

A modified phase-fitted Runge–Kutta method for the numerical solution of the Schrödinger equation

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A modified phase-fitted Runge–Kutta method (i.e., a method with phase-lag of order infinity) for the numerical solution of periodic initial-value problems is constructed in this paper. This new modified method is based on the Runge–Kutta fifth algebraic order method of Dormand and Prince [33]. The numerical results indicate that this new method is more efficient for the numerical solution of periodic initial-value problems than the well known Runge–Kutta method of Dormand and Prince [33] with algebraic order five.

KEY WORDS: Runge–Kutta methods, phase-lag, phase-fitted, explicit methods

1. Introduction

The numerical solution of second order differential equations of the form

$$y''(t) = f(t, y(t)) \quad (1)$$

has been the subject of great activity in numerous scientific areas. In (1) the function f is independent of the first derivative of y . For the solution of the above problem many methods have been used.

For the approximate solution of the above problem many categories of methods have been developed (see, for example, [1–7 and references therein]). For the efficient solution of the above problem some special methods have also been obtained (see [8–26 and references therein]). Lambert and Watson [27] presented the symmetric methods for the first time and showed that their interval of periodicity is nonvanishing, which is assuring of the existence of periodic solutions in it (the interval of periodicity is determined by the application of the symmetric multistep method to the test equation $y''(t) = -p^2y(t)$; if $p^2h^2 \in (0, T_0^2)$, where h is the step length of the integration, then this interval is called *interval of periodicity*). They developed symmetric multistep methods, in order to solve

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Table 1
6-stage modified explicit Runge–Kutta method.

0						
c_2	g_2	a_{21}				
c_3	g_3	a_{31}	a_{32}			
c_4	g_4	a_{41}	a_{42}	a_{43}		
c_5	g_5	a_{51}	a_{52}	a_{53}	a_{54}	
c_6	g_6	a_{61}	a_{62}	a_{63}	a_{64}	a_{65}
		b_1	b_2	b_3	b_4	b_5
						b_6

a problem, called *orbital instability* (when the number of steps exceeds two), which was presented from a very well known family of multistep methods for the solution of equation (1), the family of Störmer–Cowell methods. The symmetric multistep methods have been used many times for long time integrations of planetary orbits (see [28 and references therein]).

The purpose of this paper is to develop an explicit fifth algebraic order phase-fitted Runge–Kutta method (i.e., a method with phase-lag of order infinity). We introduce in this paper a new modified approach for the Runge–Kutta methods. This approach is based on the modification of the classical Butcher table for the Runge–Kutta methods. With this modification we have additional free parameters. In section 2 we give the modification of the Runge–Kutta methods. The theory of phase-lag analysis is given in section 3. The construction of the new Runge–Kutta method with phase-lag of order infinity is presented in section 4. In section 5 some numerical illustrations are given.

2. Modified Runge–Kutta methods of order 4

For first order equations of the form

$$y' = f(x, y), \quad (2)$$

the modified explicit four-stage Runge–Kutta method of order 5 as given in table 1 uses the solution at x_n , y_n in order to approximate the solution y_{n+1} at $x_{n+1} = x_n + h$ by

$$y_{n+1} = y_n + h \{ b_1 f(x_n, Y_1) + b_2 f(x_n + c_2 h, Y_2) + b_3 f(x_n + c_3 h, Y_3) + b_4 f(x_n + c_4 h, Y_4) + b_5 f(x_n + c_5 h, Y_5) + b_6 f(x_n + c_6 h, Y_6) \}, \quad (3)$$

where

$$\begin{aligned} Y_1 &= y_n, \\ Y_2 &= g_2 y_n + h a_{21} f(x_n, Y_1), \\ Y_3 &= g_3 y_n + h \{ a_{31} f(x_n, Y_1) + a_{32} f(x_n + c_2 h, Y_2) \}, \\ Y_4 &= g_4 y_n + h \{ a_{41} f(x_n, Y_1) + a_{42} f(x_n + c_2 h, Y_2) + a_{43} f(x_n + c_3 h, Y_3) \}, \end{aligned} \quad (4)$$

Table 2
m-stage modified explicit Runge–Kutta method.

