Theory and numerics of solitary waves: Talk about split-step methods

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1 Notation

We consider an autonomous problem

$$\dot{y} = f(y), \quad y(t_0) = y_0 \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}^n$ is sufficiently differentiable.

We denote its exact flow by φ_t. Φ_h will refer to a numerical one-step method with step-size h.

The *adjoint method* Φ_h^* of a method Φ_h is the inverse map of the original method with reversed time step $-h$, i.e.,

$$\Phi_h^* := \Phi_{-h}^{-1}.$$

In other words, $y_1 = \Phi_h^*(y_0)$ is implicitly defined by $\Phi_{-h}(y_1) = y_0$. A method for which $\Phi * _h = \Phi_h$ is called *symmetric*.

Note that $\varphi_{-t}^{-1} = \varphi_t$, but in general $\Phi_h^* = \Phi_{-h}^{-1} \neq \Phi_h$. The adjoint method satisfies $(\Phi_h^*)^* = \Phi_h$ and $(\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^*$.

Theorem 1 *Let φ_t be the exact flow (1) and let Φ_h be a one-step method of order p satisfying*

$$\Phi_h(y_0) = \varphi_h(y_0) + C(y_0)h^{p+1} + \mathcal{O}(h^{p+1}).$$

The adjoint method Φ_h^* then has the same order p and we have

$$\Phi_h^*(y_0) = \varphi_h(y_0) + (-1)^p C(y_0)h^{p+1} + \mathcal{O}(h^{p+1}).$$

If the method is symmetric, its (maximal) order is even.

The proof can be found in [1], Section II.3.

2 Split-Step Methods

Once decomposes the vector field into integrable pieces and treats them separately.

We consider an arbitrary system $\dot{y} = f(y)$ in $\mathbb{R}^n$, and suppose that the vector field is "split" as

$$\dot{y} = f^{[1]}(y) + f^{[2]}(y). \tag{2}$$

It then, by chance, the exact flows $\phi_t^{[1]}$ and $\Phi_t^{[2]}$ of the systems $\dot{y} = f^{[1]}(y)$ and $\dot{y} = f^{[2]}(y)$ can be calculated explicitly, we can, from a given initial value y_0, first solve the first system to obtain a value $y_{1/2}$, and from this value integrate the second system to obtain y_1. In this way we have introduced the numerical methods

$$\begin{aligned} \Phi_h^* &= \varphi_h^{[2]} \circ \varphi_h^{[1]} \\ \Phi_h &= \varphi_h^{[1]} \circ \varphi_h^{[2]} \end{aligned} \tag{3}$$

where one is the adjoint of the other. These formulas are often called the *Lie-Trotter splitting* (Trotter 1959). By Taylor expansion we find that $(\varphi_h^{[1]} \circ \varphi_h^{[2]})(y_0) = \varphi_h(y_0) + \mathcal{O}(h^2)$, so that both methods give approximations of order 1 to the solution of (2). Another idea is to use a symmetric version and put

$$\Phi_h^{[S]} = \varphi_{h/2}^{[1]} \circ \varphi_h^{[2]} \circ \varphi_{h/2}^{[1]}, \tag{4}$$

which is known as the *Strang splitting* (Strang 1968), and sometimes as the *Marchuk splitting* (Marchuk 1968). By breaking up in (4) $\varphi_h^{[2]} = \varphi_{h/2}^{[2]} \circ \varphi_{h/2}^{[2]}$, we see that the Strang splitting $\Phi_h^{[S]} = \Phi_{h/2} \circ \Phi_{h/2}^*$ is the composition of the Lie-Trotter method and its adjoint with halved step sizes. The Strang splitting formula is therefore symmetric and of order 2.

2.1 General Splitting Procedure

In a similar way to the general idea of composition methods, we can form with arbitrary coefficients $a_1, b_1, a_2, \ldots, a_m, b_m$ (where, eventually, a_1 or b_m, or both, are zero)

$$\Psi_h = \varphi_{b_m h}^{[2]} \circ \varphi_{a_m h}^{[1]} \circ \varphi_{b_{m-1} h}^{[2]} \circ \cdots \circ \varphi_{a_2 h}^{[1]} \circ \varphi_{b_1 h}^{[2]} \circ \varphi_{a_1 h}^{[1]} \tag{5}$$

and try to increase the order of the scheme by suitably determining the free coefficients. We will show a method how to do that later.

