Finite Element Design Sensitivity Analysis for Nonlinear Potential Problems

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Abstract

Design sensitivity analysis is performed for the finite element system arising from the discretization of nonlinear potential problems using isoparametric Lagrangian elements. The calculated sensitivity formulae are given in a simple matrix form. Applications to design of electromagnets and airfoils are given.

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1 Introduction

Shape optimization problems are optimal control problems where the control is some geometrical parameter[4,5,7]. Traditionally optimal shape design is associated with structural optimization. However, any shape optimization problem which is governed by an elliptic partial differential equation can be solved numerically using the same techniques. In this work we consider the case where the state problem is approximated by the finite element method. Although the continuous setting of the problem may be a distributed control problem, the numerical optimization problem always has a finite number of parameters.

By design sensitivity analysis we mean computing derivatives of the finite element solution with respect to nodal coordinates of the finite element mesh. Although the geometric sensitivity analysis is one of the most crucial steps in numerical shape optimization, it is still considered extremely elaborate and difficult even for linear problems. This is probably due to the bad form in which most of the sensitivity formulae are presented. In these formulae there are usually too much explicit dependence on certain application or element type. This implies nonstructured programs which are difficult to debug and maintain.

In what follows, we develop the geometric sensitivity analysis in matrix form for a class of nonlinear potential equations. We assume that the continuous problem is discretized using isoparametric Lagrangian elements. A sensitivity analysis of this type for linear elasticity problems has already been done by Brockman[2,3]. Also Zolesio[8,9] has performed the sensitivity analysis in the linear case using the so-called speed method for domain deformations. The speed method gives the same sensitivity formulae, although the derivation of the formulae is quite different. In addition we show how to compute efficiently the sensitivity of a functional depending on the finite element solution. The results can be applied in numerical realization of optimal shape design problems, where the system is governed by these nonlinear problems.

2 Sensitivity of the discrete solution vector of a nonlinear potential equation

Consider the nonlinear potential problem with mixed boundary conditions

$$\begin{cases} -\nabla \cdot \left(\rho(x, |\nabla u|^2)\nabla u\right) = f & \text{in } \Omega \subset \mathbb{R}^n,\ n = 2, 3 \\ u = 0 & \text{on } \Gamma_1 \\ \rho(x, |\nabla u|^2)\nabla u \cdot n = g & \text{on } \Gamma_2. \end{cases} \tag{1}$$

Here $\partial\Omega = \Gamma_1 \cup \Gamma_2$, $f \in L^2(\Omega)$, $g \in L^2(\Gamma_2)$ and $\rho : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is a given smooth function. We assssume that for given data the problem (1) is an elliptic problem and has an unique (weak) solution.

We discretize the problem (1) using Lagrangian finite elements of order k. Then the discrete analoque of problem (1) reads as

$$u_h \in V_h : \quad \int_{\Omega_h} \rho(x, |\nabla u_h|^2) \nabla u_h \cdot \nabla v_h \, dx$$
$$= \int_{\Omega_h} f v_h \, dx + \int_{\Gamma_{2h}} g v_h \, ds \quad \forall v_h \in V_h, \tag{2}$$

where $V_h = \{\varphi \in C^0(\Omega_h) \mid \varphi|_{T_e} \in P^k(T_e),\ \varphi|_{\Gamma_{1h}} = 0\}$ is the piecewise polynomial finite element space and $\Omega_h = \cup T_e$ is the finite element mesh. The matrix form of problem (2) is the system of nonlinear equations

$$\mathbf{K}(\mathbf{q})\,\mathbf{q} = \mathbf{f}, \tag{3}$$

where $\mathbf{K}(\mathbf{q})$ is the "stiffness" matrix and $\mathbf{f}$ is the "force" vector respectively. The unknown vector $\mathbf{q}$ contains the nodal values of u_h.

Suppose now that the nodes of the finite element mesh depend on a real parameter α. Our aim is to find the sensitivity of the solution vector $\mathbf{q}$ with respect to α, i.e. to find $\partial\mathbf{q}/\partial\alpha$. In what follows we will denote $(\ )' = \partial(\ )/\partial\alpha$.

