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A GRADIENT-TYPE OPTIMIZATION TECHNIQUE FOR THE OPTIMAL CONTROL FOR SCHRODINGER EQUATIONS

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Abstract: *In this paper, we are considered with the optimal control of a schrodinger equation. Based on the formulation for the variation of the cost functional, a gradient-type optimization technique utilizing the finite difference method is then developed to solve the constrained optimization problem. Finally, a numerical example is given and the results show that the method of solution is robust.*

Keywords: *Optimal control, schrodinger equation, Existence and uniqueness theory, Gradient method.*

AMS subject classification: *49J20, 49M29, 49M30, 49K20*

1. Introduction

Optimal control of systems governed by partial differential equations is an application-driven are of mathematics involving the formulation and solution of minimization problems [1,3]. In this paper, we are considered with the optimal control of a schrodinger equation. Based on the formulation for the variation of the cost functional, a gradient-type optimization technique utilizing the finite difference method is then developed to solve the constrained optimization problem. Finally, a numerical example is given and the results show that the method of solution is robust.

2. Problem Formulation

We consider the functional on the form

$$(1)\quad J(u) = \alpha_0 \int_0^T |y(0,t) - f_0(t)|^2\, dt + \alpha_1 \int_0^T |y(l,t) - f_1(t)|^2\, dt$$

which is to minimized under the conditions

$$(2)\quad i\frac{\partial y}{\partial t} + B_0 \frac{\partial^2 y}{\partial x^2} - u\, y = f(x,t),\ (x,t) \in \Omega = (0,l) \times (0,T)$$

$$(3)\quad y(x,0) = 0,\ x \in (0,l)$$

$$(4)\quad \frac{\partial y(0,t)}{\partial x} = \frac{\partial y(l,t)}{\partial x} = 0,\ t \in (0,T)$$

over the class

$$U = \left\{ u : u(x,t) \in W_2^{0,1}(\Omega),\ \alpha_0 \le u(x,t) \le \alpha_1,\ |u_t| \le \alpha_2,\ \forall (x,t) \in \Omega \right\}$$

where $\alpha_k \ge 0,\ k = \overline{0,2},\ \alpha_1 + \alpha_2 \ne 0,\ l, T, B_0 > 0$ are given numbers and $f_0(t),\ f_1(t) \in W_2^1(0,T), \varphi(x) \in W_2^1\ (0,l)$, are given functions.

Definition 1.

The problem of finding the function $y(x,t) \in V_2^{0,1}(\Omega)$ from condition (2)-(4) at given $u \in U$ is called the reduced problem.

Definition 2.

A function $y(x,t) \in V_2^{0,1}(\Omega)$ is said to be a solution of the problem (2)-(4), if for all $\eta = \eta(x,t) \in W_2^{1,1}(\Omega)$ the equation

$$(5)\quad \int_\Omega \left[-iy\frac{\partial \eta}{\partial t} - B_0 \frac{\partial y}{\partial x}\frac{\partial \eta}{\partial x} - uy\bar{\eta}\right] dx\,dt = \int_\Omega f(x,t)\,\bar{\eta}\,dx\,dt + i\int_0^l \varphi\,\bar{\eta}(x,0)\,dx$$

is valid and $\eta(x,T) = 0$, but $\bar{\eta}$ is the adjoint of η .

Proposition 1

Let $f(x,t) \in W_2^{0,1}(\Omega)$ and $\varphi(x,t) \in W_2^1\ (0,l)$. Then the problem (2)-(4) has a unique solution and satisfies the following estimate

$$(6)\quad \|y\|^2_{V_2^{1,0}(\Omega)} \le C_1 \left[\|\varphi\|^2_{W_2^1(0,l)} + \|f\|^2_{W_2^{0,1}(0,l)}\right]$$ is valid and $C_1 > 0$ is dos not depend on φ and f .

Proposition 2

Let $\varphi(x,t) \in W_2^2\ (0,l)$. Then the solution of the reduced problem (2)-(4) $y(x,t) \in V_2^{0,1}(\Omega)$ belongs to the space $W_2^{2,1}(\Omega)$ and satisfies the following estimate

$$(7)\quad \|y\|^2_{W_2^2(\Omega)} + \|y_t\|^2_{L_2(0,l)} \le C_2\left[\|\varphi\|^2_{W_2^2(0,l)} + \|f\|^2_{W_2^{0,1}(\Omega)}\right]$$ is valid and $\forall t \in [0,T], C_2 > 0$ is dos not depend on φ and f .