There is a close connection between the theories of splitting methods and of composition methods. If we put $\beta_1 = a_1$ and break up $\varphi_{b_1 h}^{[2]} = \varphi_{\alpha_1 h}^{[2]} \circ \varphi_{\beta_1 h}^{[2]}$ (group property of the exact flow) and so on, we see that with

$$\Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]} \quad \text{so that} \quad \Phi_h^* = \varphi_h^{[2]} \circ \varphi_h^{[1]} \tag{6}$$

Ψ_h is identical with the Ψ_h of a composition method. The αs and βs for $m = 3$ are given below.

$$\begin{aligned} a_1 &= \beta_1 \\ b_1 &= \beta_1 + \alpha_1 \\ a_2 &= \alpha_1 + \beta_2 \\ b_2 &= \beta_2 + \alpha_2 \\ a_3 &= \alpha_2 + \beta_3 \\ b_3 &= \beta_3 \end{aligned} \tag{7}$$

A necessary and sufficient condition for the existence of α_i and β_i satisfying (7) is that $\sum a_i = \sum b_i$, which is the consistency condition anyway for (5).

2.2 Combining Exact and Numerical Flows

It may happen that the differential equation $\dot{y} = f(y)$ can be split according to (2), such that only the flow of, say, $\dot{y} = f^{[1]}(y)$ can be computed exactly. If $f^{[1]}(y)$ constitutes the dominant part of the vector field, it is natural to search for integrators that exploit this information. We just consider

$$\Phi_h = \varphi_h^{[1]} \circ \Phi_h^{[2]}, \quad \Phi_h^* = \Phi_h^{[2]*} \circ \varphi_h^{[1]} \tag{8}$$

as the basis of the composition method. Here $\varphi_t^{[1]}$ is the exact flow of $\dot{y} = f^{[1]}(y)$, and $\Phi_h^{[2]}$ is some first-order integrator applied to $\dot{y} = f^{[2]}(y)$. Since Φ_h of (8) is consistent with (2), the resulting method has the desired high order. It is given by

$$\Psi_h = \varphi^{[1]}_{\alpha_s h} \circ \Phi^{[2]}_{\alpha_s h} \circ \Phi^{[2]*}_{\beta_s h} \circ \varphi^{[1]}_{(\beta_s+\alpha_{s-1})2h} \circ \Phi^{[2]}_{\alpha_{s-1}1h} \circ \cdots \circ \Phi^{[2]*}_{\beta_1 h} \circ \varphi^{[1]}_{\beta_1 h}. \tag{9}$$

Notice that replacing $\varphi_t^{[2]}$ with a low-order approximation $\Phi_t^{[2]}$ in (5) would not retain the high order of the composition, because $\Phi_t^{[2]}$ does not satisfy the group property.

2.3 Splitting into More than Two Vector Fields

Consider a differential equation

$$\dot{y} = f^{[1]}(y) + f^{[2]}(y) + \cdots + f^{[N]}(y), \tag{10}$$

where we assume that the flows $\varphi_t^{[j]}$ of the individual problems $\dot{y} = f^{[j]}(y)$ can be computed exactly. In this case there are many possibilities for extending (5) and for writing the method as a composition of $\varphi^{[1]}_{a_j h}, \varphi^{[2]}_{b_j h}, \varphi^{[3]}_{c_j h}, \ldots$. This makes it difficult to find optimal compositions of high order. A simple and efficient way is to consider the first-order method

$$\Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]} \circ \cdots \circ \varphi_h^{[N]} \tag{11}$$

together with its adjoint as the basis for a composition method. Without any additional effort this yields splitting methods for (10) of arbitrary high order.

