfield) one may be more convenient then another:

(iia) Choice of discrete gradient.

Each discrete gradient must satisfy the discrete identity (6), and must be consistent:

$$\left(\frac{\Delta I}{\Delta x}\right)(x, x') = \frac{DI}{Dx}(x) + \mathcal{O}(\tau). \tag{24}$$

A discrete gradient satisfying (15) and (24) was given by Itoh and Abe [10], cf. also [12]:

$$\left(\frac{\Delta I}{\Delta x}\right)_1 (x, x') := \begin{pmatrix} \frac{I(x_1', x_2, x_3, x_4, \cdots, x_n) - I(x_1, x_2, x_3, x_4, \cdots, x_n)}{x_1' - x_1} \\ \frac{I(x_1', x_2', x_3, x_4, \cdots, x_n) - I(x_1', x_2, x_3, x_4, \cdots, x_n)}{x_2' - x_2} \\ \frac{I(x_1', x_2', x_3', x_4, \cdots, x_n) - I(x_1', x_2', x_3, x_4, \cdots, x_n)}{x_3' - x_3} \\ \cdot \\ \cdot \\ \cdot \\ \frac{I(x_1', x_2', \cdots x_{n-1}', x_n') - I(x_1', x_2', \cdots, x_{n-1}', x_n)}{x_n' - x_n} \end{pmatrix}. \tag{25}$$

An equally good discrete gradient is obtained by performing an arbitrary permutation π of the indices $1, \ldots, n$:

$$\left(\frac{\Delta I}{\Delta(\pi x)}\right)_{(j)} (x, x') := \frac{(E_j - 1)}{x_j' - x_j} \left(\prod_{\ell=1}^{\pi^{-1}(j)-1} E_{\pi(\ell)}\right) I(x_1, \cdots, x_n), \tag{26}$$

where the ℓth time shift operator E_ℓ is defined by

$$E_\ell g(\cdots, x_\ell, \cdots) := g(\cdots, x_\ell', \cdots), \quad (\ell = 1, \cdots, n), \tag{27}$$

where g is any function and the dots in (27) denote the other $n-1$ (primed or unprimed) variables. This allows us to construct a quite general discrete gradient:

$$\left(\frac{\Delta I}{\Delta x}\right)_2 (x, x') := \frac{\sum_\pi c(\pi) \frac{\Delta I}{\Delta(\pi x)}}{\sum_\pi c(\pi)} \tag{28}$$

where the $c(\pi)$ are arbitrary coefficients. Choosing

$$\begin{aligned} c(\pi) &= 1, && \text{if } \pi = \text{ identity}, \\ c(\pi) &= 0, && \text{otherwise}, \end{aligned} \tag{29}$$

we recover $(\Delta I/\Delta x)_1$. Choosing

$$\begin{aligned} c(\pi) &= \frac{1}{2}, && \text{if } \pi = \text{ identity}, \\ c(\pi) &= \frac{1}{2}, && \text{if } \pi(1, \cdots, n) = (n, \cdots, 1), \\ c(\pi) &= 0, && \text{otherwise}, \end{aligned} \tag{30}$$

we obtain

$$\left(\frac{\Delta I}{\Delta x}\right)_3(x,x') = \frac{\left(\frac{\Delta I}{\Delta x}\right)_1(x,x') + \left(\frac{\Delta I}{\Delta x}\right)_1(x',x)}{2}. \tag{31}$$

A more symmetric IPI is obtained choosing

$$c(\pi) = \frac{1}{n!}, \qquad \forall\pi, \tag{32}$$

leading to

$$\left(\frac{\Delta I}{\Delta x}\right)_4(x,x') = \frac{1}{n!}\sum_\pi \frac{\Delta I}{\Delta(\pi x)}(x,x'). \tag{33}$$

Note that any discrete gradient can be obtained from any other by adding a solution of the (homogeneous) equations

$$\begin{aligned} (x'-x)a(x,x') &= 0, \\ a(x,x') &= \mathcal{O}(\tau). \end{aligned} \tag{34}$$

The solution to (34) is

$$a(x,x') = b(x,x') - (x'-x)\frac{(x'-x)\cdot b(x,x')}{(x'-x)\cdot(x'-x)}, \tag{35}$$

where b is an arbitrary vector of order τ.