0					
c_2	g_2	a_{21}			
c_3	g_3	a_{31}	a_{32}		
\vdots		\vdots	\vdots		
c_m	g_m	$a_{m,1}$	$a_{m,2}$	\dots	$a_{m,m-1}$
		b_1	b_2	\dots	b_{m-1} b_m

$$\begin{aligned}
 Y_5 &= g_5 y_n + h \{ a_{51} f(x_n, Y_1) + a_{52} f(x_n + c_2 h, Y_2) + a_{53} f(x_n + c_3 h, Y_3) \\
 &\quad + a_{54} f(x_n + c_4 h, Y_4) \}, \\
 Y_6 &= g_6 y_n + h \{ a_{61} f(x_n, Y_1) + a_{62} f(x_n + c_2 h, Y_2) + a_{63} f(x_n + c_3 h, Y_3) \\
 &\quad + a_{64} f(x_n + c_4 h, Y_4) + a_{65} f(x_n + c_5 h, Y_5) \}.
 \end{aligned}
 \tag{5}$$

It is easy to see that table 1 is different from the Butcher table for the classical 6-stage Runge–Kutta method of order five. The method presented in table 1 is called modified Runge–Kutta, since in the well-known classical Runge–Kutta methods the values of $g_i, i = 2(1)4$, are equal to 1. In the present paper and based on the requirement of infinite order of the phase-lag it can be seen that one of the values of $g_i, i = 2(1)6$, is not equal to 1.

3. Phase-lag analysis for Runge–Kutta methods

To develop the new method we use the test equation,

$$y' = ivy, \quad v \text{ real.} \tag{6}$$

We shall confine our considerations to homogeneous phase-lag based on the reasons fully described by Houwen and Sommeijer [29]. Based also on its definition given in [29], we shall use a test equation with an exact solution of the form e^{ivx} . By comparing the exact and the numerical solution for this equation, and by requiring that these solutions are in phase with maximal order in the step size h , we derive the so-called *dispersion relation* or *phase-lag relation*.

For first-order equations we write the m -stage modified explicit Runge–Kutta method in the matrix form given in table 2. Application of the above method to (6) yields the numerical solution

$$y_n = a_*^n y_0 \quad \text{and} \quad a_* = A_m(H^2) + iHB_m(H^2), \quad H = vh, \tag{7}$$

where

$$\begin{aligned}
 A_m(H^2) &= 1 - t_2 H^2 + t_4 H^4 + t_6 H^6 + \dots, \\
 B_m(H^2) &= 1 - t_3 H^2 + t_5 H^4 + t_7 H^6 + \dots
 \end{aligned}
 \tag{8}$$

are polynomials in H^2 , completely defined by Runge–Kutta parameters c_i , a_{ij} , g_i and b_k , $i = 2, \dots, m$, $j = 1, \dots, i - 1$, $k = 1, \dots, m$. The amplification factor is $a_* = a_*(H)$, and y_n denotes the approximation to $y(x_n)$.

A comparison of (7) with the solution of (6) leads to the following definition of the *dispersion or phase error or phase-lag and the amplification error*.

Definition 1 [30]. In the explicit m -stage modified Runge–Kutta method, presented in table 2, the quantities:

$$t(H) = H - \arg [a_*(H)], \quad a(H) = 1 - |a_*(H)| \quad (9)$$

are respectively called the dispersion or phase error or phase-lag and the amplification error. If $t(H) = O(H^{r+1})$ and $a(H) = O(H^{s+1})$ then the method is said to be phase-lag order r and dissipative order s .

Remark 1 [30]. From the definition (9) it follows that

$$a(H) = 1 - \sqrt{[A_m^2(H^2) + H^2 B_m^2(H^2)]}. \quad (10)$$

The interval $(0, H)$ for which $a(H) \geq 0$ is called *interval of imaginary stability*.