If the nodes of the finite element mesh depend smoothly on α, we may use the implicit function theorem and differentiate (3) to obtain

$$\mathbf{K}(\mathbf{q})'\,\mathbf{q} + \mathbf{K}(\mathbf{q})\,\mathbf{q}' = \mathbf{f}'. \tag{4}$$

The terms $\mathbf{K}(\mathbf{q})'\,\mathbf{q}$ and $\mathbf{f}$ can be computed element by element using the relations

$$\mathbf{K}(\mathbf{q})\,\mathbf{q} = \sum_e \mathbf{P}^e \mathbf{K}^e(\mathbf{q}^e)\,\mathbf{q}^e \quad \text{and} \quad \mathbf{f} = \sum_e \mathbf{P}^e \mathbf{f}^e. \tag{5}$$

Here $\mathbf{P}^e$ is the "local-to-global" expanding matrix, $\mathbf{P}^{e^{\mathrm{T}}}$ is the "global-to-local" gathering matrix and $\mathbf{q}^e = \mathbf{P}^{e^{\mathrm{T}}}\mathbf{q}$ (vector of nodal values of u_h associated to the e:th element).

In the case of isoparametric elements each element T_e is obtained from the parent element $\widehat{T}$ ($[-1,1]^n$, for example) by the mapping $\widehat{T} \to T_e : \xi \mapsto x(\xi)$. Let

$$\mathbf{N} = \begin{bmatrix} \varphi_1 \\ \vdots \\ \varphi_m \end{bmatrix} \quad \text{and} \quad \mathbf{L} = \begin{bmatrix} \partial\varphi_1/\partial\xi_1 & \dots & \partial\varphi_m/\partial\xi_1 \\ \vdots & \ddots & \vdots \\ \partial\varphi_1/\partial\xi_n & \dots & \partial\varphi_m/\partial\xi_n \end{bmatrix} \tag{6}$$

be the matrices containing the values of the shape functions and their derivatives for the parent element. Denote by $\mathbf{J} = \left[\frac{\partial x_j}{\partial \xi_i}\right]_{i,j=1}^{n}$ the Jacobian of the mapping $\xi \mapsto x(\xi)$. Finally let

$$\mathbf{X}^e = \begin{bmatrix} X_1^1 & \dots & X_n^1 \\ \vdots & \ddots & \vdots \\ X_1^m & \dots & X_n^m \end{bmatrix} \tag{7}$$

be the matrix containing the nodal coordinates of the e:th element. (In what follows, we omit the superscript e as we are now working with the e:th element). At a point $x(\xi)$ the cartesian derivatives of the shape functions are now given by $\mathbf{B} = \mathbf{J}^{-1}\mathbf{L}$ and the Jacobian by $\mathbf{J} = \mathbf{L}\mathbf{X}$.

Gaussian quadrature with integration points and weights (ξ^k, W_k), $k = 1, \dots, K$ is then used to perform the numerical integration needed for computing the element stiffness matrix, resulting

$$\mathbf{K}^e(\mathbf{q}^e) = \sum_{k=1}^{K} W_k\, \rho(x^k, s_k)\, \mathbf{B}_k^{\mathrm{T}} \mathbf{B}_k |\mathbf{J}_k|, \tag{8}$$

where $s_k = |\nabla u_h(x^k)|^2$, $x^k = x(\xi^k)$, $\mathbf{B}_k = \mathbf{B}(\xi^k)$, $\mathbf{J}_k = \mathbf{J}(\xi^k)$ and $|\mathbf{J}_k| = \det \mathbf{J}_k$.

Lemma 1. *The sensitivity of the "strain-displacement" matrix* $\mathbf{B}_k$ *is given by*

$$\mathbf{B}_k' = -\mathbf{B}_k \mathbf{X}' \mathbf{B}_k. \tag{9}$$

Proof: As $\mathbf{B}_k = \mathbf{J}_k^{-1}\mathbf{L}_k$, we have

$$(\mathbf{J}_k\mathbf{B}_k)' = \mathbf{J}_k'\mathbf{B}_k + \mathbf{J}_k\mathbf{B}_k' = \mathbf{L}_k' = 0,$$

and therefore

$$\mathbf{B}_k' = -\mathbf{J}_k^{-1}\mathbf{J}_k'\mathbf{B}_k = -\mathbf{J}_k^{-1}\mathbf{L}_k\mathbf{X}'\mathbf{B}_k = -\mathbf{B}_k\mathbf{X}'\mathbf{B}_k. \qquad \square$$

