

CUBIC SPLINE ON SPLINE METHOD FOR THE SOLUTION OF TWO DIMENSIONAL DIFFUSION EQUATION

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ABSTRACT

In this paper a cubic spline on spline method is applied in conjunction with an alternating direction approach to solve a two dimensional diffusion equation. Theoretical error estimates and stability analysis of the method are carried on. To illustrate the implementation of the method, numerical results for a test problem are obtained.

1. INTRODUCTION

The diffusion equation arises in many engineering problems such as; heat transfer, propagation of smoke, pollution, just to name a few. Exact solutions for the diffusion equation can only be obtained for certain simple boundary and initial conditions. Therefore we rely on numerical methods such as finite difference methods, finite element methods, boundary element methods and spline methods for the solution of the diffusion equation subject to complex boundary and initial conditions.

Cubic splines and cubic splines on splines together with finite difference approximations have been used for the solution of one dimensional spatial diffusion equation [1], [2].

In this paper we consider the solution of two dimensional spatial diffusion equation using cubic spline on spline technique together with an alternating direction approach. Consider the two dimensional diffusion equation namely

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad (1)$$

over the region defined by $x \in [0,1]$ and $y \in [0,1]$, and subject to the initial condition at $t=0$

$$u(x, y, 0) = g(x, y)$$

and boundary conditions for $t > 0$

$$\begin{aligned} u(0,y,t) = f_1(y,t) & \quad u(x,0,t) = h_1(x,t) \\ u(1,y,t) = f_2(y,t) & \quad u(x,1,t) = h_2(x,t) \end{aligned}$$

2- DESCRIPTION OF THE PROPOSED ALGORITHM

Let the x interval be subdivided into n equal subintervals of length h , such that

$$x_i = i h \quad i = 1, 2, \dots, n;$$

Similarly the y interval is subdivided into m equal subintervals of length k , such that

$$y_j = j k \quad j = 1, 2, \dots, m$$

The time step is denoted by L which leads to

$$t_q = q L \quad q = 1, 2, \dots$$

Using an alternating direction approach we replace the time derivative and the y derivative over half the time step by their equivalent finite differences, we obtain

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i,j,q+1/2} - u_{i,j,q}}{L/2} - \left[\frac{u_{i,j+1,q} - 2u_{i,j,q} + u_{i,j-1,q}}{k^2} \right] \quad (2)$$

which can be written as

$$\frac{d^2 U_1(x)}{dx^2} = F(U_1, x) \quad (3)$$

where U_1 is considered as a function in x only at $y = jk$ and $t = qL$ upon the above discretization given in (2).

Over the following half time step we replace the x derivative and the time derivative by their equivalent finite difference approximations, to get:

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{1,j,q+1} - u_{1,j,q+1/2} - u_{1+1,j,q+1/2} - 2u_{1,j,q+1/2} + u_{1-1,j,q+1/2}}{L/2} \quad (4)$$

which can be written as

$$\frac{d^2 U_3(y)}{dy^2} = G(U_3, y) \quad (5)$$

where U_3 is the corresponding function in y only at $x = ih$ and $t = (q + 1/2)L$.

Equations (3) and (5) can be reduced to a system of 1st order differential equations.

$$\frac{dU_1}{dx} = U_2 = F_1 \quad (3-a)$$

$$\frac{dU_2}{dx} = F(U_1, x) = F_2 \quad (3-b)$$

(3-a) and (3-b) can be written as

$$\frac{dU_p}{dx} = F_p(U_1, U_2, x) \quad p = 1, 2 \quad (6)$$

also

$$\frac{dU_3}{dy} = U_4 = G_3 \quad (5-a)$$

$$\frac{dU_4}{dy} = G(U_3, y) = G_4 \quad (5-b)$$

i.e.

$$\frac{dU_p}{dy} = G_p(U_3, U_4, y) \quad p = 3, 4 \quad (7)$$

Following the procedure detailed in [3], integrating equations (6) from x_{i-1} to x_i at $y = jk$ and $t = qL$, and denoting the resulting quantities by $\phi_{p,i}(u)$ we have

$$\phi_{p,i}(u) = \int_{x_{i-1}}^{x_i} \frac{dU_p}{dx} dx - \int_{x_{i-1}}^{x_i} F_p(U_1, U_2, x) dx = 0 \quad (8)$$

$$\phi_{p,i}(u) = U_{p,i} - U_{p,i-1} - \int_{x_{i-1}}^{x_i} F_p(U_1, U_2, x) dx = 0 \quad p = 1, 2 \quad (9)$$