3 Example: Low order splitting methods for the 1D Nonlinear Schrödinger Equation (NLS)

For repetition: the 1D nonlinear Schrödinger equation

$$iu_t + u_{xx} + |u|^2 u = 0 \tag{12}$$

It will be convenient to rewrite the NLS to

$$u_t = i\mathcal{L}u + i\mathcal{N}(u)u, \qquad -\infty < x < \infty, \tag{13}$$

where

$$\mathcal{L}u := u_{xx} \qquad \mathcal{N}(u) := |u|^2 \tag{14}$$

As a first step, we see, that the solution of (12) may be advanced from one time-level to the next by means of the following formula

$$u(x, t+\tau) \approx e^{i\tau(\mathcal{L}+\mathcal{N}(u))} \cdot u(x,t), \tag{15}$$

where τ denotes the timestep. In general (15) is first order accurate, but under scpecial circumstances $|u|^2$ is time-independent in which case (15) turns out to be exact.

The time-splitting procedure now consists of replacing the right-hand side of (15) by

$$e^{i\tau(\mathcal{L}+\mathcal{N}(u))}u(x,t) \approx e^{i\tau\mathcal{L}}e^{i\tau\mathcal{N}(u)}u(x,t) \tag{16}$$

This expression is exact whenever $\mathcal{L}$ and $\mathcal{N}$ commute. Otherwise the splitting is first order accurate. Accordingly, we use

$$U(x, t+\tau) = e^{i\tau\mathcal{L}}e^{i\tau\mathcal{N}(U)}U(x,t) \tag{17}$$

where $U(x,t)$ denotes the approximation of $u(x,t)$.

Next, we introduce the quantity

$$V^m := e^{i\tau\mathcal{N}(U^m)}U^m \tag{18}$$

where U^m denotes the approximation at the time $m\tau$. Then the split-step scheme (17) may be written as

$$U^{m+1} = e^{i\tau\mathcal{L}}V^m. \tag{19}$$

4 High order splitting methods for Hamiltonian PDE systems

Symplectic integrators are numerical integrations schemes for Hamiltonian systems, which conserve the symplectic two-form $dp^d q$ exactly, so that $(q(0), p(0)) \to (q(\tau), p(\tau))$ is a canonical transformation. We will show here, how to construct explicit symplectic integrators for a Hamiltonian

$$H = T(p) + V(q). \tag{20}$$

4.1 The Problem

Let A and B be non-commutative operators and τ a small real number. For a given positive integer n which will be called the *order of integrator*, find a set of real numbers $(c_1, c_2, \ldots, c_k)$ and $(d_1, d_2, \ldots, d_k)$ such that the difference of the exponential function $\exp[\tau(A+B)]$ and the product of exponential functions

$$\exp(c_1\tau A)\exp(d_1\tau B)\exp(c_2\tau A)\exp(d_2\tau B) \times \cdots \times \exp(c_k\tau A)\exp(d_k\tau B) \tag{21}$$

is of the order τ^{n+1}, i.e., the following equation holds,

$$\exp[\tau(A+B)] = \prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B) + o(\tau^{n+1}). \tag{22}$$

This is equivalent to

$$\begin{array}{ll} S(\tau) & := \prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B) \\ & = \exp([\tau(A+B) + o(\tau^{n+1})]. \end{array} \tag{23}$$

For example, as we saw before, when $n = 1$, a trivial solution is $c_1 = d_1 = 1$ ($k = 1$), and we have

$$\exp[\tau(A+B)] = \exp(\tau A) \exp(\tau B) + o(\tau^2) \tag{24}$$

When $n = 2$, we find that $c_1 = c_2 = \frac{1}{2}, d_1 = 1, d_2 = 0$ ($k = 2$), thus

$$\exp[\tau(A+B)] = \exp(\frac{1}{2}\tau A) \exp(\tau B) \exp(\frac{1}{2}\tau B) + o(\tau^3) \tag{25}$$