Proposition 3

Let all the conditions Proposition 2 be valid. Then the optimal control problem (1)-(4) has at least one solution.

3. Variation of the Cost Functional

3.1 The Adjoint Problem

Results [4] imply that the function $\Phi = \Phi(x,t,u)$ is a solution in $L_2\ (\Omega)$ of the adjoint problem

$$(8)\qquad i\frac{\partial \Phi}{\partial t} + B_0\frac{\partial^2 \Phi}{\partial x^2} - u\Phi = 0,\ (x,t) \in \Omega = (0,l)\ x\ (0,T)$$

$$\Phi(x,T) = 0, \quad x \in (0,1)$$

$$(9) \quad \frac{\partial \Phi(0,t)}{\partial x} = -\frac{2\alpha_0}{B_0}[y(0,t) - f_0(t)], \quad t \in (0,T)$$

$$\frac{\partial \Phi(1,t)}{\partial x} = \frac{2\alpha_1}{B_0}[y(1,t) - f_1(t)], \quad t \in (0,T)$$

where $y(x,t)$ is the solution of (1)-(4) corresponding to $u \in U$.

Definition 3.

For each $u \in U$, a function $\Phi(x,t;u)$ is a solution of the adjoint problem (8)-(9) belonging to the control u iff

(I) $\Phi(x,t;u) \in L_2(\Omega)$,

(II) The integral identity

$$(10) \quad \int_\Omega \Phi \left[i \frac{\partial \overline{\eta_1}}{\partial t} + B_0 \frac{\partial^2 \overline{\eta_1}}{\partial x^2} - u\,\overline{\eta_1} \right] dx\, dt$$

$$= -2\alpha_1 \int_0^T [y(1,t) - f_1(t)]\, \overline{\eta_1}(1,t)\, dt$$

$$+ 2\alpha_0 \int_0^T [y(0,t) - f_0(t)]\, \overline{\eta_1}(0,t)\, dt$$

is valid $\forall\ \eta_1 \in W_2^{2,1}(\Omega)$, $\eta_1(x,0) = (\eta_1)_x|_{x=0} = (\eta_1)_x|_{x=1} = 0.$

On the basis of the above assumptions and the results [5], we have the following proposition:

Proposition 4.

The adjoint problem (8)-(9)has a unique solution from $L_2(\Omega)$ and he following estimate

$$(11) \quad \|\Phi\|^2_{L_2(\Omega)} \le C_3[\Gamma_1 + \Gamma_2], \qquad \text{where}$$

$$\Gamma_1 = \|y(0,t) - f_0(t)\|^2_{W_2^{\frac{1}{2}}(0,T)}, \quad \Gamma_1 = \|y(1,t) - f_1(t)\|^2_{W_2^{\frac{1}{2}}(0,T)}$$

is valid and c_3 is a certain constant.

3.2 The Gradient Formulae of Cost Functional

The sufficient differentiability conditions of the functional (5) and its gradient formulae will be given as follows:

Theorem 1.

Let the above assumptions be satisfied. Then $J(u)$ is Gato differentiable, and its gradient satisfies

$$(12) \quad \delta J(u) = -\int_\Omega \mathrm{Re}(y\,\Phi)\,\omega\, dx\, dt, \quad \forall\ \omega \in W_\infty^{0,1}(\Omega).$$

Proof :

Suppose that $u \in U$ and $\delta u \in W_\infty^{0,1}(\Omega)$ such that $u + \delta u \in U$ and denoting $\delta y(x,t) = y(x,t;u+\delta u) - y(x,t;u)$. Then $\delta y(x,t;\delta u)$ is the solution of the boundary value problem:

$$(13)\qquad i\frac{\partial \delta y}{\partial t}+B_0\frac{\partial^2 \delta y}{\partial x^2}-(u+\delta u)\,\delta y = y(x,t)\,\delta u,\ (x,t)\in\Omega,$$

$$(14)\quad \delta y(x,0)=0,\ \ x\in(0,l),\ \ \frac{\partial\,\delta y(0,t)}{\partial x}=\frac{\partial \delta y(l,t)}{\partial x}=0,\ \ t\in(0,T)$$

and the solution of the above boundary value problem satisfies the following estimation

$$(15)\quad \|\delta y\|^2_{W_2^{2,0}(\Omega)} \le C_4\,\|\delta u\ y\|^2_{W_2^{0,1}(\Omega)}$$

where C_4 is a constant and independent of δu.