Similarly, integrating equations (7) from y_{j-1} to y_j at $x = ih$ and $t = (q + 1/2)L$ we have:

$$\Psi_{p,j}(u) = U_{p,j} - U_{p,j-1} - \int_{y_{j-1}}^{y_j} G_p(U_3, U_4, y) dy = 0 \quad p = 3, 4 \quad (10)$$

There are various numerical schemes to evaluate the above integrals in (9) and (10), among them is the following scheme that involves the numerical derivatives of F and G [4] leading to:

$$\begin{aligned} \phi_{p,i}(u) &= U_{p,i} - U_{p,i-1} - \frac{h}{2} (F_{p,i} + F_{p,i-1}) \\ &+ \frac{h^2}{10} (F'_{p,i} - F'_{p,i-1}) - \frac{h^3}{120} (F''_{p,i} + F''_{p,i-1}) + O(h^7) = 0 \quad p = 1, 2 \end{aligned} \quad (11)$$

$$\begin{aligned} \Psi_{p,j}(u) &= U_{p,j} - U_{p,j-1} - \frac{k}{2} (G_{p,j} + G_{p,j-1}) \\ &+ \frac{k^2}{10} (G'_{p,j} - G'_{p,j-1}) - \frac{k^3}{120} (G''_{p,j} + G''_{p,j-1}) + O(k^7) = 0 \quad p = 3, 4 \end{aligned} \quad (12)$$

For simplicity the subscript p will be dropped from now on.

To determine the derivatives F' and F'' from F we use a cubic spline S on F to obtain F' , then we use another cubic spline \bar{S} on S' to evaluate F'' .

Similarly to determine the derivatives G' and G''

from G we use a cubic spline Z on G to obtain G', then we use another cubic spline \bar{Z} on Z' to evaluate G'.

3- CONSTRUCTION OF THE CUBIC SPLINES

Let S and Z denote cubic interpolating splines such that

$$S(x_i) = F_i \quad \text{for } i = 0, 1, 2, \dots, n$$

$$Z(y_j) = G_j \quad \text{for } j = 0, 1, 2, \dots, m$$

It is known that if

$$S'_0 = F'_0 \quad \text{and} \quad S'_n = F'_n$$

$$Z'_0 = G'_0 \quad \text{and} \quad Z'_m = G'_m$$

then S and Z are unique [5]

S' and Z' may be directly computed from F_i and G_j using the well known formula [5]

$$S'_{i+1} + 4S'_i + S'_{i-1} = \frac{3}{h} (F_{i+1} - F_{i-1}) \quad (13)$$

$$Z'_{j+1} + 4Z'_j + Z'_{j-1} = \frac{3}{k} (G_{j+1} - G_{j-1}) \quad (14)$$

At end points, approximations of first and second derivatives can be used in a manner similar to that implemented in [6], [7]

$$F'_0 = \frac{1}{12h} [-25F_0 + 48F_1 - 36F_2 + 16F_3 - 3F_4] + O(h^4)$$

$$F_0^2 = \frac{1}{h^2} [2F_0 - 5F_1 + 4F_2 - F_3] + O(h^2)$$

$$G'_0 = \frac{1}{12k} [-25G_0 + 48G_1 - 36G_2 + 16G_3 - 3G_4] + O(k^4)$$

$$G_0^2 = \frac{1}{k^2} [2G_0 - 5G_1 + 4G_2 - G_3] + O(k^2)$$

Corresponding formulae for F'_n and G'_m are skew symmetric to that of F'_0 and G'_0. Formulae for F_n^2 and G_m^2 are symmetric to that of F_0^2 and G_0^2. The

superscripts on S, Z, F and G above denote the order of their derivatives.