4.2 Basic formulas

We could look closer at this method now, but because it is almost hopeless to obtain a much higher integrator, we skip this and advance to a much better method using the **Baker-Campbell-Hausdorff (BCH) formula**. For any non-commutative operators X and Y, the product of the two exponential functions, $\exp(X)\exp(Y)$, can be expressed in the form of a single exponential function as

$$\exp(X)\exp(Y) = \exp(Z)$$

where

$$\begin{array}{ll} Z & = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}([X,X,Y] + [Y,Y,X]) + \frac{1}{24}[X,Y,Y,X] \\ & -\frac{1}{720}([Y,Y,Y,Y,X] + [X,X,X,X,Y]) + \frac{1}{360}([Y,X,X,X,Y] + [X,Y,Y,Y,X]) \\ & +\frac{1}{120}([X,X,Y,Y,X] + [Y,Y,X,X,Y]) + \dots \ . \end{array} \tag{26}$$

Here we used the notation of the commutator $[X,Y] := XY - YX$, and higher order commutators like $[X,X,Y] = [X,[X,Y]]$. A remarkable feature of this BCH formula is that there appear only commutators of X and Y exept for the linear terms in the series.

By repeated application of the BCH formula (26), we find

$$\exp(X)\exp(Y)\exp(X) = \exp(W),$$

where

$$\begin{array}{ll} Z & = 2X + Y + \frac{1}{6}[Y,Y,X] - \frac{1}{6}[X,X,Y] + \frac{7}{360}[X,X,X,X,Y] \\ & -\frac{1}{360}[Y,Y,Y,Y,X] + \frac{1}{90}[X,Y,Y,Y,X] + \frac{1}{45}[Y,X,X,X,Y] \\ & -\frac{1}{60}[X,X,Y,Y,X] + \frac{1}{30}[Y,Y,X,X,Y] + \dots \ . \end{array} \tag{27}$$

Thus the operator for the 2nd order symplectic integrator (25) can be written in the form

$$\begin{array}{ll} S_{2nd}(\tau) & := \exp(\frac{1}{2}\tau A) \exp(\tau B) \exp(\frac{1}{2}\tau A) \\ & = \exp(\tau\alpha_1 + \tau^3\alpha_3 + \tau^5\alpha_5 + \tau^7\alpha_7 + \dots), \end{array} \tag{28}$$

where

$$\begin{array}{l} \alpha_1 := A + B, \quad \alpha_3 = \frac{1}{12}[B,B,A] - \frac{1}{24}[A,A,B], \\ \alpha_5 := \frac{7}{5760}[A,A,A,A,B] + \dots \ . \end{array}$$

In the expression (28) there exist no terms of even powers of τ, i.e., $\alpha_2 = \alpha_4 = \alpha_6 = \cdots = 0$. This comes from the fact that the operator $S_{2nd}(\tau)$ is symmetric and has the exact time reversibility

$$S(\tau)S(-\tau) = S(-\tau)S(\tau) = identity \tag{29}$$

Indeed this is an example of a more general statement as follows.

Lemma 1 *Let $S(\tau)$ be an operator of the form (23) which has the time reversibility (29). If we expand $S(\tau)$ in the from*

$$S(\tau) = \exp(\tau\gamma_1 + \tau^2\gamma_2 + \tau^3\gamma_3 + \tau^4\gamma_4 + \dots) \tag{30}$$

then

$$\gamma_2 = \gamma_4 = \gamma_6 = \cdots = 0$$

The proof can be found in [3].

Therefore if a symplectic integrator has a symmetric form so that (29) holds, it is automatically of an even order. Keeping this fact in mind, we now construct symplectic integrators (4th, 6th, 8th, ...) by a symmetric product of symplectic integrators of lower order.

4.3 Symmetric integrator with exact coefficients

A 4th order integrator is obtained by a symmetric repetition (product) of the 2nd order integrator (28) in the form

$$S_{4th}(\tau) := S_{2nd}(x_1\tau)S_{2nd}(x_0\tau)S_{2nd}(x_1\tau) \tag{31}$$

where x_0 and x_1 are two real unknowns to be determined. If we apply formula (27) to 31, we have

$$\begin{aligned} S_{4th}(\tau) \quad &= \exp[\tau(x_0 + 2x_1)\alpha_1 + \tau^3(x_0^3 + 2x_1^3)\alpha_3 \\ &\quad +\tau^5(x_0^5 + 2x_1^5)\alpha_5 + \dots]. \end{aligned} \tag{32}$$

