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SYMMETRIC PROJECTION METHODS FOR DIFFERENTIAL EQUATIONS ON MANIFOLDS *

E. HAIRER

Section de mathématiques, Université de Genève, 2-4 rue du Lièvre, CH-1211 Genève 24, Switzerland. email: Ernst.Hairer@math.unige.ch

Abstract.

Projection methods are a standard approach for the numerical solution of differential equations on manifolds. It is known that geometric properties (such as symplecticity or reversibility) are usually destroyed by such a discretization, even when the basic method is symplectic or symmetric. In this article, we introduce a new kind of projection methods, which allows us to recover the time-reversibility, an important property for long-time integrations.

AMS subject classification: 65L06.

Key words: Differential equations on manifolds, symmetric Runge–Kutta methods, projection methods, numerical geometric integration, long-time integration.

1 Differential equations on manifolds.

We consider the initial value problem

$$y' = f(y), \qquad y(0) = y_0, \tag{1.1}$$

and we assume the existence of an invariant manifold

$$\mathcal{M} = \{y \in \mathbf{R}^n \,;\, g(y) = 0\} \tag{1.2}$$

for its flow, i.e., $g'(y)f(y) = 0$ for $y \in \mathcal{M}$. The functions $g : \mathbf{R}^n \to \mathbf{R}^m$ and $f : \mathbf{R}^n \to \mathbf{R}^n$ are assumed to be sufficiently differentiable. Examples are differential-algebraic equations which, by repeated differentiation of the constraints, are brought to an index 1 system, from which the algebraic variables are eliminated [10]. Further problems of this type arise in the simulation of mechanical systems whose configuration space is a matrix Lie group (see Example 4.1 below).

Numerical methods for the solution of differential equations on manifolds, which avoid the use of local coordinates, can be divided into two groups: (i) methods for which the numerical solution automatically stays on $\mathcal{M}$ without using explicitly the function $g(y)$, and (ii) methods which, after every successful step, project the numerical approximation onto the manifold $\mathcal{M}$. To the first

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class belong symplectic one-step methods, if $g(y) = y^T C y$ is a quadratic first integral (i.e., $g'(y)f(y) = 0$ for all y in a neighborhood of the solution). Also the methods of Crouch and Grossman [2] and Lie group methods, such as those proposed by Munthe-Kaas [9], yield numerical solutions which automatically lie on $\mathcal{M}$. They, however, require a special formulation of the vector field. Projection methods form the second class of numerical integrators for our problem. They need that the vector field $f(y)$ is defined in a neighborhood of the manifold $\mathcal{M}$ (what is usually fulfilled in practical applications). The idea of projection methods is to perform in every step the following two operations (1.1, left):

- compute $\widehat{y}_1 = \widehat{\Phi}_h(y_0)$ by an arbitrary one-step method,
- project the value $\widehat{y}_1$ onto the manifold $\mathcal{M}$ to obtain $y_1 \in \mathcal{M}$.

For $y_0 \in \mathcal{M}$ the distance of $\widehat{y}_1$ to the manifold $\mathcal{M}$ is of the size of the local error, i.e., $\mathcal{O}(h^{p+1})$. We therefore also have $y_1 - y(h) = \mathcal{O}(h^{p+1})$, so that the projection does not deteriorate the convergence order of the method. Projection methods are thoroughly investigated in the context of differential-algebraic problems (see e.g., [6, Section VII.2] and [3, Section 5.3]).

Here, we are mainly interested in problems where the flow on the manifold $\mathcal{M}$ has additional geometric properties such as symplecticity or reversibility. It is known that even in the case where the basic method is symplectic or symmetric, a discretization with the above projection algorithm destroys the geometric properties and makes it inappropriate for long-time integrations. The same is true for Lie group methods. For this reason, Zanna, Engø, and Munthe-Kaas [11] introduced selfadjoint Lie group methods which have more favorable properties for long-time integrations.

In the present article, we introduce a new kind of projection methods. It retains the time-reversibility of the basic one-step method and allows for an efficient implementation (Section 2). In Section 3 we present a backward error analysis for these methods. Their excellent long-time behavior is illustrated in Section 4 on some typical examples.