The following Lemma is due to Brockman[2]:

Lemma 2. *For the sensitivity of the determinant we have*

$$|\mathbf{J}_k|' = |\mathbf{J}_k| \sum_{j=1}^{m} \nabla\varphi_j(x^k)^T (X^j)'. \tag{10}$$

Lemma 3. *The sensitivities of* s_k *and* x^k *are given by*

$$(x^k)' = (\mathbf{X}')^T \mathbf{N}_k \tag{11}$$

and

$$s_k' = 2\,(\mathbf{B}_k \mathbf{q}^e)^T \mathbf{B}_k' \mathbf{q}^e + 2\,(\mathbf{B}_k \mathbf{q}^e)^T \mathbf{B}_k (\mathbf{q}^e)'. \tag{12}$$

Proof: The result immediately follows from the relations

$$x^k = \mathbf{X}^{\mathrm{T}} \mathbf{N}_k \quad \text{and} \quad s_k = (\mathbf{B}_k \mathbf{q}^e)^{\mathrm{T}} (\mathbf{B}_k \mathbf{q}^e). \qquad \square$$

Lemma 4. *The sensitivity of* $\rho(x^k, s_k)$ *is given by*

$$\rho(x^k, s_k)' = 2\,\frac{\partial \rho(x^k, s_k)}{\partial s} (\mathbf{B}_k \mathbf{q}^e)^T \mathbf{B}_k' \mathbf{q}^e + (\nabla_x \rho(x^k, s_k))^T (\mathbf{X}')^T \mathbf{N}_k + 2\,\frac{\partial \rho(x^k, s_k)}{\partial s} (\mathbf{B}_k \mathbf{q}^e)^T \mathbf{B}_k (\mathbf{q}^e)' \tag{13}$$

Proof: The result follows from Lemma 3. $\square$

Theorem 1. *The term* $\mathbf{K}^e(\mathbf{q}^e)'\,\mathbf{q}^e$ *is given by*

$$\mathbf{K}^e(\mathbf{q}^e)'\,\mathbf{q}^e = \mathbf{S}^e(\mathbf{q}^e)\,\mathbf{q}^{e\prime} + \mathbf{T}^e(\mathbf{q}^e)\,\mathbf{q}^e, \tag{14}$$

where

$$\mathbf{S}^e(\mathbf{q}^e) = \sum_{k=1}^{K} C_k\,\mathbf{B}_k^T \mathbf{B}_k \mathbf{q}^e \mathbf{q}^{eT} \mathbf{B}_k^T \mathbf{B}_k \tag{15}$$

$$\mathbf{T}^e(\mathbf{q}^e) = \sum_{k=1}^{K} \Big(C_k\,\mathbf{B}_k^T \mathbf{B}_k \mathbf{q}^e \mathbf{q}^{eT} \mathbf{B}_k^T \mathbf{B}_k' + D_k\,(\mathbf{B}_k')^T \mathbf{B}_k + D_k\,\mathbf{B}_k^T \mathbf{B}_k' + E_k\,\mathbf{B}_k^T \mathbf{B}_k + F_k\,\mathbf{B}_k^T \mathbf{B}_k \Big) \tag{16}$$

and

$$\begin{aligned} C_k &= 2\,W_k |\mathbf{J}_k| \partial \rho(x^k, s_k)/\partial s, & D_k &= W_k |\mathbf{J}_k| \rho(x^k, s_k) \\ E_k &= W_k |\mathbf{J}_k| (\nabla_x \rho(x^k, s_k))^T (\mathbf{X}')^T \mathbf{N}_k, & F_k &= W_k |\mathbf{J}_k|' \rho(x^k, s_k). \end{aligned} \tag{17}$$

Proof: The result follows from Lemma 4 and the facts that $(\mathbf{B}_k\mathbf{q}^e)^{\mathrm{T}}\mathbf{B}_k\mathbf{q}^{e\prime}$ and $(\mathbf{B}_k^{\mathrm{T}}\mathbf{q}^e)^{\mathrm{T}}\mathbf{B}_k'\mathbf{q}^e$ are scalars. $\square$