4- CONSTRUCTION OF CUBIC SPLINE ON SPLINE INTERPOLANTS

Let \bar{S} and \bar{Z} be cubic interpolating splines on the S'_i and Z'_j values computed in (13) and (14). The first derivatives of \bar{S} and \bar{Z} at x_i and y_j respectively are computed from a formula similar to that mentioned above hence

$$\bar{S}'_{i+1} + 4\bar{S}'_i + \bar{S}'_{i-1} = \frac{3}{h} (S'_{i+1} - S'_{i-1}) \quad (15)$$

with

$$\bar{S}'_0 = F_0^2 \quad \text{and} \quad \bar{S}'_n = F_n^2$$

$$\text{also } \bar{Z}'_{j+1} + 4\bar{Z}'_j + \bar{Z}'_{j-1} = \frac{3}{h} (Z'_{j+1} - Z'_{j-1}) \quad (16)$$

with

$$\bar{Z}'_0 = G_0^2 \quad \text{and} \quad \bar{Z}'_m = G_m^2$$

5- ESTIMATION OF ERROR BOUNDS

In this section error bounds for the function and its derivatives are estimated, that is estimates for

$$|F'_i - S'_i|, |F_i^2 - \bar{S}'_i|, |G'_j - Z'_j| \text{ and } |G_j^2 - \bar{Z}'_j|$$

are to be determined.

Let e_i denote the difference between F'_i and S'_i i.e. e_i = F'_i - S'_i, and d_j the difference between G'_j and Z'_j, d_j = G'_j - Z'_j.

Let us consider the maximum norm, defined by

$$\|F(x)\| = \max_x |F(x)|$$

$$\|e\| = \max_{0 \leq i \leq n} |e_i|$$

$$\|G(y)\| = \max_y |G(y)|$$

$$\|d\| = \max_{0 \leq j \leq m} |d_j|$$

In the following section we give some theoretical results related to these error bounds.

Theorem 1:

If S and Z are cubic interpolating splines on F and G such that

$$S'_{i+1} + 4 S'_i + S'_{i-1} = \frac{3}{h} (F_{i+1} - F_{i-1}) \quad (17)$$

with

$$S'_0 = F'_0, \quad S_0^2 = F_0^2$$

$$S'_n = F'_n, \quad S_n^2 = F_n^2$$

and

$$Z'_{j+1} + 4 Z'_j + Z'_{j-1} = \frac{3}{k} (G_{j+1} - G_{j-1}) \quad (18)$$

with

$$Z'_0 = G'_0, \quad Z_0^2 = G_0^2$$

$$Z'_m = G'_m, \quad Z_m^2 = G_m^2$$

then

$$\|e\| = O(h^4)$$

$$\|d\| = O(k^4)$$

Proof

By subtracting $F'_{i+1} + 4F'_i + F'_{i-1}$ from both sides of equation (17), we get

$$e_{i+1} + 4 e_i + e_{i-1} = F'_{i+1} + 4F'_i + F'_{i-1} - \frac{3}{h} (F_{i+1} - F_{i-1})$$

Using Taylor's expansion, this equation leads to;

$$e_{i+1} + 4 e_i + e_{i-1} = \frac{h^4}{4} \left[\frac{1}{3} F^5(\eta_i) - \frac{1}{5} F^5(\xi_i) \right]$$

where $x_{i-1} \leq \eta_i, \xi_i \leq x_{i+1}$

Furthermore, for any function W and V defined at the knots such that

$$W_{i+1} + 4 W_i + W_{i-1} = V_i,$$

by the maximum principle argument for difference equation it follows that

$$\|W\| < |W_0| + |W_n| + \frac{1}{2} \max_{0 < i < n} |V_i|.$$

Let $W = e$ and since by assumption $e_0 = e_n = 0$ therefore

$$\|e\| \leq \frac{1}{2} \max_{0 < i < n} \frac{h^4}{4} \left| \frac{1}{3} F^5(\eta_i) - \frac{1}{5} F^5(\xi_i) \right|,$$

$$\|e\| \leq \frac{1}{15} h^4 \|F^5\|. \quad (19)$$

Following a similar argument, it can be shown that

$$\|d\| \leq \frac{1}{15} k^4 \|G^5\|, \quad (20)$$

which completes the proof.