Choosing

$$b(x,x') = \frac{DI}{Dx}(z(x,x')) - \left(\frac{\Delta I}{\Delta x}\right)_1(x,x'), \tag{36}$$

where $z(x,x') = x + \mathcal{O}(\tau)$. Substituting in (35) and adding to (25) we obtain

$$\left(\frac{\Delta I}{\Delta x}\right)_5(x,x') = \frac{DI}{Dx}(z) - (x'-x)\frac{(x'-x)\cdot\frac{DI}{Dx}(z) - I(x') - I(x)}{(x'-x)\cdot(x'-x)}. \tag{37}$$

This very nice solution was discovered by Gonzalez.

(iib) Choice of skew symmetric matrix.

To be consistent each skew matrix must satisfy

$$\tilde{S}(x,x',\tau) = S(x) + \mathcal{O}(\tau). \tag{38}$$

Two simple choices are therefore

$$\tilde{S}_1(x,x',\tau) = S(x) \tag{39}$$

or

$$\tilde{S}_2(x,x',\tau) = S\left(\frac{x+x'}{2}\right) \tag{40}$$

(iic) Combining the discrete gradient and the skew-matrix. A simple first-order IPI is

$$\frac{x'-x}{\tau} = S(x)\left(\frac{\Delta I}{\Delta x}\right)_1 (x,x'). \tag{41}$$

To obtain a second-order IPI we impose the additional requirement of "time-symmetry", i.e.

$$\tilde{S}(x,x',\tau) = \tilde{S}(x',x,-\tau) \tag{42}$$

$$\left(\frac{\Delta I}{\Delta x}\right)(x,x') = \left(\frac{\Delta I}{\Delta x}\right)(x',x). \tag{43}$$

Eq. (42) is satisfied by $\tilde{S}_2$, and eq. (43) is satisfied e.g. by $(\Delta I/\Delta x)_3$, $(\Delta I/\Delta x)_4$, and, if $z(x,x') = z(x',x)$, by $(\Delta I/\Delta x)_5$ [19].

The "time-symmetry" (42-43) makes these integrators suitable building blocks for constructing integrators of arbitrary order using Yoshida's method [22].

4. A numerical example.

To illustrate the fact that standard methods [23] in general do not preserve first integrals, we have compared the performance of three numerical integration methods on the ODE

$$\begin{aligned} \dot{x} &= x + yz + 0.1xy^2 + xy^3 + 0.1xy^5 \\ \dot{y} &= -x^2 + z^2 - 0.1x^2y^2 \\ \dot{z} &= -z - xy - y^3 z, \end{aligned} \tag{44}$$

with initial conditions $x(0) = z(0) = 1$, $y(0) = 2$. Note that the system (44) has the first integral

$$I = \frac{x^2}{2} + \frac{y^4}{4} + y + \frac{z^2}{2}. \tag{45}$$

The level surfaces of this integral are all compact. The three 4th order methods we used are: an explicit linear multi-step method (LM4), an explicit Runge-Kutta method (RK4), and one of our new implicit IPI's (QT4). Timesteps τ have been adjusted such that the amount of numerical work done by the three methods is identical.

LM4: This is the 4th-order Adams-Bashforth method.

RK4: The standard 4th-order Runge-Kutta method defined by the Butcher tableau:

$$\begin{array}{cccc} \frac{1}{2} & & & \\ 0 & \frac{1}{2} & & \\ 0 & 0 & 1 & \\ \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array} . \tag{46}$$

QT4: Note that (44) can be written in skew-gradient form (11), with

$$S = \begin{pmatrix} 0 & x + 0.1xy^2 & y \\ -x - 0.1xy^2 & 0 & z \\ -y & -z & 0 \end{pmatrix}. \tag{47}$$

QT4 was obtained by first constructing a 2nd-order IPI, using (17) with (31) and (43), and then applying Yoshida's method to get a 4th order IPI [22].