In the absence of surface terms (i.e. $g \equiv 0$) the element force vector is given by

$$\mathbf{f}^e = \sum_k W_k f(x^k)\mathbf{N}_k|\mathbf{J}_k|. \tag{18}$$

Differentiating (18) we get

Theorem 2. *The sensitivity of* $\mathbf{f}^e$ *is given by*

$$(\mathbf{f}^e)' = \sum_k W_k \left(\nabla_x f(x^k)^T (x^k)'\mathbf{N}_k|\mathbf{J}_k| + f(x^k)\mathbf{N}_k|\mathbf{J}_k|'\right). \qquad \square \tag{19}$$

Performing the assembly process, we get the following expression for the sensitivity of the solution vector:

Theorem 3. *The sensitivity of* $\mathbf{q}$ *is given as the solution of the linear system of equations*

$$\Big(\mathbf{K}(\mathbf{q}) + \mathbf{S}(\mathbf{q})\Big)\,\mathbf{q}' = \mathbf{f}' - \mathbf{T}(\mathbf{q})\,\mathbf{q}. \qquad \square \tag{20}$$

Remark 1. In the equations (9)–(19) the only matrix depending on a specific application (mesh topology, design parametrization, etc.) is $\mathbf{X}'$. All other matrices are available from the assembly of the system (3).

Remark 2. In practise the nonlinear system (3) is solved only approximately. Therefore the equation (20) also holds approximately only. To get accurate numerical values for the sensitivities it is recommended to solve system (3) as accurately as possible.

3 On the adjoint state technique for the sensitivity of a functional

Let $\alpha = (\alpha_1, ..., \alpha_M) \in \mathbb{R}^M$ be a parameter vector and let $F : \mathbb{R}^M \times \mathbb{R}^N \to \mathbb{R} : (\alpha, \mathbf{q}) \mapsto F(\alpha, \mathbf{q})$ be a functional. The sensitivity of F with respect to α_s, $s = 1, ..., M$ is given by

$$\frac{dF}{d\alpha_s} = \frac{\partial F}{\partial \alpha_s} + (\nabla_q F)^{\mathrm{T}} \frac{\partial \mathbf{q}}{\partial \alpha_s}. \tag{21}$$

The form of equation (21) is not suitable when the gradient of F with respect to α is needed as it requires M solutions of the linear system (20). Employing the standard adjoint equation technique of optimal control theory to eliminate $\frac{\partial \mathbf{q}}{\partial \alpha_s}$ we obtain

$$\frac{dF}{d\alpha_s} = \frac{\partial F}{\partial \alpha_s} + \mathbf{p}^{\mathrm{T}}\left(\frac{\partial \mathbf{f}}{\partial \alpha_s} - \mathbf{T}(\mathbf{q})\,\mathbf{q}\right), \tag{22}$$

where $\mathbf{p}$ is the solution of the adjoint equation

$$\Big(\mathbf{K}(\mathbf{q}) + \mathbf{S}(\mathbf{q})\Big)\mathbf{p} = \nabla_q F. \tag{23}$$

Now the computation of $\nabla_\alpha F$ requires only one solution of the linear system (23).

As an example consider the cost functional $F(\alpha, \mathbf{q}) = \int_{\Omega_h(\alpha)} u_h^2\, dx$. We can write it as a sum

$$F(\alpha, \mathbf{q}) = \sum_e \int_{T_e} u_h^2\, dx$$

To compute the terms required in (22) and (23) we first use the isoparametric mapping technique and Gaussian quadrature to obtain

$$\int_{\widehat{T}} u_h^2 |\mathbf{J}^e|\, d\xi \approx \sum_{k=1}^{K} W_k (\mathbf{N}_k{}^{\mathrm{T}} \mathbf{q}^e)^2 |\mathbf{J}_k| \equiv F^e(\alpha, \mathbf{q}).$$

Then by differentiation we obtain

$$\begin{cases} \dfrac{\partial F^e}{\partial \alpha_s} = \displaystyle\sum_{k=1}^{K} W_k (\mathbf{N}_k{}^{\mathrm{T}} \mathbf{q}^e)^2 \frac{\partial |\mathbf{J}_k|}{\partial \alpha_s} \\ \dfrac{\partial F^e}{\partial q_j^e} = \displaystyle\sum_{k=1}^{K} W_k 2\,(\mathbf{N}_k{}^{\mathrm{T}} \mathbf{q}^e) \varphi_j(\xi^k) |\mathbf{J}_k|, \quad j = 1, \ldots, m. \end{cases}$$

Thus all calculations needed for (22) and (23) can be done using element-by-element techniques.

