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FINITE DIFFERENCE METHOD FOR AN OPTIMAL CONTROL PROBLEM OF QUANTUM PROCESSES

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0. INTRODUCTION

In recent years there has been growing interest in general problems of control of objects governed by equations of quantum mechanics, electrodynamics and quantum fields. See [1] and [2 — 6] for an up-to-date survey and an extensive bibliography. A typical class of these problems is encountered in nuclear energetics, automatics and computer engineering techniques. Unfortunately, theoretical researches have been extensively developped, only few results have been published on approximate methods for these problems [7].

The aim of the present paper is to suggest a scheme based on the finite difference method for approximating a nonlinear optimal control problem of quantum processes governed by nonstationary Schrödinger equations.

In Section 1 we describe the optimal control problem to be studied. Then in Section 2 we develop the finite difference scheme for this prblem. The main results are formulated in Section 3 and established in Section 4.

Throughout the paper we shall use the notations of [8].

1. OPTIMAL CONTROL PROBLEM OF QUANTUM PROCESSES

Let Ω be a bounded domain of R^n, T be a given finite, positive number. Let $Q = \Omega \times [0, T]$, $S = \Gamma \times [0, T]$, where Γ is the boundary of Ω. Consider the following system

$$\frac{\partial \Psi}{\partial t} - i \sum_{k, j=1}^{n} \frac{\partial}{\partial x_k}\left(a_{kj}(x) \frac{\partial \Psi}{\partial x_j}\right) + ia(x)\Psi + iu(x)\Psi = 0 \qquad (1.1)$$

$$(x, t) \in Q$$

$$\Psi|_s = 0, \qquad (1.2)$$

$$\Psi|_{t=0} = \varphi(x),\ x \in \Omega, \tag{1.3}$$

$$\|\varphi\| = 1,\ \|\cdot\| = \|\cdot\|_{L_2}(\Omega), \tag{1.4}$$

where

(i) a_{kj}, $a(x)$ belong to the real functional space $L_\infty(\Omega)$,

(ii) $u(x) \in L_q(\Omega)$, $q = \begin{cases} \alpha > 1 & n = 1 \\ n + \varepsilon & \forall\ \varepsilon > 0,\ n = 2 \\ n & n > 2 \end{cases}$

(iii) $a(x)$, $u(x) > 0$ almost everywhere in Ω;

(iv) $a_{kj}(x) = a_{jk}(x) \quad k,j \in [1,2,\dots, n]$,

(v) $\mu_1|\xi|^2 \leqslant \sum_{k,j=1}^{n} a_{kj}(x)\,\xi_k\,\xi_j \leqslant \mu_2|\xi|^2$,

(vi) $|\partial a_{kj} / \partial x_l| \leqslant \mu_3$,

(vii) Ω is a ball, or a ball layer, or a parallelepiped or Ω can be transformed into one of these domains with the aid of a regular transformation $y = y(x) \in C^2(\overline{\Omega})$. μ_1, μ_2, μ_3 are fixed and positive constants, $\xi = (\xi_1, \dots, \xi_n)$ is an arbitrary vector of R^n, $|\xi|^2 = \xi_1^2 + \dots + \xi_n^2$.

DEFINITION. A function ψ is said to be a generalized solution in $W_2^{1,1}(Q)$ of the problem (1.1) — (1.3), if ψ belongs to $W_2^{1,1}(Q)$ and satisfies

$$\int_Q \Big(-\psi\overline{\eta}_t + i\sum_{k,j=1}^{n} a_{kj}\psi_{x_k}\overline{\eta}_{x_j} + ia\,\psi\,\overline{\eta}\Big)\,dx\,dt + i\int_Q u\,\psi\,\overline{\eta}\,dx\,dt = \int_\Omega \varphi\,\overline{\eta(x,0)}\,dx \tag{1.5}$$

for all η from $\widehat{W}^1_{2,0}(Q)$.