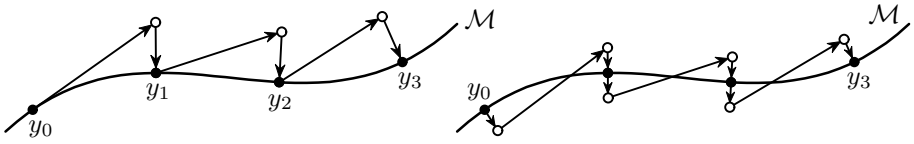

Figure 1.1: Standard projection (left) compared to symmetric projection (right).

2 Symmetric projection methods.

The idea of symmetric projection methods is very simple. We first perturb the initial value $y_0 \in \mathcal{M}$ out of the manifold, we then apply one step of a symmetric method, and, finally, we project back to the manifold $\mathcal{M}$ (Figure 1.1, right picture). Care has to be taken about the choice of the perturbation and the projection in order to make the procedure symmetric. Using orthogonal

projections this yields:

$$\widehat{y}_0 = y_0 + G^T(y_0)\mu \qquad \text{where} \quad g(y_0) = 0, \tag{2.1}$$

$$\widehat{y}_1 = \widehat{\Phi}_h(\widehat{y}_0), \qquad \text{(symmetric one-step method applied to (1.1))} \tag{2.2}$$

$$y_1 = \widehat{y}_1 + G^T(y_1)\mu \qquad \text{with } \mu \text{ such that} \quad g(y_1) = 0. \tag{2.3}$$

Here, $G(y) = g'(y)$ denotes the Jacobian of $g(y)$. It is important to take the same vector μ in (2.1) and (2.3).

A closely related symmetric projection has recently been proposed by Ascher and Reich [1]. They consider the implicit midpoint rule and perform a symmetric projection step in order to enforce conservation of energy.

Existence of numerical solution. The vector μ is implicitly defined by

$$F(\mu) = g\Big(\widehat{\Phi}_h\big(y_0 + G^T(y_0)\mu\big) + G^T(y_1)\mu\Big) = 0, \tag{2.4}$$

and can be computed by Newton-type iterations. We have

$$F'(\mu) = 2G(y_1)G^T(y_1) + \mathcal{O}(h).$$

Hence, if $G(y)$ is of maximal rank m, the inverse of $F'(\mu)$ is bounded, and the Newton–Kantorovich theorem implies existence and local uniqueness of the solution μ of (2.4). Since $F(0) = \mathcal{O}(h^{p+1})$, this solution is of size $\mu = \mathcal{O}(h^{p+1})$.

Symmetry. Assuming the basic method $\widehat{\Phi}_h$ to be symmetric, i.e., $\widehat{\Phi}_h = \widehat{\Phi}_{-h}^{-1}$, the projection method $y_1 = \Phi_h(y_0)$ defined by (2.1)–(2.3) is also symmetric. This follows from the fact that exchanging $h \leftrightarrow -h$, $y_0 \leftrightarrow y_1$, $\widehat{y}_0 \leftrightarrow \widehat{y}_1$, and $\mu \leftrightarrow -\mu$, yields the same formulas.

Modifications of the algorithm. In some particular situations, it may be advantageous to modify the projection steps (2.1) and (2.3). Without deteriorating the symmetry of the method, it is possible to replace the arguments of $G^T(y)$ in (2.1) and (2.3) with $y_{1/2} = (y_0 + y_1)/2$ (which is natural for the implicit midpoint rule), or with a suitable internal stage approximation of the method $\widehat{\Phi}_h$.

Sometimes, it may also be advantageous to replace the Jacobian $G(y) = g'(y)$ with some suitable approximation. If the same kind of approximation is used in (2.1) and (2.3), the symmetry of the method is retained. For example, in multibody systems (see Example 4.2 below) the computation of the second derivative of the position constraint can be avoided, if we first project onto the position constraint and then onto the velocity constraint. This is a standard approach in multibody simulation.