4 Applications

In this section we shortly list some state equations of form (1) which have appeared in optimal design litterature.

Axisymmetric Poisson's equation

An important application is the axisymmetric Poisson's equation

$$-\nabla \cdot \Big(2\pi r \nabla u(r,z)\Big) = 2\pi r\, f(r,z). \tag{24}$$

In this case $\rho(x,s) = 2\pi\, x_1$. As the problem is linear the adjoint problem (23) has the same coefficient matrix. When direct methods are used for the solution of (3) one may solve (23) eficiently using the existing factorization of the coefficient matrix.

Sensitivity analysis for magnetic field calculations

Electromagnetic behaviour is governed by the Maxwell's equations for the magnetic field $\vec{H}$ and the magnetic induction $\vec{B}$. Introducing the vector potential $\vec{A}$, $\vec{B} = \nabla \times \vec{A}$ the Maxwell's equations reduce into equation

$$-\nabla \times (\rho \nabla \times \vec{A}) = \vec{j}, \tag{25}$$

where $\vec{j}$ is the current density and ρ is the magnetic reluctivity. Let the domain under consideration be given as $\Omega = \Omega_{air} \cup \Omega_{copper} \cup \Omega_{iron}$. In this case the function ρ is of the form

$$\rho(x,s) = \begin{cases} \text{const}, & x \in \Omega_{air} \cup \Omega_{copper} \\ r(s), & x \in \Omega_{iron}. \end{cases} \tag{26}$$

Assuming that $\vec{A} = (0,0,u)$ and $\vec{j} = (0,0,j_3)$, the problem then reduces into the nonlinear potential problem

$$-\nabla \cdot (\rho(x, |\nabla u|^2) \nabla u) = j_3. \tag{27}$$

Although the mapping $x \mapsto \rho(x,s)$ is not continuous, no problems arise if the finite element boundaries coincide with the material boundaries. The results of Theorems 1–2 are now directly applicape.

We note that in refs. 1 and 6 the sensitivity analysis was performed for this problem in the case of P^1 triangular elements. As in both cases area coordinates were employed the sensitivity formulae presented there cannot be utilized in the case of higher order elements.

Sensitivity analysis for subsonic compressible flow

The design of airfoils with good aerodynamical properties is an important problem for the designers of turbomachines and aircrafts. In two dimensions compressible gas flow is described by the compressible potential equation

$$\nabla \cdot \left(\rho(|\nabla u|^2)\nabla u\right) = 0. \tag{28}$$

The velocity of the flow is given by $\vec{v} = \nabla u$ and the density of the gas by

$$\rho(|\vec{v}|^2) = \rho_0 \left(1 - \frac{\gamma - 1}{\gamma + 1}|\vec{v}|^2\right)^{\frac{1}{\gamma-1}} \quad (\rho_0 \text{ and } \gamma \text{ positive constants}). \tag{29}$$

When the flow is subsonic then the equation (29) with suitable boundary conditions is an elliptic boundary value problem. In the transonic case the problem is of mixed elliptic-hyperbolic type. For the optimization problem formulation (cost function, constraints, etc.) we refer to the book of Pironneau[7]. Again Theorem 1 gives a direct formula for sensitivity calculations.

5 Numerical example

Let us consider the following boundary value problem depending on a parameter $\alpha \in \mathbb{R}$:

$$\begin{cases} -\nabla \cdot \left(\rho(|\nabla u|^2)\nabla u\right) = \dfrac{1}{10}, & \text{in } \Omega(\alpha) \\ u = 0, & \text{on } \Gamma_1 \\ \rho(|\nabla u|^2) \cdot n = 0, & \text{on } \Gamma(\alpha) \cup \Gamma_2 \cup \Gamma_3. \end{cases}$$