Further, let

$$\varphi \in W^2_{2,0}(\Omega). \tag{1.6}$$

Then the problem (1.1) — (1.3) has a unique generalized solution in $W_2^{1,1}(Q)$ ([2]). Furthermore, this solution be longs to $W_2^{2,1}(Q)$. Consequently, $\psi(x, T; u)$ makes sense and $\psi(x, T; u) \in W_2^2(Q)$. From [2] we also have

$$\|\psi(x, t; u)\| = \|\varphi\| = 1, \quad \forall\, t \in [0,T] \tag{1.7}$$

Let $z(x)$ be a given function from $W^2_{2,0}(\Omega)$. Suppose that the control $u(x)$ belongs to a bounded closed and convex subset $\mathcal{U}$ of $L_q^+(\Omega)$ ($L_q^+(\Omega) = \{u(x) \mid u(x) \in L_q(\Omega),\ u(x) \geqslant 0$ almost everywhere in $\Omega\}$). The control problem we are concerned with is to minimize the functional

$$\mathcal{J}(u)=\int_{\Omega} | \psi(x, T; u)-z(x) |^{2} dx=\| \psi(x, T; u)-z(x) \|^{2} \quad (18)$$

subject to the above constraints.

This problem arises from the control of quantum processes ([1], [6]). It is known [6] that under the above mentioned conditions it always has a solution.

2. FINITE DIFFERENCE SCHEME FOR THE PROBLEM

Let the upper-half space $E_n \times [0, \infty)$ of variables (x, t) be covered by a grid $x_i = k_i h_i$, $h_i > 0$, $k_i \in \{0, \pm 1, \pm 2, \ldots\}$, $i \in \{1, 2, \ldots, n\}$ and $t = k_o \tau$, > 0, $k_o \in \{0, 1, 2, \ldots\}$. Let $Q_{(k, k_0)} = \omega_{(kh)} \times (k_0 \tau, (k_0+1)\tau) = \{(x, t): k_i h_i < x_i < (k_i+1) h_i,\ k_0 \tau < t < (k_0+1)\tau\}$. By $\overline{\Omega}_h$ we denote the closed domain consisting of these cells $\overline{\omega}_{(kh)}$ which are contained in $\overline{\Omega}$. Let S_h be the boundary of $\overline{\Omega}_h$ and $\Omega_h = \overline{\Omega}_h - S_h$. For functions ψ defined on our grid we use the notation ψ_h, but occasionally for the sake of simplicity we write ψ instead of ψ_h if no confusion is possible. Further, $\psi_h(k)$ denotes the restriction of the grid function ψ_h to the layer $t = t_k = k\tau$.

Let

$$\sigma \psi_h(k) = \frac{1}{2} [\psi_h(k) + \psi_h(k+1)],$$

$$u_h \Big|_{(kh)} = (\Delta h)^{-1} \int_{\omega_{(kh)}} u(x) dx, \quad \Delta h = h_1 h_2 \ldots h_n,$$

$$\xi_h \Big|_{x=(kh),\ t=k_0\tau} = (\Delta h)^{-1} \tau^{-1} \int_{(k_0-1)\tau}^{k_0 \tau} \int_{\omega(kh)} \zeta(x,t)\, dx dt,$$

where $\zeta(x, t)$ is any function from $L_2(Q_T)$.

For any grid Ω_h consider the following problem

$$I_{h,\tau}([u]_h) = (\Delta h)^2 \sum_{\Omega_h} | \psi_h(N) - z_h |^2 \to \inf, \quad (2.1)$$

$$\frac{\psi_h(k+1) - \psi_h(k)}{\tau} - i \sum_{l,j=1}^{n} (a_{ljh}\, \sigma \psi_{x_j}(k))_{\overline{x}_l} + i\, a_h\, \sigma \psi_h(k) + i u_h\, \sigma \psi_h(k) = 0, \quad (2.2)$$

in Ω_h, $k \in \{0, 1, 2, \ldots, N = \left[\frac{T}{\tau}\right]\}$,

$$\psi_h(k) | S_h = 0, \quad (2.3)$$

$$\psi_h(0) = \varphi_h \text{ in } \Omega_h, \tag{2.4}$$

$$[u]_h \in U_h = \{ [u]_h = \{u_h\},\ u_h \in \mathcal{U} \}, \tag{2.5}$$

where $\psi_h(k, [u]_h)$ is a solution of the problem (2.2)—(2.4) corresponding to control $[u]_h$.