Numerical results are given in Figure 1

FIGURE 1

5. Reduction of Discrete Gradient Method to previous methods.

1. *Quadratic integrals: reduction to implicit midpoint rule.*

From the arguments given above it follows that there formally exists a matrix S such that

$$f(x) = S(x) \cdot \frac{DI(x)}{Dx}. \tag{48}$$

Now use an IPI with $\tilde{S}_2$ and e.g. $(\Delta I/\Delta x)_4$ or $(\Delta I/\Delta x)_5$ (with $z = \frac{x+x'}{2}$). It can be shown that if I is quadratic, then

$$\left(\frac{\Delta I}{\Delta x}\right)_4 (x, x') = \left(\frac{\Delta I}{\Delta x}\right)_5 (x, x') = \frac{DI}{Dx}\left(\frac{x + x'}{2}\right), \tag{49}$$

and using (48) we see this reduces to the implicit midpoint rule (5).

By the same token, any IPI with (40) preserves all quadratic Casimirs.

2. *Hamiltonian systems: reduction to the Itoh-Abe and Gonzalez methods.*

For standard Hamiltonian systems we can take $I = H$ and $S = \tilde{S} = \omega$. The Itoh-Abe method is then recovered choosing the discrete gradient $(\Delta H/\Delta x)_1$. Gonzalez' method is obtained choosing the discrete gradient $(\Delta I/\Delta x)_5$ with $z = \frac{x+x'}{2}$.

3. *Reduction to integral-preserving splitting methods.*

The ODE (11) is equivalent to the vectorfield

$$v = \sum_{i<j} v_{i,j}, \tag{50}$$

where

$$v_{i,j} := S_{i,j}\left(\frac{\partial I}{\partial x_j}\frac{\partial}{\partial x_i} - \frac{\partial I}{\partial x_i}\frac{\partial}{\partial x_j}\right), \tag{51}$$

and each vectorfield $v_{i,j}$ preserves the integral I. Using the splitting (50) we obtain the method of Quispel and Capel [16]. Using various other partitions of the set $\{v_{i,j}\}$, there are many ways in which the n-dimensional vectorfield v can be split into lower-dimensional vectorfields that each preserve I.

6. Concluding remark.

Associated with the continuous system (11) there is a bracket formulation

$$\frac{dh(x)}{dt} = \{h, I\}_C, \tag{52}$$

where the continuous bracket is defined by

$$\{h, g\}_C := \frac{Dh}{Dx} \cdot S \cdot \frac{Dg}{Dx}. \tag{53}$$

If $\{h, I\}_C \equiv 0$, then h is a first integral.

Associated with the discrete system (17) there is also a bracket formulation

$$\frac{h(x') - h(x)}{\tau} = \{h, I\}_D, \tag{54}$$

where the discrete bracket is given by

$$\{h, g\}_D := \frac{\Delta h}{\Delta x} \cdot \tilde{S} \cdot \frac{\Delta g}{\Delta x}. \tag{55}$$

If $\{h, I\}_D \equiv 0$, then h is a first integral.