Here $\rho(|\nabla u|^2) = (1 + |\nabla u|^2)^{1/2}$, $\Omega(\alpha) = \{(x, y) \in \mathbb{R}^2 \mid 0 < y < 1,\ 0 < x < 1 + \alpha(y - y^2)\}$, $\Gamma_1 = [0, 1] \times \{0\}$, $\Gamma_2 = \{0\} \times [0, 1]$, $\Gamma_3 = [0, 1] \times \{1\}$ and $\Gamma(\alpha) = \{(x, y) \in \mathbb{R}^2 \mid 0 < y < 1,\ x = 1 + \alpha(y - y^2)\}$. The solution of this problem is approximated by the finite element method using isoparametric four-node quadrilateral elements. The nodal coordinates of the finite element mesh used (see Figure 1) are given by

$$\begin{cases} x_{i,j} = \dfrac{i-1}{20}\left(1 + \alpha(y_{21,j} - y_{21,j}^2)\right), & i, j = 1, \ldots, 21 \\ y_{i,j} = \dfrac{j-1}{20}, \quad i, j = 1, \ldots, 21. \end{cases}$$

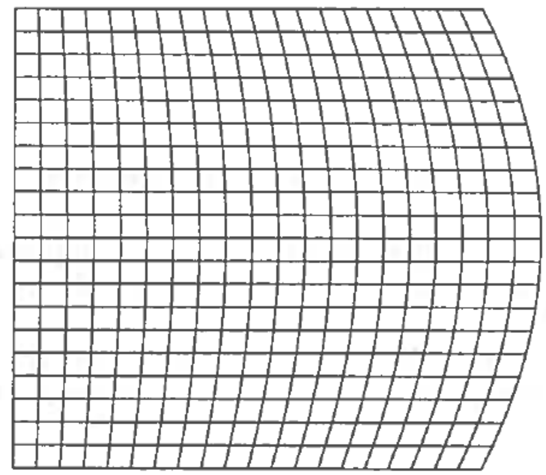

Figure 1: Structure of the finite element mesh (with $\alpha = \frac{1}{2}$).

In Figure 2 a contour plot of the sensitivity of the finite element solution $\partial u_h(\alpha)/\partial\alpha|_{\alpha=0}$ is shown. Computations were done in double precision using HP9000/340-computer.

The correctness of the sensitivity solution was confirmed by comparing the nodal values of $\partial u_h/\partial\alpha|_{\alpha=0}$ with those obtained by finite differencing. By solving the nonlinear and linear systems (3) and (20) as accurate as possible and searching an optimal differencing parameter the analytic and finite difference sensitivities were found to have at least five digits in common at each node.

6 Conclusions

The sensitivity formulae presented in this paper are both simple to program correctly and efficient as basic linear algebra subroutine (BLAS) packages can be utilized. Our approach is general as it applies to all isoparametric Lagrangian finite elements. General purpose programs can be easily developed as the dependence on the specific application can be isolated into separate modules. The same approach can clearly be applied to different state problems (elasticity, Navier-Stokes, etc).

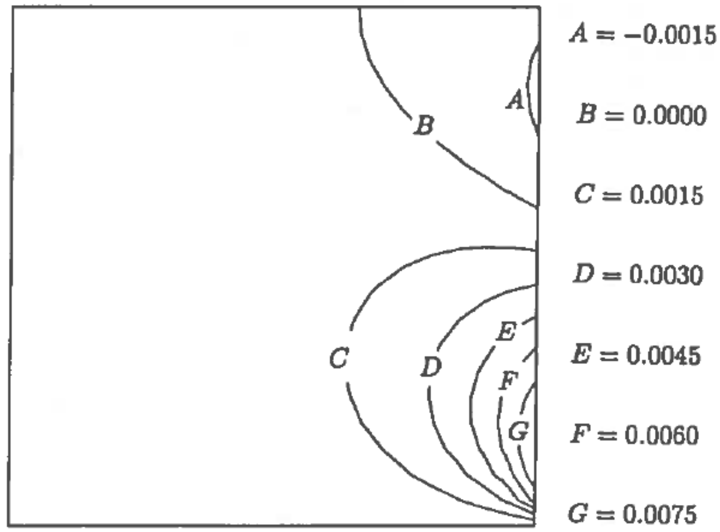

Figure 2: Contour plot of the sensitivity of $u_h(\alpha)$ at $\alpha = 0$.

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