Implementation. The symmetric one-step method used in (2.2) is in general implicit (e.g., trapezoidal rule, implicit midpoint rule, implicit Runge–Kutta method) and can be written as $\widehat{y}_1 = \widehat{y}_0 + h\Psi(h, \widehat{y}_0, \widehat{y}_1)$. It is then natural to solve the nonlinear equation (2.4) in tandem with (2.2). This can be done by simplified Newton iterations as follows: suppose that y_1 and μ are given

approximations to the solution, then compute $\widehat{y}_0$ and $\widehat{y}_1$ from (2.1) and (2.3), and let $d := \widehat{y}_1 - \widehat{y}_0 - h\Psi(h, \widehat{y}_0, \widehat{y}_1)$ be the defect of the one-step method. The increments for y_1 and μ can then be computed from

$$\begin{pmatrix} I & -2G^T \\ G & 0 \end{pmatrix} \begin{pmatrix} \Delta y_1 \\ \Delta \mu \end{pmatrix} = - \begin{pmatrix} d \\ g(y_1) \end{pmatrix}.$$

Convergence of this iteration is usually as fast as that for the basic method without projection.

We remark that this implementation can conveniently be combined with the reversible stepsize strategy of Stoffer (see [5]).

3 Backward error analysis.

If $f(y)$ and $g(y)$ are defined in a neighborhood of $\mathcal{M}$, we can extend our projection algorithm to initial values $y_0 \notin \mathcal{M}$ by replacing the condition "$g(y_1) = 0$" with "$g(y_1) = g(y_0)$". This yields a symmetric one-step method $y_1 = \Phi_h(y_0)$ which is defined on an open set of $\mathbf{R}^n$, and where $\Phi_h(y_0)$ is as smooth as the functions $f(y)$, $g(y)$, and $\widehat{\Phi}_h(y)$. We are thus in the position where standard backward error analysis can be applied (see e.g., [4, Chapter V]). This extended one-step method is consistent with the differential equation

$$y' = P(y)f(y), \qquad P = I - G^T(GG^T)^{-1}G, \tag{3.1}$$

which, on the manifold $\mathcal{M}$, reduces to (1.1) (if $g(y)$ is a first integral of (1.1), then $P(y)f(y) = f(y)$ for all $y \in \mathbf{R}^n$). Hence, its numerical solution is (formally) equal to $y_n = \widetilde{\varphi}_{nh}(y_0)$, where $\widetilde{\varphi}_t(y_0)$ is the flow of the modified equation

$$y' \;=\; f_0(y) + h^2 f_2(y) + h^4 f_4(y) + \cdots \tag{3.2}$$

(with $f_0(y) = P(y)f(y)$), which due to the symmetry of the method is a series in even powers of h. If the basic method (2.2) is of order p, i.e., $\widehat{\Phi}_h(y) - \varphi_h(y) = h^{p+1}d_p(y) + \mathcal{O}(h^{p+2})$, where $\varphi_t(y)$ denotes the flow of (1.1), then, restricted to the manifold $\mathcal{M}$, the modified equation (3.2) becomes

$$y' \;=\; f(y) + h^p f_p(y) + h^{p+2} f_{p+2}(y) + \cdots \tag{3.3}$$

with $f_p(y) = P(y)d_p(y)$ for $y \in \mathcal{M}$. Hence, $f_p(y)$ is just the projected local error.

THEOREM 3.1. *The coefficient functions of the modified equation* (3.2) *satisfy*

$$g'(y)f_j(y) = 0 \qquad \textit{for all} \quad y \in \mathbf{R}^n. \tag{3.4}$$

Hence, $g(y)$ is a first integral of the modified equation (when truncated at an arbitrary power of h) and therefore has $\mathcal{M}$ as invariant manifold.

PROOF. The proof is by induction and follows standard arguments. The statement (3.4) is obviously true for $j = 0$. Assume now that (3.4) holds for $j \le r$, and denote by $\varphi_{r,t}(y)$ the flow of (3.2) where the series is truncated

after the $\mathcal{O}(h^r)$ term. By definition of $f_{r+2}(y)$ in the modified equation, we have $\Phi_h(y) = \varphi_{r,h}(y) + h^{r+2} f_{r+2}(y) + \mathcal{O}(h^{r+3})$. Since $g\big(\Phi_h(y)\big) = g(y)$ and $g\big(\varphi_{r,h}(y)\big) = g(y)$ for all h and all $y \in \mathbf{R}^n$, this implies that

$$\begin{aligned} 0 \;=\; g\big(\Phi_h(y)\big) - g\big(\varphi_{r,h}(y)\big) &= g'\big(\varphi_{r,h}(y)\big) h^{r+2} f_{r+2}(y) + \mathcal{O}(h^{r+3}) \\ &= h^{r+2} g'(y) f_{r+2}(y) + \mathcal{O}(h^{r+3}). \end{aligned}$$