Also we have the following theorem (for the detailed proof, see [30]).

Theorem 1. For the Runge–Kutta method given by table 2 and (7) we have the following formula for the direct calculation of the phase-lag order r and the phase-lag constant q :

$$\tan(H) - H \left[\frac{B_m(H^2)}{A_m(H^2)} \right] = qH^{r+1} + O(H^{r+3}). \quad (11)$$

4. Derivation of the new Runge–Kutta method

Based on the procedure described above, on (8) and on the 6-stage modified explicit Runge–Kutta method presented in table 1 we have that

$$\begin{aligned} A_6(H^2) = & 1 - H^6 b_6 a_{65} a_{54} a_{43} a_{32} a_{21} - H^2 b_6 a_{63} g_3 - H^2 b_6 a_{64} g_4 - H^2 b_6 a_{65} g_5 \\ & - H^2 b_6 a_{61} - H^2 b_6 a_{62} g_2 - H^2 b_5 a_{53} g_3 - H^2 b_5 a_{54} g_4 - H^2 b_5 a_{51} \\ & - H^2 b_5 a_{52} g_2 + H^4 b_6 a_{65} a_{54} a_{43} g_3 - H^2 b_2 a_{21} + H^4 b_6 a_{65} a_{54} a_{41} \\ & + H^4 b_6 a_{65} a_{54} a_{42} g_2 + H^4 b_6 a_{65} a_{53} a_{32} g_2 - H^2 b_3 a_{31} + H^4 b_6 a_{65} a_{52} a_{21} \\ & + H^4 b_6 a_{65} a_{53} a_{31} + H^4 b_6 a_{64} a_{43} a_{31} + H^4 b_6 a_{64} a_{43} a_{32} g_2 \\ & + H^4 b_5 a_{54} a_{43} a_{32} g_2 + H^4 b_6 a_{63} a_{32} a_{21} + H^4 b_5 a_{54} a_{43} a_{31} + H^4 b_6 a_{64} a_{42} a_{21} \\ & + H^4 b_5 a_{54} a_{42} a_{21} - H^2 b_3 a_{32} g_2 + H^4 b_5 a_{53} a_{32} a_{21} - H^2 b_4 a_{41} \\ & + H^4 b_4 a_{43} a_{32} a_{21} - H^2 b_4 a_{42} g_2 - H^2 b_4 a_{43} g_3, \end{aligned} \quad (12)$$

$$\begin{aligned}
B_6(H^2) = & b_1 - H^2 b_6 a_{65} a_{54} g_4 + b_4 g_4 - H^2 b_6 a_{64} a_{43} g_3 - H^2 b_6 a_{65} a_{51} \\
& - H^2 b_6 a_{65} a_{52} g_2 - H^2 b_6 a_{65} a_{53} g_3 - H^2 b_6 a_{63} a_{32} g_2 - H^2 b_6 a_{64} a_{41} \\
& - H^2 b_6 a_{64} a_{42} g_2 - H^2 b_5 a_{54} a_{42} g_2 - H^2 b_5 a_{54} a_{43} g_3 - H^2 b_6 a_{62} a_{21} \\
& - H^2 b_6 a_{63} a_{31} - H^2 b_5 a_{52} a_{21} - H^2 b_5 a_{53} a_{31} - H^2 b_5 a_{53} a_{32} g_2 \\
& - H^2 b_5 a_{54} a_{41} - H^2 b_3 a_{32} a_{21} - H^2 b_4 a_{42} a_{21} - H^2 b_4 a_{43} a_{31} \\
& - H^2 b_4 a_{43} a_{32} g_2 + H^4 b_6 a_{65} a_{54} a_{42} a_{21} + H^4 b_6 a_{65} a_{54} a_{43} a_{31} \\
& + H^4 b_6 a_{65} a_{54} a_{43} a_{32} g_2 + b_6 g_6 + H^4 b_5 a_{54} a_{43} a_{32} a_{21} \\
& + H^4 b_6 a_{64} a_{43} a_{32} a_{21} + H^4 b_6 a_{65} a_{53} a_{32} a_{21} + b_2 g_2 + b_3 g_3 + b_5 g_5. \quad (13)
\end{aligned}$$