We shall assume that for every grid $\Omega_h \times \omega_\tau$ by any available minimization method one can compute the approximate value $I^*_{h,\tau} + \varepsilon_{h,\tau}$ of the infimum $I^*_{h,\tau}$ of the function $I_{h,\tau}$ in U_h subject to conditions (2.2) — (2.5) and approximate control $[u]_{h,\varepsilon} = \{u_h\}$, $u_h \in \mathcal{U}$ such that

$$I^*_{h,\tau} \leqslant I_{h,\tau}([u]_{h,\varepsilon}) \leqslant I^*_{h,\tau} + \varepsilon_{h,\tau}, \tag{2.6}$$

where $\varepsilon_{h,\tau}$ converges to zero as $h_1, h, \ldots, h_n$ and τ tend simultaneously to zero.

3. FORMULATION OF THE MAIN RESULTS

For every functoin $\psi_{h,\tau}(k)$ defined on a grid $\Omega_h \times \omega_\tau$ we put

$$\tilde{\psi}_{h,\tau}(x,t) = \begin{cases} \psi_h(\tau)_{h=kh},\ \tau = k_0\tau', & (x,t) \in \omega_{(kh)} \times \omega_\tau \\ 0, & (x,t) \overline{\in} \omega_{(kh)} \times \omega_\tau. \end{cases}$$

THEOREM 1. The finite difference scheme (2.2) – (2.4) has a unique grip solution $\Psi_{h,\tau}$ and its interpolation $\psi_{h,\tau}(x,t)$ strongly converges in $\overset{\circ}{W}{}^{1,1}_2(Q)$ to the generalized solution in $\overset{\circ}{W}{}^{1,1}_2(Q)$ of the problem (1.1) — (1.3) ψ (x,t) as $h_1, h_2, \ldots, h_n$ and τ tend simultaneously to zero. Furthermore

$$\| \tilde{\psi}_{h,\tau} \| = \| \tilde{\varphi}_h \| \tag{2.7}$$

and

$$\| \psi(x,t) \big|_{t=t_k} - \tilde{\Psi}_{h,\tau}(x,t) \big|_{t=t_k} \|^2 \leqslant c\,(\tau + (\Delta h)^2), \tag{2.8}$$

where the constant c does not depend on τ and h, but depends only on the domain Ω and the coefficients of equation (1.1).

THEOREM 2. *Let u^* be a solution of the problem (1.8). Then*

$$\lim_{\substack{h_1, h_2, \ldots, h_n \to 0 \\ \tau \to 0}} I^*_{h,\tau} = J^* = \inf_{u \in \mathcal{U}} J(u),$$

$$-c_1(\omega_{u^*}(h) + \sqrt{\tau + (\Delta h)^2}) \leqslant I^*_{h,\tau} - J^* \leqslant c_2 \sqrt{\tau + (\Delta h)^2}, \tag{2.9}$$

where $\omega_u(h)$ *is the module of continuity of* $u(x)$ *in* $L_q(\Omega)$. *If the sequence* $\{[u]_{h,\varepsilon}\}$ *is determined from (2.6), then*

$$0 \leqslant J([u]_{h,\varepsilon}) - J^* \leqslant c_3\,(\omega_u(h) + \sqrt{\tau + \Delta h)^2}) + \varepsilon_{h,\tau} \tag{2.10}$$

4. PROOFS OF THE CONVERGENCE THEOREMS

Proof of Theorem 1. From (2.2) we have

$$\psi_h(k+1) - i\frac{\tau}{2}\sum_{l,j=1}^{n}(a_{ljh}6\psi_{xj}(k+1))_{\bar{x}_l} + i\frac{\tau}{2}(a_h + u_h)\Psi_h(k+1) =$$

$$= \Psi_h(k) + i\frac{\tau}{2}\sum_{l\,j=l}^{n}(a_{ljh}6\Psi_{xj}(k))_{\bar{x}_l} - i\frac{\tau}{2}a_h + u_h)\Psi_h(k) \tag{4.1}$$

in Ω_h, $k \in [0,1,\ldots, N-1]$.

Let $\psi(k) = \{\psi_h(k)\}$, let H_h be the linear space of all vector-functions defined in Ω_h. From (4.1), (2.3), (2.4) we have

$$(E - i\frac{\tau}{2}L_h)\Psi(k+1) = (E + i\frac{\tau}{2}L_h)\Psi(k), \tag{4.2}$$

where E is the identity operator in H_h, L_h is the operator defined by the system (4.1) and the condition (2.3).