For $h \to 0$, we thus get (3.4) with $j = r + 2$. □

THEOREM 3.2. *If* (1.1) *is ρ-reversible with an orthogonal matrix ρ, i.e., $f(\rho y) = -\rho f(y)$ for $y \in \mathbf{R}^n$, and if $g(\rho y) = \sigma g(y)$ with some invertible matrix σ and for $y \in \mathbf{R}^n$, then it holds that*

$$f_j(\rho y) = -\rho f_j(y) \quad \textit{for } y \in \mathbf{R}^n \textit{ and for all } j,$$

and therefore the modified differential equation (3.2) *is also ρ-reversible.*

PROOF. For numerical methods satisfying $\Phi_{-h}(\rho y) = \rho \Phi_h(y)$, their symmetry is necessary and sufficient for the modified equation being ρ-reversible (see [4, Theorem V.2.1]). Without having formulated it explicitly, we assume that $\widehat{\Phi}_h$ satisfies this relation (this is trivially true for all Runge–Kutta methods). Differentiating $g(\rho y) = \sigma g(y)$, we get $\rho^T G^T(\rho y) = G^T(y)\sigma^T$ and, due to the orthogonality of ρ, we see that (2.1) is equivalent to

$$\rho \widehat{y}_0 = \rho y_0 + G^T(\rho y_0)\sigma^{-T}\mu, \qquad g(\rho y_0) = 0.$$

This, together with a similar relation for (2.3), implies $\Phi_{-h}(\rho y) = \rho \Phi_h(y)$ for the symmetric projection method. □

All results on the long-time behavior of symmetric methods, applied to ρ-reversible systems in an Euclidean space, remain therefore valid for symmetric projection methods and ρ-reversible differential equations on manifolds.

4 Numerical illustrations.

Let us illustrate the qualitative performance of symmetric projection methods at two representative examples.

EXAMPLE 4.1 (*Rigid body).* A commonly used test problem for Lie group methods are the equations of motion of a rigid body

$$\begin{aligned} y_1' &= a_1 y_2 y_3, \qquad a_1 = (I_2 - I_3)/(I_2 I_3), \\ y_2' &= a_2 y_3 y_1, \qquad a_2 = (I_3 - I_1)/(I_3 I_1), \\ y_3' &= a_3 y_1 y_2, \qquad a_3 = (I_1 - I_2)/(I_1 I_2), \end{aligned} \tag{4.1}$$

where the vector $y = (y_1, y_2, y_3)^T$ represents the angular momentum in the body frame, and I_1, I_2, I_3 are the principal moments of inertia (see [8, Chapter 15] for a detailed description). This is a differential equation on the manifold defined by