Based on the formula for the direct calculation of the phase-lag (11) and on the above formulae (12) and (13) and substituting the following coefficients:

$$\begin{aligned}
a_{21} &= \frac{1}{5}, & a_{31} &= \frac{3}{40}, & a_{32} &= \frac{9}{40}, & c_i &= \sum_{j=1}^{i-1} a_{ij}, \quad i = 2(1)6, \\
a_{41} &= \frac{3}{10}, & a_{42} &= -\frac{9}{10}, & a_{43} &= \frac{6}{5}, \\
a_{51} &= \frac{226}{729}, & a_{52} &= -\frac{25}{27}, & a_{53} &= \frac{880}{729}, & a_{54} &= \frac{55}{729}, \\
a_{61} &= -\frac{181}{270}, & a_{62} &= \frac{5}{2}, & a_{63} &= -\frac{266}{297}, & a_{64} &= -\frac{91}{27}, & a_{65} &= -\frac{189}{55}, \quad (14) \\
b_1 &= \frac{19}{216}, & b_2 &= 0, & b_3 &= \frac{1000}{2079}, \\
b_4 &= -\frac{125}{216}, & b_5 &= \frac{81}{88}, & b_6 &= \frac{5}{56}, \\
g_3 &= g_4 = g_5 = g_6 = 1,
\end{aligned}$$

we have that in order to have a phase-lag of order infinity the following relation must hold:

$$\begin{aligned}
\tan(H) &= H \left[\frac{B_6(H^2)}{A_6(H^2)} \right] = 0 \Rightarrow \\
g_2 &= -\frac{1}{15} \frac{2400H - 400H^3 + 5H^5 + \tan(H)(-2400 + 1200H^2 - 100H^4 + 3H^6)}{H^5}. \quad (15)
\end{aligned}$$

Numerical considerations indicate that Taylor series should be used when $H < 10^{-3}$.

The Taylor series expansion for g_2 given by the above formula (15) is

$$\begin{aligned}
g_2 &= 1 - \frac{H^2}{105} + \frac{11H^4}{2835} + \frac{262H^6}{155925} + \frac{4163H^8}{6081075} + \frac{1418H^{10}}{5108103} \\
&+ \frac{407098H^{12}}{3618239625} + \frac{6510824H^{14}}{142781302125} + \dots \quad (16)
\end{aligned}$$

The order condition equations (for more details, see [1]) for the developed method (and for $H \rightarrow 0$) are given by

$$\begin{aligned}
\sum_i b_i &= 1, & \sum_i b_i c_i &= \frac{1}{2}, & \sum_i b_i c_i^2 &= \frac{1}{3}, \\
\sum_{ij} b_i a_{ij} c_j &= \frac{1}{6}, & \sum_i b_i c_i^3 &= \frac{1}{4}, & \sum_{ij} b_i c_i a_{ij} c_j &= \frac{1}{8}, \\
\sum_{ij} b_i a_{ij} c_j^2 &= \frac{1}{12}, & \sum_{ijk} b_i a_{ij} a_{jk} c_k &= \frac{1}{24}, & \sum_i b_i c_i^4 &= \frac{1}{5}, \\
\sum_{ij} b_i c_i^2 a_{ij} c_j &= \frac{1}{10}, & \sum_{ijk} b_i a_{ij} c_j a_{ik} c_k &= \frac{1}{20}, & \sum_{ij} b_i c_i a_{ij} c_j^2 &= \frac{1}{15}, \\
\sum_{ij} b_i a_{ij} c_j^3 &= \frac{1}{20}, & \sum_{ijk} b_i c_i a_{ij} a_{jk} c_k &= \frac{1}{30}, & \sum_{ijk} b_i a_{ij} c_j a_{jk} c_k &= \frac{1}{40}, \\
\sum_{ijk} b_i a_{ij} a_{jk} c_k^2 &= \frac{1}{60}, & \sum_{ijkm} b_i a_{ij} a_{jk} a_{km} c_m &= \frac{1}{120},
\end{aligned} \tag{17}$$

i.e., the method is of algebraic order five. We note here that the above system of order condition equations represents also the present modified Runge–Kutta method since the coefficient g_2 is determined in order the Taylor series expansion to be of the form given in (16), i.e., for $H \rightarrow 0$ the coefficient g_2 to be equal to 1, i.e., to be equal to the value for fifth order Runge–Kutta Dormand and Prince method.