Furthermore, error bounds on the cubic splines on splines used to interpolate the derivatives of S and Z are derived in the following theorem.

Theorem 2:

Let \bar{S} and \bar{Z} denote cubic interpolating splines on S'_i and Z'_j computed in (17) and (18). If the first derivatives \bar{S}' and \bar{Z}' at x_i and y_j are computed from (15) and (16) then:

$$|F_i^2 - \bar{S}'_i| = O(h^3),$$

and $|G_j^2 - \bar{Z}'_j| = O(k^3).$

Proof

Subtracting $F_{i+1}^2 + 4F_i^2 + F_{i-1}^2$ from both sides of equation (15) and let

$$F_i^2 - \bar{S}'_i = E_i \text{ then;}$$

$$E_{i+1} + 4E_i + E_{i-1} = -\frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2.$$

The right-hand side of the above equation can be rewritten as:

$$\begin{aligned} & -\frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2 \\ &= -\frac{3}{h}[(S'_{i+1} - F'_{i+1}) - (S'_{i-1} - F'_{i-1})] \\ &+ [-\frac{3}{h}(F'_{i+1} - F'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2]. \end{aligned}$$

Expanding the terms in the 2nd bracket using Taylor series expansion about the point x_i up to order h^4 and using the result given by equation (19) in theorem 1 above, we arrive at:

$$\left| \frac{3}{h}(S'_{i+1} - S'_{i-1}) + F_{i+1}^2 + 4F_i^2 + F_{i-1}^2 \right| \leq \frac{1}{5}h^3 \|F^5\|.$$

Applying the maximum principle for difference equation, we get:

$$|F_i^2 - \bar{S}'_i| \leq \frac{1}{10}h^3 \|F^5\|.$$

Similarly

$$|G_j^2 - \bar{Z}'_j| \leq \frac{1}{10}k^3 \|G^5\|,$$

which completes the assertion of the given theorem.

6- COMPUTATIONAL PROCEDURE

Substituting F'_i, F_i^2, G'_j and G_j^2 in equations (11) and (12) by S'_i, \bar{S}'_i, Z'_j and \bar{Z}'_j respectively we obtain

$$\begin{aligned} \phi_i(u) &= u_i - u_{i-1} - \frac{h}{2}(F_i + F_{i-1}) + \frac{h^2}{10}(S'_i - S'_{i-1}) \\ &\quad - \frac{h^3}{120}(\bar{S}'_i + \bar{S}'_{i-1}) + O(h^6) \end{aligned} \quad (21)$$

$$\begin{aligned} \psi_j(u) &= u_j - u_{j-1} - \frac{k}{2}(G_j + G_{j-1}) + \frac{k^2}{10}(Z'_j - Z'_{j-1}) \\ &\quad - \frac{k^3}{120}(\bar{Z}'_j + \bar{Z}'_{j-1}) + O(k^6) \end{aligned} \quad (22)$$

In order to solve the system of equations (21), let

$$\phi_i(u) = V_i(u) + W_i(u), \quad (23)$$

where

$$V_i = u_i - u_{i-1} - \frac{h}{2}(F_i + F_{i-1}), \quad (24)$$

$$W_i = \frac{h^2}{10}[(S'_i - S'_{i-1}) - \frac{h}{12}(\bar{S}'_i + \bar{S}'_{i-1})]. \quad (25)$$

Using the modified Newton's non-linear iterative technique, we have;

$$u^{(k+1)} = u^{(k)} - J^{-1}(V) \phi(u^{(k)}) \quad k = 0, 1, 2, \dots (26)$$

where $J(V)$ is the Jacobian of the values of V given by equation (24).

In a similar way the system of equations (22) is solved. The convergence of the modified Newton technique is proved in [8]. It is evident that $J(V)$ has a sparse structure and has only few elements per row. Various sparse matrix techniques can be used for the solution of equation (26), for details of such techniques we refer to the work given in [9].

7- STABILITY ANALYSIS OF THE METHOD

Round-off errors cannot be avoided due to the use of a finite number of decimal places in all computations.