From (15) and using the theorem of imbedding [6], we have

$$(16)\quad \|\delta y(0,t)\|_{L_2(0,T)}+\|\delta y(l,t)\|_{L_2(0,T)}\le C_5\,\|\delta u\ y(x,t)\|_{W_2^{0,1}(\Omega)}$$

where C_5 is a constant and independent of δu.

The increment of the functional $J(u)$ can be expressed as:

$$(17)\qquad \delta J = J(u+\theta u)-J(u)$$

$$=2\alpha_1\,\mathrm{Re}\int_0^T [\,y(l,t)-f_1(t)\,]\,\overline{\delta y}(l,t)\,dt$$

$$+2\alpha_0\,\mathrm{Re}\int_0^T [\,y(0,t)-f_0(t)\,]\,\overline{\delta y}(0,t)\,dt$$

$$+\alpha_1\,\|\delta y(l,t)\|^2_{L_2(0,T)}+2\,\alpha_0\,\|\delta y(0,t)\|^2_{L_2(0,T)}$$

If we take complex adjoint for (10),(13), we have

$$(18)\quad \int_\Omega \overline{\Phi}\,[\,i\frac{\partial \eta_1}{\partial t}+B_0\frac{\partial^2 \eta_1}{\partial x^2}-u\,\eta_1\,]\,dx\,dt$$

$$=-2\,\alpha_1\int_0^T [\,\overline{y}(l,t)-\overline{f}_1(t)\,]\,\eta_1(l,t)\,dt$$

$$+2\,\alpha_0\int_0^T [\,\overline{y}(0,t)-\overline{f_0}(t)\,]\,\eta_1(0,t)\,dt$$

$$(19)\quad \int_\Omega [\,i\frac{\partial\overline{\delta y}}{\partial t}+B_0\frac{\partial^2\overline{\delta y}}{\partial x^2}-(u+\delta u)\,\overline{\delta y}\,]\,\eta\,dx\,dt$$

$$=\int_\Omega \overline{y}(x,t)\,\delta u\,\eta\,dx\,dt,$$

Subtracting (13) from (19), (10) from (18) and in the obtained relation we put Φ, δy instead of η, η_1, then we have

$$(20)\quad 2\,\alpha_1\ \mathrm{Re}\int_0^T [\,y(1,t)-f_1(t)\,]\,\overline{\delta y}(1,t)\,dt$$

$$+\,2\,\alpha_0\ \mathrm{Re}\int_0^T [\,y(0,t)-f_0(t)\,]\,\overline{\delta y}(0,t)\,dt$$

$$=-\frac{1}{2}\int_\Omega [\,\delta u\,\Phi\,\overline{y}+\delta u\,y\,\overline{\Phi}\,]\,dx\,dt$$

$$-\frac{1}{2}\int_\Omega [\,\delta u\,\delta y\,\overline{\Phi}+\delta u\,\Phi\,\overline{\delta y}\,]\,dx\,dt$$

$$=-\mathrm{Re}\int_\Omega y\,\overline{\Phi}\,\delta u\,dx\,dt-\mathrm{Re}\int_\Omega \delta y\,\overline{\Phi}\,\delta u\,dx\,dt\,.$$

By substituting the last relation in (17), we have

$$(21)\quad \delta J=-\mathrm{Re}\int_\Omega y\,\overline{\Phi}\delta y\,\delta u\,dx\,dt\ -\mathrm{Re}\int_\Omega \delta y\,\overline{\Phi}\,\delta u\,dx\,dt.$$

$$+\ \alpha_0\,\|\delta y(0,t)\|^2_{L_2(0,T)}+\alpha_1\,\|\delta y(l,t)\|^2_{L_2(0,T)}$$