$$g(y_1, y_2, y_3) := y_1^2 + y_2^2 + y_3^2 - R^2 = 0, \tag{4.2}$$

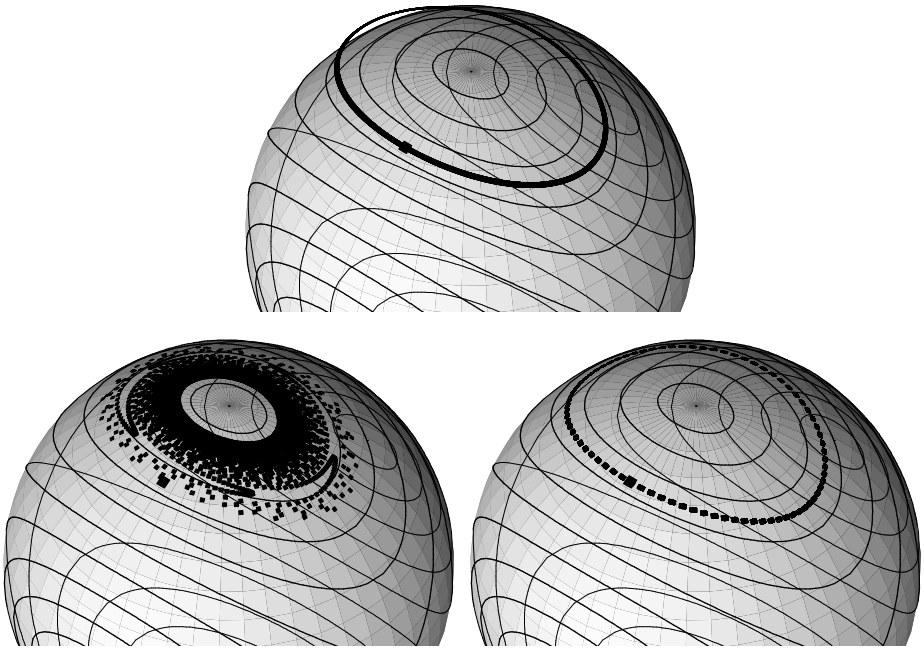

Figure 4.1: Numerical solution of the rigid body equations (4.1) obtained by the trapezoidal rule with $h = 1$ (5000 steps) without projection (upper picture), with standard projection (lower left), and with symmetric projection (lower right).

where R is the Euclidean norm of the initial vector. It is interesting to note that the system (4.1) is actually a Hamiltonian system on the sphere (4.2) with Hamiltonian

$$H(y_1, y_2, y_3) = \frac{1}{2}\Big(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3} \Big). \tag{4.3}$$

We do not explicitly use this additional invariant in our algorithm, but it is interesting to study how well it is conserved by the numerical solution. The exact solution of the problem lies on the intersection of the sphere (4.2) with the ellipsoid $H(y_1, y_2, y_3) = const$ (see Figure 4.1).

Since (4.2) and (4.3) are both quadratic first integrals of the system (4.1), it does not make sense to study the performance of symplectic methods (they exactly conserve both invariants, and a projection onto the manifold is superfluous). We therefore consider the trapezoidal rule as the basic method for our projection algorithm. We take $I_1 = 2$, $I_2 = 1$ and $I_3 = 2/3$, a large stepsize $h = 1$, and $y_0 = (R\cos(1.1), 0, R\sin(1.1))^T$ as initial value ($R = 2.3$).

The upper picture of Figure 4.1 shows the numerical solution obtained without any projections. We see that it is qualitatively correct, but it does not lie on the sphere. The lower left picture shows the numerical solution obtained with standard projection (Figure 1.1, left). Now, the solution is forced to lie on the correct manifold, but the qualitative behavior becomes completely wrong

(because standard projection destroys the symmetry of the method). The lower right picture of Figure 4.1 shows the numerical solution of method (2.1)–(2.3). This time, the numerical solution lies on the manifold, and it shows the correct qualitative behavior, as expected from the backward error analysis.

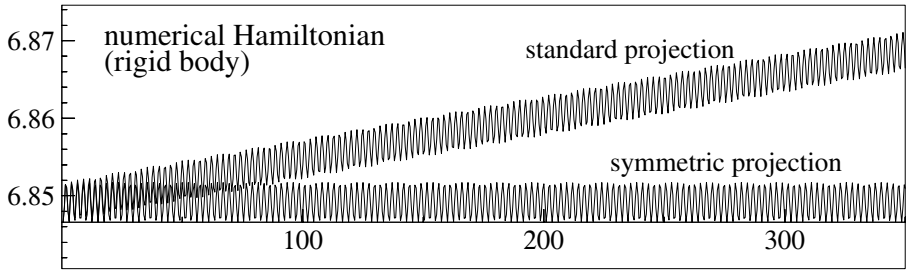

Figure 4.2: Numerical Hamiltonian for the rigid body simulation with $h = 0.5$.

In Figure 4.2 we plot the value of the Hamiltonian (4.3) along the numerical solution. This should be constant equal to the value $H(y_0) \approx 6.8466$ (horizontal axis in Figure 4.2). Standard projection shows a linear drift from the exact value, whereas symmetric projection gives a numerical Hamiltonian that stays close to the correct value for all times. The same correct behavior can be observed for symmetric methods without any projection.

Let us remark that projection as postprocessing is also possible. This means that after every step the solution is projected onto the manifold, but the integration is continued with the unprojected value. In the previous example this gives also excellent results, but it is less satisfactory, because using the vector field $f(y)$ outside the manifold may be dangerous. This is in particular the case when $g(y)$ is not a first integral.