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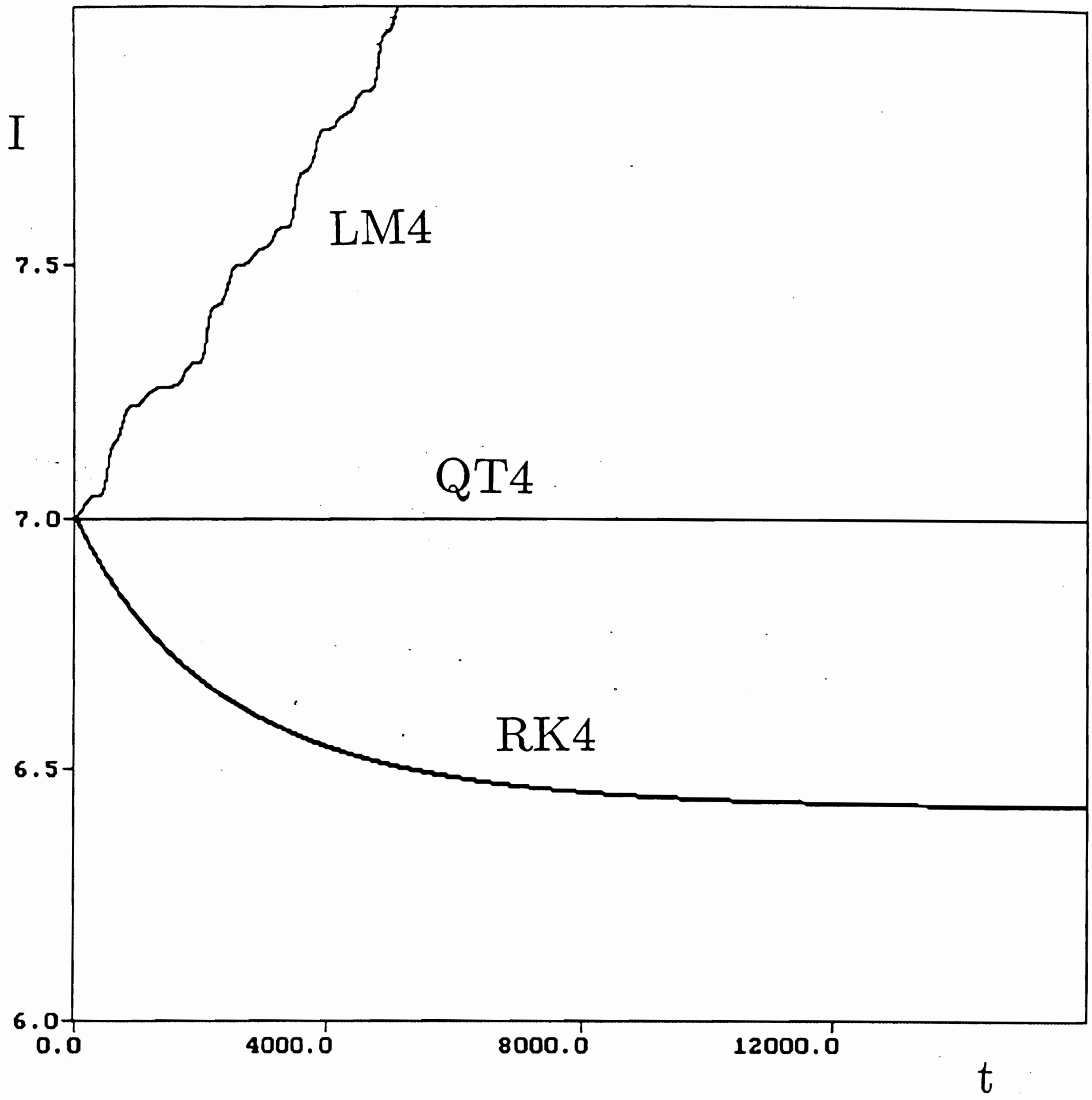
Figure 1.

This figure illustrates that conventional integration methods (RK4 and LM4) do not preserve first integrals. It shows the numerical value of the integral I, as a function of time $t = n\tau$, for the 3D test system (37). It compares the standard 4th order Runge-Kutta method (RK4; $\tau = 0.031$), a 4th order Linear Multistep method (LM4; $\tau = 0.040$), and a 4th order Discrete Gradient Method (QT4; $\tau = 0.443$). (Timesteps τ have been adjusted such that the amount of numerical work done by the three methods is equivalent.)



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