In order that (32) gives a 4th order integrator, we need two conditions

$$x_0 + 2x_1 = 1, \quad x_0^3 + 2x_1^3 = 0 \tag{33}$$

so that $S_{4th}(\tau) = \exp[\tau(A + B) + o(\tau^5)]$. The real unique solution is obviously

$$x_0 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \quad x_1 = \frac{1}{2 - 2^{1/3}}. \tag{34}$$

If we compare the operator (31 with (28), we find the relations between the two sets of coefficients:

$$d_1 = d_3 = x_1, \quad d_2 = x_0, \quad c_1 = c_4 = \frac{1}{2}x_1, \quad c_2 = c_3 = \frac{1}{2}(x_0 + x_1). \tag{35}$$

Once a 4th order integrator is found, it is easy to obtain a 6th order integrator using the 4th order one by the same process.

More generally, if a symmetric integrator of order $2n$, $S_{2n}(\tau)$, is already known, a $(2n+2)$th order integrator is obtained by the product

$$S_{2n+n}(\tau) := S_{2n}(z_1\tau)S_{2n}(z_0\tau)S_{2n}(z_1\tau), \tag{36}$$

where z_0 and z_1 must satisfy

$$z_0 + 2z_1 = 1, \quad z_0^{2n+1} + 2z_1^{2n+1} = 0 \tag{37}$$

or

$$z_0 = -\frac{2^{1/(2n+1)}}{2 - 2^{1/2(2n+1)}}, z_1 = \frac{1}{2 - 2^{1/2(2n+1)}}. \tag{38}$$

In this way we can construct symplectic integrators of an arbitrary even order with exact coefficients. However, with this construction, the $(2n)$th order integrator requires the operator S_{2nd}, 3^{n-1} times. This means that the number of steps k is $k = 3^{n-1} + 1$, which grows rapidly as n increases. In [3] an alternative method is shown to obtain more economically integrators, though the coefficients cannot be given analytically.

A computational task split step method

A.1 Setting

We want to find a stationary 1-soliton solution of (12) by numerical propagation of an initially Gaussian profile

$$u(x, 0) = 1.5e^{-x^2} \tag{39}$$

and discarding radiation. We use PML to treat the outgoing radiation, i.e., change the problem to

$$iu_t + \frac{1}{1 + \sigma e^{i\gamma}} \partial_x \left(\frac{1}{1 + \sigma e^{i\gamma}} u_x \right) + |u|^2 u = 0 \tag{40}$$

in an additional layer on the boundary as shown in [4]. After enough damping to avoid interfering reflection, we apply Dirichlet BC to cut off the remaining radiation.

The $\mathcal{L}$ will be replaced by

$$\mathcal{L}u := \frac{1}{1 + \sigma e^{i\gamma}} \partial_x \left(\frac{1}{1 + \sigma e^{i\gamma}} u_x \right) \tag{41}$$

in the damping layer.

Although the NLS equation is defined of the real line we need to impose conditions at a finite boundary when it is solved numerically. We will simulate on the interval $[-\frac{1}{2}L, \frac{1}{2}L]$. This interval is divided in $N - 50$ equal subintervals with grid spacing h, i.e.,

$$h := \frac{L}{N - 50} \tag{42}$$

At both ends of the interval, we will add a layer of 25 intervals of the length h, where we will apply PML. The grid points are denoted by

$$x_j = jh, \qquad j = -\frac{N}{2}, \ldots, \frac{N}{2}. \tag{43}$$

The approximation of $u(x_j, m\tau)$ is denoted by U_j^m.

In order to implement the split-step scheme (18) - (19) in practice, we use the following rational approximation

$$e^{i\tau\mathcal{L}} = (\mathrm{Id} - \theta i\tau\mathcal{L})^{-1}(\mathrm{Id} + (1 - \theta)i\tau\mathcal{L}) \tag{44}$$

where θ is a free parameter with $0 \leq \theta \leq 1$.