An important class of problems are conservative multibody systems with holonomic constraints.

$$q' = H_p(p,q), \tag{4.4}$$

$$p' = -H_q(p,q) - G^T(q)\lambda, \tag{4.5}$$

$$0 = g(q). \tag{4.6}$$

Here, $H : \mathbf{R}^n \times \mathbf{R}^n \to \mathbf{R}$ is the Hamiltonian function, H_p and H_q denote partial derivatives, $g : \mathbf{R}^n \to \mathbf{R}^m$ are the constraints, and $G(q) = g_q(q)$. Typically, $H(p,q) = \frac{1}{2}p^T M(q)^{-1}p + U(q)$ is the sum of the kinetic and potential energies. Differentiating the constraint (4.6) twice, we get

$$0 = G(q)H_p(p,q), \tag{4.7}$$

$$0 = \frac{d}{dq}\Big(G(q)H_p(p,q)\Big)H_p(p,q) - G(q)H_{pp}(p,q)\Big(H_q(p,q) + G^T(q)\lambda\Big), \tag{4.8}$$

and we see that λ can be expressed in terms of p and q, if $G(q)H_{pp}(p,q)G^T(q)$ is invertible. Inserting the so-obtained $\lambda = \lambda(p,q)$ into (4.5), we get a differential

equation for (q, p), whose solution stays on the manifold

$$\mathcal{M} = \{(q,p)\,;\, g(q) = 0,\, G(q)H_p(p,q) = 0\}. \tag{4.9}$$

There exist numerical methods that produce qualitatively correct solutions, e.g., the RATTLE algorithm which is much used in molecular dynamics, and the Lobatto IIIA–IIIB pair [7]. However, it is known that the numerical treatment of the index 3 problem (4.4)–(4.6) is much more difficult than that of the underlying ordinary differential equation for q and p. We show, at the example of the simple pendulum, that the symmetric projection method (2.1)–(2.3) also gives qualitatively correct numerical approximations when integrating over long times.

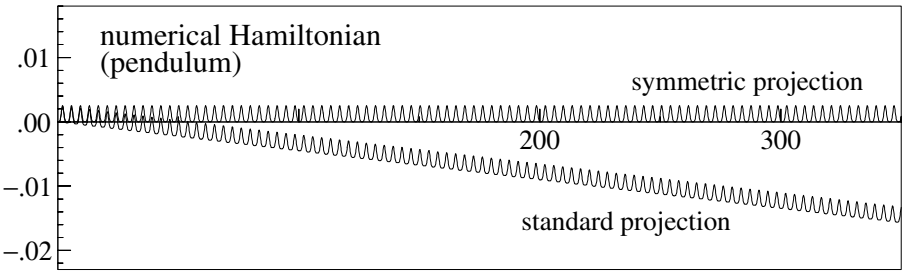

Figure 4.3: Numerical Hamiltonian for the pendulum problem with stepsize $h = 0.1$ (midpoint rule).

Example 4.2 (*Pendulum).* We consider the problem (4.4)–(4.6) with Hamiltonian $H(p,q) = (p_1^2 + p_2^2)/2 + q_2$ and constraint $g(q_1, q_2) = q_1^2 + q_2^2 - 1$. This yields the equations for the simple pendulum, expressed in Cartesian coordinates. This time we apply the implicit midpoint rule (as representative of the Gauss methods) with stepsize $h = 0.1$ and initial values $q_1(0) = 1$, $q_2(0) = 0$, $p_1(0) = 0$, and $p_2(0) = 0$. Applying this method to the underlying differential equation for (q, p), we observe that the quadratic constraint $g(q_1, q_2) = 0$ is not exactly conserved. This is not a contradiction to the symplecticity of the method, because $g(q_1, q_2)$ is not a first integral. Hence, the use of projection methods makes sense.

The numerical results are similar to those of the preceding example. Figure 4.3 shows the numerical Hamiltonian for both types of projection algorithms (see [6, Section VII.2] for a discussion of projections in multibody simulations). Again, we observe that symmetric projection yields a correct qualitative behavior, whereas standard projection cannot keep the energy close to the correct value when integrated over long times.

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