Operator L_h acts in the finite dimensional space H_h so it is bounded. Further, conditions (1.7), (1.8) and (2.3) mean that L_h is symmetric (or self-adjoint) and negative defined. Therefore, the spectrum of the operator A is real. Consequently, the operator $E - i\frac{\tau}{2}L_h$ has an inverse bounded operator.

Now, by the above and (4.2) we obtain

$$\Psi(k+1) = \left(E - i\frac{\tau}{2}L_h\right)^{-1}\left(E + i\frac{\tau}{2}L_h\right)\Psi(k).$$

Operator $K = \left(E - i\frac{\tau}{2}L_h\right)^{-1}\left(E + i\frac{\tau}{2}L_h\right)$ is the Kelleg transform of the self-adjoint operator L_h, so it is isometric ([10], point 121). Therefore

$$\|\Psi(k+1)\|^2_{H_h} = (\Delta h)^2\sum_{\Omega_h}|\psi_h(k+1)|^2$$

$$= (\Delta h)^2\sum_{\Omega_h}|\psi_h(k)|^2 = \|\psi(k)\|^2_{H_h},$$

i.e. $\|\widetilde{\psi}_h(k+1)\|^2 = \|\widetilde{\psi}_h(k)\|^2$. From this equality, it is easy to see that

$$\|\widetilde{\psi}_h(k)\|^2 = \|\widetilde{\varphi}_h\|^2, \ \forall k \in [1, 2, \ldots, N].$$

The proof of the convergence of the finite difference scheme (2.2) — (2.4) is similar to the one in [8] and [9], and therefore will be omitted. Now, we study the accuracy of this scheme.

Let

$$y_h(k) = \frac{1}{\Delta_h} \int_{\omega_{(kh)}} \psi(x, k\tau)\, dx,$$

$$z_h(k) = \psi_h(k) - y_h(k).$$

We have

$$\left(E - i\frac{\tau}{2}L_h\right) z(k+1) - \left(E + i\frac{\tau}{2}L_h\right) z(k)$$

$$= -\left(E - i\frac{\tau}{2}L_h\right) y(k+1) + \left(E + i\frac{\tau}{2}L_h\right) y(k).$$

Hence,

$$z(k+1) = Kz(k) - y(k) + Ky(z)$$

and

$$\|\widetilde{z}(k+1)\|^2 \leqslant \|\widetilde{z}(k)\|^2 + \|\widetilde{y}(k+1) - y(k)\|^2 + \|\widetilde{(E-K)}\, y(k)\|^2.$$

On the other hand

$$\|\widetilde{y}(k+1) - \widetilde{y}(k)\|^2 \leqslant \|\psi(x, (k+1)\tau) - \psi(x, k\tau)\|^2$$

$$= \tau^2 \left\|\frac{\partial \Psi(x, \theta)}{\partial t}\right\|^2 \leqslant c\tau^2, \ k\tau \leqslant \theta \leqslant (k+1)\tau.$$

From conditions (i)—(vii) it is easy to see that $\|E - K\| \leqslant c\tau$.

Hence,

$$\left\|\left(E - i\frac{\tau}{2}L_h\right)^{-1} L_h\right\|^2 \leqslant c.$$

(Throughout the sequel c, c_1, c_2,... denote a generic positive constant independent of h and τ).

Finally, we have

$$\|\widetilde{z}(k+1)\|^2 \leqslant \|\widetilde{z}(k)\|^2 + c\tau^2 \leqslant \ldots \leqslant \|z(0)\|^2 + kc\tau^2 \leqslant c\tau.$$