Suppose that

$$(22)\quad R_1=\alpha_0\,\|\delta y(0,t)\|^2_{L_2(0,T)}+\alpha_1\,\|\delta y(l,t)\|^2_{L_2(0,T)}$$

$$(23)\quad R_2=-\mathrm{Re}\int_\Omega \delta y\,\overline{\Phi}\,\delta u\,dx\,dt\,.$$

It is clear that,

$$(24)\quad |R_1|\le\alpha_0\,\|\delta y(0,t)\|^2_{L_2(0,T)}+\alpha_1\,\|\delta y(l,t)\|^2_{L_2(0,T)}.$$

From the formulae of R_2 ,it is estimated as

$$(25)\quad |R_2|\le C\,\|\delta y\,\delta u\|^2_{L_2(\Omega)}\ .$$

Then

$$(26)\quad |R_1|+|R_2|=o\,(\|\delta u\|_{W^{0,1}_\infty(\Omega)}).$$

By substituting (26) in (21), we obtain

$$(27)\quad J(u+\theta\,\delta u)-J(u)=-\int_\Omega \mathrm{Re}(y\overline{\Phi})\,(\theta\,\omega)\,dx\,dt+O\,(\theta).$$

Hence, in light of the variation functional, we have

$$(28)\quad \delta J(u,\omega)=\lim_{\theta\to 0}\frac{J(u+\theta\ u)-J(u)}{\theta}=-\int_\Omega \mathrm{Re}(y\overline{\Phi})\,\omega\,dx\,d$$

and this proves the differentiability of the functional and gradient formulae of the function $J(u)$. This completes the proof of the theorem.

Using Tikhinov method [7], we define the following functional

$$(29)\quad J_m(u)=J(u)+\alpha^m\int_0^l\int_0^T |u(x,t)-\omega(x,t)|^2\,dx\,dt\,.$$

and $\omega(x,t)\in L_2(\Omega)$.

4. Discrete Problem

We consider the set of node values $\{x_j, t_k\}$, $x_j = x_0 + Jh, j = \overline{0,M}$

$t_k = t_0 + k\tau, k = \overline{0,N}, M = \frac{l}{h}, N = \frac{T}{\tau}$ and the following notations [8]:

$$(30) \qquad (y_j^k)_{\bar{x}} = \frac{y_j^k - y_{j-1}^k}{h}, \quad (y_j^k)_x = \frac{y_{j+1}^k - y_j^k}{h},$$

$$(31) \qquad (y_j^k)_{\bar{t}} = \frac{y_j^k - y_j^{k-1}}{\tau}, \quad (y_j^k)_{\bar{x}x} = \frac{y_{j+1}^k - 2y_j^k + y_{j-1}^k}{h}$$

After applying the numerical integration formula [8],we have the discertisation of the optimal control problem (1)-(5) as follows: Let it is required to minimize the functional

$$(32) \qquad I_m([u]) = \tau \sum_{k=0}^{N} \{\alpha_0 [y_0^k - f_0^k]^2 - \alpha_1 [y_M^k - f_1^k]^2 \}$$

$$+\nu^m \tau \sum_{k=1}^{N} \{h \sum_{j=1}^{M-1} \left| u_0^k - \omega_0^k \right|^2 + \frac{1}{2} \left| u_M^k - \omega_M^k \right|^2 + \frac{1}{2} \left| u_j^k - \omega_j^k \right|^2 \}$$

on the control set

$$U_N^M = \left\{ \begin{array}{l} [u] : [u] = (u_j^k),\ \alpha_0 \le u_j^k \le \alpha_1,\ j = \overline{0,M},\ k = \overline{0,N}, \\ \left| (u_j^k)_t \right| \le \alpha_2,\ j = \overline{0,M},\ k = \overline{2,N} \end{array} \right\}$$

under the conditions

$$(33) \quad i(y_j^k)_{\bar{t}} + B_0 (y_j^k)_{\bar{x}x} - u_j^k y_j^k = f_j^k,\ j = \overline{1,M-1}, k = \overline{1,N}$$

$$(34) \qquad y_j^0 = 0, \quad j = \overline{0,M},$$

$$(35) \quad \frac{2B_0}{h} (y_0^k)_x = f_0^k - i[(u_0^k)_{\bar{t}} - u_0^k y_0^k], k = \overline{1,N}$$

$$(36) \quad -\frac{2B_0}{h} (y_M^k)_x = f_M^k - i[(u_M^k)_{\bar{t}} - u_M^k y_M^k], k = \overline{1,N}$$