In order to study the stability of the numerical scheme the Von Neumann technique is applied. The round-off errors, that is the difference between the exact numerical solutions and the computed ones at each node are assumed that they can be expressed as a series consisting of the product of an exponential function in time multiplied by a harmonic one in space.

Due to the linearity of the problem dealt with a single term of the series can be considered.

Let us denote these errors for the function u_p , the cubic splines S'_p and \bar{S}'_p over the first half of the time step by E_{u_p} , E_{s_p} and $E_{s'_p}$ respectively ($p = 1,2$). Following the above argument we take the following;

$$E_{u_p} = a_p e^{i i \beta h} e^{i j \gamma k} e^{q \alpha L}$$

$$E_{s'_p} = b_p e^{i i \beta h} e^{i j \gamma k} e^{q \alpha L}$$

$$E_{s_p} = c_p e^{i i \beta h} e^{i j \gamma k} e^{q \alpha L} \quad p = 1,2$$

where $a_p, b_p, c_p, \alpha, \beta$ and γ are arbitrary constants and $\hat{i} = \sqrt{-1}$.

These expressions are known to satisfy similar equations as (13), (15) and (21) respectively.

Hence it follows that equations (13) and (15) lead to

$$b_1 (2 + \text{Cos } \beta h) = \frac{3}{h} a_2 \hat{i} \text{Sin } \beta h \quad (27)$$

$$b_2 (2 + \text{Cos } \beta h) e^{\alpha L/2} = \frac{6}{hL} a_1 \hat{i} \text{Sin } \beta h$$

$$[(e^{\alpha L/2} - 1) - \frac{L}{k^2} (\text{Cos } \gamma k - 1)], \quad (28)$$

$$c_1 (2 + \text{Cos } \beta h) = \frac{3}{h} b_1 \hat{i} \text{Sin } \beta h, \quad (29)$$

$$c_2 (2 + \text{Cos } \beta h) = \frac{3}{h} b_2 \hat{i} \text{Sin } \beta h, \quad (30)$$

From equation (21) we get

$$2 a_1 \hat{i} \text{Sin } \beta h - h a_2 (1 + \text{Cos } \beta h) + \hat{i} \frac{h^2}{5} b_1 \text{Sin } \beta h - \frac{h^3}{60} c_1 (1 + \text{Cos } \beta h) = 0, \quad (31)$$

$$2 a_2 \hat{i} \text{Sin } \beta h e^{\alpha L/2} - \frac{2h}{L} a_1 (1 + \text{Cos } \beta h) [(e^{\alpha L/2} - 1) - \frac{L}{k^2} (\text{Cos } \gamma k - 1)]$$

$$+ \hat{i} \frac{h^2}{5} b_2 \text{Sin } \beta h e^{\alpha L/2} - \frac{h^3}{60} e^{\alpha L/2} c_2 (1 + \text{Cos } \beta h) = 0. \quad (32)$$

The above system of equation (27-32) leads to:

$$e^{\alpha L/2} = \frac{[1 + s(\text{Cos } \gamma k - 1)](1 + \text{Cos } \beta h)(11 \text{Cos}^2 \beta h + 68 \text{Cos } \beta h + 101)^2}{(1 + \text{Cos } \beta h)(11 \text{Cos}^2 \beta h + 68 \text{Cos } \beta h + 101)^2 + 800r(1 - \text{Cos } \beta h)(2 + \text{Cos } \beta h)^4}$$

where $r = \frac{L}{h^2}$ and $s = \frac{L}{k^2}$.

Over the second half of the time step a similar system of equations is obtained leading to:

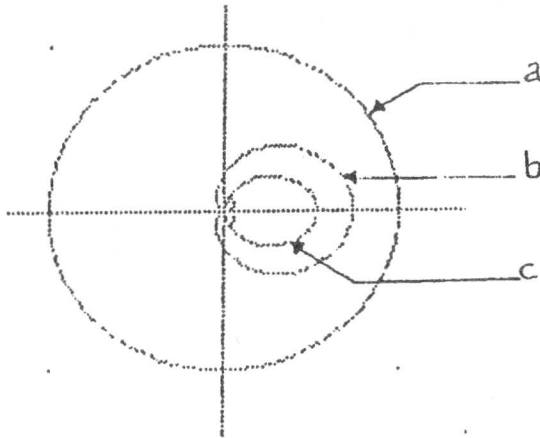
$$e^{\alpha L/2} = \frac{[1 + r(\text{Cos } \beta h - 1)](1 + \text{Cos } \gamma k)(11 \text{Cos}^2 \gamma k + 68 \text{Cos } \gamma k + 101)^2}{(1 + \text{Cos } \gamma k)(11 \text{Cos}^2 \gamma k + 68 \text{Cos } \gamma k + 101)^2 + 800s(1 - \text{Cos } \gamma k)(2 + \text{Cos } \gamma k)^4}$$