Consequently,

$$\|\widetilde{\Psi}_h(k+1) - \Psi(x, (k+1)\tau)\|^2 \leqslant \|\widetilde{\Psi}_h(k+1) - \widetilde{y}_h(k+1)\|^2$$

$$+ \|\widetilde{y}_h(k+1) - \Psi(x, (k+1)\tau\|^2 \leqslant c\tau + \|\widetilde{y}_h(k+1) - \Psi(x, (k+1)\tau)\|^2$$

$$\leqslant c\tau + \sum_{\Omega_h} \left\|\frac{1}{\Delta h}\int_{\omega_{(kh)}} \Psi(x, (k+1)\tau)\, dx - \Psi(x, (k+1)\tau)\right\|^2_{\omega_{(kh)}}$$

$$= c\tau + \sum_{\Omega_h} \| \int_{\omega_{(kh)}} (\Psi(x,(k+1)\tau) - \Psi(\xi,(k+1)\tau))\, d\xi \|^2_{\omega_{(kh)}}$$

$$= c\tau + \sum_{\Omega_h} \int_{\omega_{(kh)}} \left| \frac{1}{\Delta h} \int_{\omega_{(kh)}} \Psi(x, k+1)\tau) - \Psi(\xi, (k+1)\tau))\, d\xi \right|^2 dx$$

$$= c\tau + \sum_{\Omega_h} \int_{\omega_{(kh)}} \left| \frac{1}{\Delta h} \int_{\omega_{(kh)}} d\xi \int \frac{\partial \psi}{\partial \eta} d\eta \right|^2 dx$$

$$\leqslant c\tau + \sum_{\Omega_h} \int_{\omega_{(kh)}} \left| \frac{1}{\Delta h} \int_{\omega_{(kh)}} d\xi \int_{\omega_{(kh)}} \left| \frac{\partial \Psi}{\partial \eta} \right| d\eta \right|^2 dx$$

$$= c\tau + \sum_{\Omega_h} \Delta h \left(\int_{\omega_{(kh)}} \left| \frac{\partial \psi}{\partial \eta} \right| d\eta \right)^2$$

$$\leqslant c\tau + \sum_{\Omega_h} (\Delta h)^2 \int_{\omega_{(kh)}} \left| \frac{\partial \psi}{\partial \eta} \right|^2 d\eta$$

$$\leqslant c\tau + (\Delta h)^2 \left\| \frac{\partial \Psi}{\partial \eta} \right\|^2 \leqslant c(\tau + (\Delta h)^2).$$

Thus,

$$\|\widetilde{\Psi}_h(k+1) - \Psi(x, (k+1)\tau)\|^2 \leqslant c(\tau + (\Delta h)^2).$$

Theorem 1 is proved.

Proof of Theorem 2. We shall need some lemmas.

LEMMA 1. (F.P. Vasiliev ([11], p. 299)). Let U be a convex, closed set of $L_q(\Omega)$, $u(x)$ an element of U. Then

$$u_h = \frac{1}{\Delta h} \int_{\omega_{(kh)}} u(x)\, dx \in U. \tag{4.3}$$

LEMMA 2. Let all the conditions of Theorem 1 hold. Then for every $u \in U$ we have

$$|J(u) - I_{h,\tau}([u]_h)| \leqslant c\sqrt[4]{\tau + (\Delta h)^2}. \tag{4.4}$$

Proof. From Lemma 4.1 [8] (p. 301) we have

$$\|\widetilde{z}(x) - z(x)\| \to 0 \text{ as } h \to 0.$$

Further, since $z(x) \in W^2_{2,0}(\Omega)$ it follows that

$$\|\widetilde{z}(x) - z(x)\|^2 \leqslant c(\Delta h)^2 \left\| \frac{\partial z}{\partial x} \right\|^2. \tag{4.5}$$

On the other hand

$$I_{h,\tau}([u]_h) = (\Delta h)^2 \sum_{\Omega_h} \left| \Psi_{h,\tau}(N,[u]_h) - z_h \right|^2$$

$$= \|\widetilde{\Psi}_{h,\tau}(x, T; u) - \widetilde{z}(x)\|^2.$$

ence

$$\left|J(u) - I_{h,\tau}([u]_h)\right| = \Big| \| \Psi(x,T;\, u) - z(x) \|^2 - \| \tilde{\Psi}_{h,\tau}(x,T;\, u) - \tilde{z}(x) \|^2 \Big|$$

$$\leqslant (\| \Psi(x,T;\ u) \| + \| \tilde{\Psi}_{h,\tau}(x,T;\ u \| + \| z(x) \| + \| \tilde{z}(x) \|)\times$$

$$(\| \tilde{\Psi}(x,T;\ u) - \tilde{\Psi}_{h,\tau}(x,T;\, u) \| + \| z(x) - \tilde{z}(x) \|).$$