Now, the discrete gradient formulae will be given as follows:

Theorem 2

The functional $J_m(u)$ is differentiable, and its gradient satisfies

$$(37) \quad (I_m^{/}([u]))_j^k = -\mathrm{Re}\,(y_j^k \Phi_j^k) + 2\alpha^m (u_j^k - \omega_j^k),$$

where $j = \overline{0,M-1}, k = \overline{1,N}$ and Φ_j^k is the solution of discrete adjoint problem:

$$(38) \quad i(\Phi_j^k)_{\bar{t}} + B_0 (\Phi_j^k)_{\bar{x}x} - u_j^k \Phi_j^k = 0, j = \overline{1,M-1}, k = \overline{1,N-1}$$

$$(39) \qquad \Phi_j^N = 0, \quad j = \overline{0,M},$$

$$(40) \quad (\Phi_j^k)_x + \frac{2\alpha_0}{B_0} [y_0^k - f_0^k] = \frac{h}{B_0} [u_0^k \Phi_0^k - i(\Phi_0^k)_t], k = \overline{1,N-1}$$

$$(41)\quad (\Phi_j^k)_{\bar{x}} + \frac{2\alpha_0}{B_0}[y_M^k - f_1^k] = \frac{h}{B_0}[u_M^k \Phi_M^k - i\,(\Phi_M^k)_t],\ k=\overline{1,N-1}$$

5. Solution of Control Problem

5.1 The Projection Gradient Method

Here we describe the projection gradient method [9] for the solution of the optimal control problem such as: construct a sequence $u_{n+1\,m}$ by setting

$$(42)\quad [u]_{n+1m} = P_{U_N^M}\left\{ [u]_{nm} - \nu_n \left(I_m^l([u]_{nm})\right)\right\}$$

where $P_{U_N^M}(u)$ is the project on the set U_N^M . In the first we define $(\bar{u}_j^k)_{nm}$ in the form

$$(43)\quad (u_j^k)_{n+1m} = \begin{cases} \Psi_1 & \alpha_0 \le \Psi_2 \le \alpha_1 \\ \alpha_0 & \Psi_2 < \alpha_0 \\ \alpha_1 & \Psi_2 > \alpha_1 \end{cases}$$

where

$$(44)\quad \Psi_2 = [u_j^k]_{nm} - \nu_n \left(I_m^l([u]_{nm})\right)_j^k$$

$$(45)\quad \Psi_1 = [u_j^k]_{nm} + \nu_n \left(I_m^l([u]_{nm})\right)_j^k$$

and $j=\overline{0,M}$, $k = \overline{1,N}$, $n=0,1,\ldots$, $m = 0,1,\ldots$

Using the above sequence we construct the project in the form

$$(46)\quad (u_j^1)_{n+1m} = (\bar{u}_j^1)_{n+1m}$$

$$(47)\quad (u_j^k)_{n+1m} = \begin{cases} \Theta_0 & \Theta_1 \le \Psi_2 \le \Theta_2 \\ \Theta_1 & (u_j^k)_{nm} < \Theta_1 \\ \Theta_2 & (u_j^k)_{nm} > \Theta_2 \end{cases}$$

where

$$\Theta_0 = (\bar{u}_j^k)_{n+1m} + \nu_n \left(I_m^l([u]_{nm})\right)_j^k$$

$$\Theta_1 = -\tau\,\alpha_2 + (\bar{u}_j^{k-1})_{n+1m}\ ,\quad \Theta_2 = \tau\,\alpha_2 + (\bar{u}_j^{k-1})_{n+1m}$$

$j=\overline{0,M}$, $k = \overline{2,N}$, $n=0,1,\ldots$, $m = 0,1,\ldots$

5.2 Numerical Algorithm

With the gradient obtained, the following gradient type algorithm can then be developed for the optimal value of u^* based on the projection gradient method (PGM)which described in the above section.

The outlined of the algorithm for solving control problem are as follows:

Step 1: Choose an initial control $u^{(n)} \in U,\ n=0$.

If $I'(u^{(n)})=0$, $u^{(n)}$ is the solution of the problem.