5. Numerical illustrations

The one-dimensional or radial Schrödinger equation has the form

$$y''(x) + q(x)y(x) = 0, \tag{18}$$

where $0 \leq x < \infty$ and $q(x) = E - l(l+1)/x^2 - V(x)$. We call the term $l(l+1)/x^2$ the *centrifugal potential*, and the function $V(x)$ the *potential*, where $V(x) \rightarrow 0$ as $x \rightarrow \infty$. In (18), E is a real number denoting the *energy*, l is a given integer and V is a given function which denotes the *potential*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes the *effective potential*, which satisfies $W(x) \rightarrow 0$ as $x \rightarrow \infty$. The boundary conditions are

$$y(0) = 0 \tag{19}$$

and a second boundary condition, for large values of x , determined by physical considerations.

In order to illustrate the efficiency of the new method given by (14) and (15), we apply it to the radial Schrödinger equation.

In order to apply the new method to the Schrödinger equation the value of parameter v is needed. For every problem of the radial Schrödinger equation given by (18) the parameter v is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}. \tag{20}$$

For some well-known potentials, such as Woods–Saxon potential, the definition of parameter v is given not as a function of x but based on some critical points which have been defined from the study of the appropriate potential (for details, see [23]).

5.1. Radial Schrödinger equation – Bound-states problem

We apply the new method to the Schrödinger equation (18) with the boundary conditions

$$y(0) = 0, \quad y(x) \approx \exp(-\sqrt{-E}x), \quad x \rightarrow \infty. \quad (21)$$

In order to solve this problem numerically we use a strategy which has been proposed by Cooley [31] and has been improved by Blatt [32]. This strategy involves integrating forward from the point $x = 0$, backward from the point $x_{\text{end}} = 15$ and matching up the solution at some internal point in the range of integration. As initial condition for the backward integration we take (see [20])

$$y(x_{\text{end}}) = \exp(-\sqrt{-E}x_{\text{end}}), \quad (22)$$

where h is the step length of integration of the numerical method.

5.1.1. Woods–Saxon potential

We use as potential the well-known Woods–Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z^2)} \quad (23)$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.

We compute the approximate eigenenergies of the Woods–Saxon bound-states problem using the classical Runge–Kutta Dormand and Prince method [33] (method [a]), the Runge–Kutta method developed by Houwen and Sommeijer of third algebraic order with phase-lag of order 10 ([29p. 606, scheme (3.9)]) (method [b]) and the new method (method [c]). The computed eigenenergies are compared with exact ones. In table 3 we present the maximum absolute error $|E_{\text{calculated}} - E_{\text{accurate}}|$ of the eigenenergies E_0 , E_4 , E_8 , E_{12} , as multiples of 10^{-9} , using the step size h given in the second column.

For the purpose of obtaining our numerical results it is appropriate to choose v as follows (for details, see [22,23]):

$$v = \begin{cases} \sqrt{-50 - E} & \text{for } x \in [0, 6.5 - 2h], \\ \sqrt{-37.5 - E} & \text{for } x = 6.5 - h, \\ \sqrt{-25 - E} & \text{for } x = 6.5, \\ \sqrt{-12.5 - E} & \text{for } x = 6.5 + h, \\ \sqrt{-E} & \text{for } x \in [6.5 + 2h, 15]. \end{cases} \quad (24)$$

Table 3

Radial Schrödinger equation. Bound-states problem. Woods–Saxon potential. Comparison of the maximum errors in the computation of the eigenvalues in 10^{-9} units using the methods [a]–[c].