From (1.7), (4.5) and (2.8) we get

$$\left| J(u) - I_{h,\tau}([u]_h) \right| \leqslant c\sqrt{\tau + (\Delta h)^2}.$$

LEMMA 3. *Let all the conditions of Theorem 1 hold and* [u] *be any control rom U. Then*

$$\left| J(\widetilde{[u]}_h) - I_{h,\tau}([u]_h) \right| \leqslant c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}), \tag{4.6}$$

where $\omega_u(h)$ *is the module of continuity of* $u(x)$ *in* $L_q(\Omega)$.

Proof. Using the inequality for the coefficients of the equation (1.1) ([2] and 6], p. 18) we can write

$$\left| J(\widetilde{[u]}_h) - I_{h,\tau}([u]_h) \right| \leqslant c(\| \Psi(x,T;\, \widetilde{[u]}_h)$$

$$- \tilde{\Psi}_{h,\tau}(x,T;\, [u]_h) \| + \| z(x) - \tilde{z}(x) \|)$$

$$\leqslant c(\| \Psi(x,T;\ \widetilde{[u]}_h) - \Psi(x,T;\, u) \| + \| \Psi(x,T;\, u) -$$

$$- \tilde{\Psi}_{h,\tau}(x,T;\, [u]_h) \| + \| z(x) - \tilde{z}(x) \|)$$

$$\leqslant c(\| \widetilde{[u]}_h - u \|_q + \sqrt{\tau + (\Delta h)^2} + \Delta h)$$

$$\leqslant c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}),$$

Let us now prove Theorem 2. As seen above, the set of all optimal controls of the problem (1.8) U_* is non empty. Let us pick $u^* \in U_*$. According to Lemna 1 $[u^*]_h \in U$. Consequently, it follows from Lemma 2 that

$$I^*_{h,\tau} \leqslant I_{h,\tau}([u^*]_h \leqslant J(u^*) + c\sqrt{\tau + (\Delta h)^2}$$
$$= J^* + c\sqrt{\tau + (\Delta h)^2}. \tag{4.7}$$

Further, the function $I_{h,\tau}([u]_h)$ attains its infimum on the compact set U_h, i.e. $I^*_{h,\tau} > -\infty$, $U^*_h \neq \varnothing$, Since U is convex we have $\widetilde{[u]}^*_h \in U$. Now, from Lemma 3 we get

$$J^* \leqslant J(\widetilde{[u]}^*_h < I_{h,\tau}([u]^*_h) + c(\omega u^*(h) +$$
$$+ \sqrt{\tau + (\Delta h)^2}) = I^*_{h,\tau} + c(\omega_{u^*}(h) + \sqrt{\tau + (\Delta h)^2}). \tag{4.8}$$

Hence,

$$-c(\omega_{u^*}(h)+\sqrt{\tau+(\Delta h)^2}) \leqslant I^*_{h,\tau} - J^* \leqslant c\sqrt{\tau+(\Delta h)^2}.$$

Since $\omega_u(h) \to 0$ as $h \to 0$ ([12]), §3), we get

$$\lim_{(h,\tau)\to 0} I^*_{h,\tau} = J^*.$$

Consider a sequence $\{[u]_{h,\varepsilon}\}$ determined by (2. 6). Clearly, $[\widetilde{u}]_{h,\varepsilon} \in U$ and

$$0 \leqslant J([\widetilde{u}]_{h,\varepsilon}) - J^* = [J([\widetilde{u}]_{h,\varepsilon}) - I_{h,\tau}([u]_{h,\varepsilon})]$$
$$+ [I_{h,\tau}([u]_{h,\tau}) - \overset{*}{I}_{h,\tau}] + [\overset{*}{I}_{h,\tau} - J^*].$$

From (2. 6), (4. 4), (4, 6) we then oblain

$$J[(u]_{h,\varepsilon}) - J^* \leqslant c(\omega_u(h) + \sqrt{\tau+(\Delta h)^2}) + \varepsilon_{h,\tau}.$$

This means that the sequence $\{[u]_{h,\varepsilon}\}$ is a minimizing sequence for the problem (1. 8).

The proof of Theorem 2 is complete.

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