Equation (19) now becomes

$$(\mathrm{Id} - \theta i\tau\mathcal{L})U^{m+1} = (\mathrm{Id} + (1 - \theta)i\tau\mathcal{L})V^m. \tag{45}$$

The space variable may be discretized by replacing $\mathcal{L}$ by $\mathcal{L}_h$ where

$$\mathcal{L}_h U_j := (U_{j+1} - 2U_j + U_{j-1})/h^2 \tag{46}$$

for $j = -\frac{N}{2} + 25, \ldots, \frac{N}{2} - 25$ and

$$\mathcal{L}_h U_j := \frac{1}{(1+\sigma_j e^{i\gamma})^2}\left((U_{j+1} - 2U_j + U_{j-1})/h^2 - \frac{\sigma_j' e^{i\gamma}}{1+\sigma_j e^{i\gamma}}(U_{j+1} - U_j)/h\right) \tag{47}$$

for $j = -\frac{N}{2}, \ldots, -\frac{N}{2} + 24$ or $j = \frac{N}{2} - 24, \ldots, \frac{N}{2}$.

Hence the scheme (45) may be written in matrix notation as

$$(I - ir\theta\mathbf{S})\mathbf{U}^{m+1} = (I + ir(1-\theta)\mathbf{S})\mathbf{V}^m \tag{48}$$

where I is the identity matrix, and

$$r := \frac{\tau}{h^2}, \qquad \mathbf{U} := (U_{-\frac{N}{2}}, \ldots, U_{\frac{N}{2}}), \tag{49}$$

$$V_j^m := e^{i\tau|U_j^m|^2} U_j^m \tag{50}$$

and

$$\mathbf{S} := \begin{pmatrix}
b_{-\frac{N}{2}} & c_{-\frac{N}{2}} & & & & & & \\
a_{-\frac{N}{2}+1} & b_{-\frac{N}{2}+1} & c_{-\frac{N}{2}+1} & & & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & a_{-\frac{N}{2}+24} & b_{-\frac{N}{2}+24} & c_{-\frac{N}{2}+24} & & & & \\
 & & 1 & -2 & 1 & & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & 1 & -2 & 1 & & \\
 & & & & a_{\frac{N}{2}-24} & b_{\frac{N}{2}-24} & c_{\frac{N}{2}-24} & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & a_{\frac{N}{2}-1} & b_{\frac{N}{2}-1} & c_{\frac{N}{2}-1} \\
 & & & & & & a_{\frac{N}{2}} & b_{\frac{N}{2}}
\end{pmatrix} \tag{51}$$

with

$$a_j := \frac{1}{(1+\sigma_j e^{i\gamma})^2} \tag{52}$$

$$b_j := \frac{1}{(1+\sigma_j e^{i\gamma})^2}\left(-2 + \frac{h\sigma_j' e^{i\gamma}}{1+\sigma_j e^{i\gamma}}\right) \tag{53}$$

$$c_j := \frac{1}{(1+\sigma_j e^{i\gamma})^2}\left(1 - \frac{h\sigma_j' e^{i\gamma}}{1+\sigma_j e^{i\gamma}}\right) \tag{54}$$

The absorbtion parameter decreases in quadratic power to an angle of $\frac{\pi}{4}$ and with a maximum absorption parameter of 100.

$$\gamma := \frac{\pi}{4} \tag{55}$$

$$\sigma_j := 100 \begin{cases} \left(\frac{j+(\frac{N}{2}-24)}{25}\right)^2 & \text{if } j < 0 \\ \left(\frac{j-(\frac{N}{2}-24)}{25}\right)^2 & \text{if } j > 0 \end{cases} \quad ,j \in \left\{-\frac{N}{2}, \ldots, -\frac{N}{2}+24, \frac{N}{2}-24, \ldots, \frac{N}{2}\right\} \tag{56}$$

$$\sigma_j' := 200 \begin{cases} \left(\frac{j+(\frac{N}{2}-24)}{25}\right) & \text{if } j < 0 \\ \left(\frac{j-(\frac{N}{2}-24)}{25}\right) & \text{if } j > 0 \end{cases} \quad ,j \in \left\{-\frac{N}{2}, \ldots, -\frac{N}{2}+24, \frac{N}{2}-24, \ldots, \frac{N}{2}\right\} \tag{57}$$

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