Step 2 : At each iteration n do

Solve the state problem, then find $y(.,u^{(n)})$.

Solve the adjoint problem for (1)-(3), then find

$\Phi(.,u^{(n)})$. Find optimal control $u_*^{(n+1)}$ using PGM.

End do.

Step 3: Test the optimality of $u^{(n+1)}$.

If $u^{(n+1)}$ is optimum, stop the process.

Otherwise, go to Step 4.

Step 4 Set $u^{(n+1)} = u^{(n)}$, $n = n+1$ and go to Step 2.

6. Numerical Results

Designed algorithm is implemented as a FORTRAN routine [10]. Numerical experiment is carried out to check its performance. The initial data of the problem (1)-(5) are taken as follows:

$$\alpha_0 = \alpha_1 = \alpha_2 = l = T = 1,\ \varepsilon = 0.5E-03$$

$$f_0 = it,\ f_1 = i(1+t),\ \varphi(x) = i\,x,\ u^{(0)} = 1.0$$

$$\omega(x,t) = 1 + \frac{x+t}{2},\ f(x,t) = -1 - i\,(x+t)(x^2+t+1)$$

The number of division of the intervals was taken as $N = M = 20$. The computed control values of $u_j^{13},\ j=\overline{0,N}$ the values of relative error are shown in Tables 1 ,2 and the 3D plots of the optimal control and initial values are presented in Figures 1,2 . The optimal value of the cost functional is $J_* = \inf_{u\in U} J(u) = J(u_*) = 0.48526\,E-03$.

The computed control values of $u_j^{13},\ j=\overline{0,N}$			
0.15592E+01	0.15950E+01	0.16301E+01	0.16641E+01
0.17221E+01	0.17464E+01	0.17714E+01	0.18021E+01
0.18332E+01	0.18602E+01	0.19112E+01	0.19830E+01
0.20679E+01	0.21474E+01	0.22155E+01	0.22837E+01
0.23625E+01	0.24368E+01	0.24078E+01	0.24324E+01
0.24718E+01			

The values of relative error of $u_j^{13},\ j=\overline{0,N}$			
0.025528	0.004683	0.012478	0.02563
0.050038	0.030459	0.048194	0.046236
0.041988	0.032024	0.033075	0.042328
0.055069	0.061758	0.060028	0.056052
0.054668	0.049211	0.000924	0.028029
0.049297			

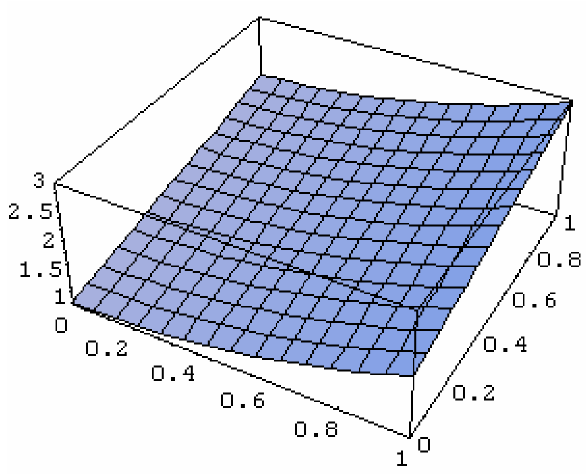

Fig. 1. Optimal control $u_*(x,t)$

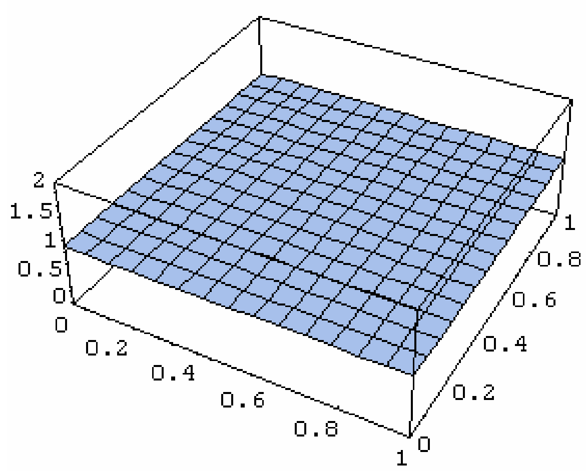

Fig. 2. Initial control $u_0(x,t)$

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