Energy	h	Method [a]	Method [b]	Method [c]
$E_0 = -49.457788728$	1/4	45	11672	0
	1/8	2	138	0
	1/16	0	17	0
$E_4 = -41.232607772$	1/4	32859	1246281	12
	1/8	1042	157290	1
	1/16	17	19759	0
$E_8 = -26.873448915$	1/4	1072313	7860877	1987
	1/8	52020	1001651	307
	1/16	1069	125908	8
$E_{12} = -8.676081670$	1/4	45860449	19869742	12341
	1/8	348351	2764957	123
	1/16	10218	347898	31

5.2. Radial Schrödinger equation – The resonance problem

Consider the numerical solution of the Schrödinger equation (18) in the well-known case where the potential is the Woods–Saxon potential (23). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider equation (18) in a rather large domain of energies, i.e., $E \in [1, 1000]$.

In the case of positive energies, $E = k^2$, the potential dies away faster than the term $l(l+1)/x^2$ and the Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2} \right) y(x) = 0 \quad (25)$$

for x greater than some value X .

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$ where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions, respectively. Thus, the solution of equation (1) has (when $x \rightarrow 0$) the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC \left[\sin \left(kx - \frac{l\pi}{2} \right) + \tan \delta_l \cos \left(kx - \frac{l\pi}{2} \right) \right], \end{aligned} \quad (26)$$

where δ_l is the phase shift that may be calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_1) - y(x_2)C(x_2)} \quad (27)$$

for x_1 and x_2 distinct points in the asymptotic region (we choose x_1 as the right-hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and

Table 4

Radial Schrödinger equation. Resonance problem. Comparison of the maximum errors in the computation of the resonances in 10^{-6} units using the methods [a]–[c]. The empty areas indicate that the corresponding maximum absolute error is larger than 1.

Energy	h	Method [a]	Method [b]	Method [c]
$E_1 = 53.588872$	1/8	108	9878	3
	1/16	12	879	0
	1/32	4	65	0
$E_2 = 163.215341$	1/8	22857	65789	12
	1/16	126	547	4
	1/32	17	67	0
$E_3 = 341.495874$	1/8			1231
	1/16	1675		213
	1/32	567	5698	22
$E_4 = 989.701916$	1/8			213421
	1/16			31562
	1/32	345621		1287

$C(x) = kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need y_0 before starting a one-step method. From the initial condition we obtain y_0 . With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l .

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift δ_l or finding those E , for $E \in [1, 1000]$, at which $\delta_l = \pi/2$. We actually solve the latter problem, known as *the resonance problem* when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are

$$y(0) = 0, \quad y(x) = \cos(\sqrt{E}x) \quad \text{for large } x. \quad (28)$$

We solve the above problem using the methods mentioned in the bound-states problem.

The numerical results obtained for the three methods were compared with the analytic solution of the Woods–Saxon potential. In table 4 we present the maximum absolute error $|E_{\text{calculated}} - E_{\text{accurate}}|$ of the resonances E_n , $n = 1(1)4$, in multiples of 10^{-6} .

For the purpose of obtaining our numerical results it is appropriate to choose v as in bound-states problem (where $-E$ is substituted by E).

From the above results it can be seen that the new method is more efficient for the numerical solution of the Schrödinger equation than other similar well-known methods in the literature such as the fifth algebraic order Runge–Kutta method of Dormand and Prince [33] and the third algebraic order Runge–Kutta method with phase-lag of order 10 developed by Houwen and Sommeijer ([29p. 606, scheme (3.9)].

All computations were carried out using double precision arithmetic (16 significant digits accuracy).

6. Conclusion

A modified fifth order Runge–Kutta method with phase-lag of order infinity is developed in this paper. The new method is based on the fifth algebraic order Dormand and Prince Runge–Kutta method and is superior in accuracy to the classical one. This method has the simplicity of the initial start up. This makes it very fruitful compared with similar multistep methods.

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