Hence, the amplification factor $e^{\alpha L}$ over a complete time step is;

$$e^{\alpha L} = \frac{[1 - s(1 - \text{Cos } \gamma k)]}{1 + \frac{800s(1 - \text{Cos } \gamma k)(2 + \text{Cos } \gamma k)^4}{(1 + \text{Cos } \gamma k)(11 \text{Cos}^2 \gamma k + 68 \text{Cos } \gamma k + 101)^2}} \cdot \frac{[1 - r(1 - \text{Cos } \beta h)]}{1 + \frac{800r(1 - \text{Cos } \beta h)(2 + \text{Cos } \beta h)^4}{(1 + \text{Cos } \beta h)(11 \text{Cos}^2 \beta h + 68 \text{Cos } \beta h + 101)^2}} \quad (33)$$

For stability, that is in order that these errors do not grow exponentially large with time, the following stability condition is imposed, namely $|e^{\alpha L}| \leq 1$.

Using a polar plot for the values of $|e^{\alpha L}|$ in equation (33) as βh varies from 0 to 2π , and for different values of r , s and γk ; it was found that all orbits lie within the unit circle which represents $|e^{\alpha L}| = 1$. Therefore the numerical scheme is unconditionally stable.



Polar plot of the amplification factor $|e^{\alpha L}|$

- (a) $|e^{\alpha L}| = 1$
- (b) with $r = s = 0.5$ and $\gamma k = \pi/4$
- (c) with $r = s = 1$ and $\gamma k = \pi/4$.

8- NUMERICAL RESULTS

In order to illustrate the above method a simple test example with known analytical solution is considered. Equation (1) is solved with the initial condition at $t = 0$

$$u(x, y, 0) = \sin \pi x \sin \pi y \quad \begin{matrix} 0 \leq x \leq 1, \\ 0 \leq y \leq 1, \end{matrix}$$

and the boundary conditions for $t > 0$

$$u(0, y, t) = u(1, y, t) = 0,$$

$$u(x, 0, t) = u(x, 1, t) = 0,$$

the spatial steps are chosen such that $h = k = 1/40$ and the time step $L = 10^{-3}$

The results are found to be in very good agreement with the analytical solution

$$u = e^{-2\pi^2 t} \sin \pi x \sin \pi y$$

The following table displays samples of these numerical results along with the values of the analytical solution.

x	y	t = 0.005		t = 0.01	
		u-Num	u-Anal	u-Num	u-Anal
0.25	0.25	0.4530211	0.4530092	0.4104563	0.4104345
0.5		0.6406679	0.6406516	0.5804715	0.5804420
0.75		0.4530203	0.4530093	0.4104549	0.4104346
0.25	0.5	0.6406680	0.6406516	0.5804719	0.5804420
0.5		0.9060411	0.9060180	0.8209105	0.8208687
0.75		0.6406678	0.6406518	0.5804715	0.5804421
0.25	0.75	0.4530204	0.4530093	0.4104551	0.4104346
0.5		0.6406678	0.6406518	0.5804713	0.5804421
0.75		0.4530208	0.4530095	0.4104559	0.4104348

9. CONCLUSION

A cubic spline on spline method is applied together with an alternating direction approach for the solution of a two dimensional diffusion equation. The stability analysis of the method shows that it is unconditionally stable, thus no restrictions in the choice of h and k (the space steps) and L (the time step) are necessary to ensure stability. Theoretical error estimates show that the method leads to approximations of at least a third order.

The numerical results for the example considered show that this method gives very good approximation for the solution of the diffusion equation.

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