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Primal-Dual Newton-Type Interior-Point Method for Topology Optimization[1]

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Abstract. We consider the problem of minimization of energy dissipation in a conductive electromagnetic medium with a fixed geometry and a priori given lower and upper bounds for the conductivity. The nonlinear optimization problem is analyzed by using the primal-dual Newton interior-point method. The elliptic differential equation for the electric potential is considered as an equality constraint. Transforming iterations for the null space decomposition of the condensed primal-dual system are applied to find the search direction. The numerical experiments treat two-dimensional isotropic systems.

1. Introduction

The development, analysis, and implementation of efficient methods for the optimal design of topology, shape, and material in continuous and discrete structural mechanics have been studied intensively during the past decade; see e.g. Bendsøe (Ref. 1). In particular, the topology optimization of solid structures involves the determination of the optimal placement of material in space; i.e., one has to determine which points of space are material points and which points should remain void (no material). On the other

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hand, not much work has been done concerning the optimal design of electronic devices and systems whose operational behavior is governed by electromagnetic fields that can be described by the Maxwell equations. Although advanced numerical techniques for the computation of electromagnetic fields have been developed in recent years [see e.g. Beck, Deuflhard, Hiptmair, Hoppe, and Wohlmuth (Ref. 2) and the references therein], the issue of structural optimization with the Maxwell equations as state constraints has not yet been investigated.

In this paper, we consider problems concerning the topology optimization in electromagnetic media described by the Maxwell equations supplemented by the respective material laws. We are looking for an optimal distribution of conductivity in a fixed geometrical configuration. In the stationary case, one obtains problem formulations in electrostatics and magnetostatics, which are similar to elastomechanical problems. The mathematical models lead to elliptic boundary-value problems corresponding to the minimization of energy dissipation given by the Joule–Lenz law. We suppose that our domain is occupied by an isotropic conductor with a finite conductivity. To simplify the presentation, we consider the stationary case; i.e., constant currents are available in the conductor.

We have concentrated our efforts on solving nonlinear nonconvex optimization problems for the minimization of the energy dissipation. We solve a constrained optimization problem, constituted by the objective just mentioned, subject to equality constraints on the elliptic electric potential equation, mass conservation, and inequality box constraints for the conductivity (i.e., a priori given lower and upper bounds). Interior-point methods, which generate iterates that satisfy strictly the inequalities in the problem formulation, are applied. A primal-dual formulation is proposed to solve the optimization problem. This formulation leads to large and sparse linear-quadratic subproblems to be solved at each iteration, which are similar to the problems studied by Maar and Schulz (Ref. 3), where primal interior-point methods are mainly investigated.

The primal-dual interior-point methods have been proposed originally by Kojima, Mizuno, and Yoshise (Ref. 4), based on the application of the classical logarithmic barrier function method to primal and dual linear programs, which was studied earlier by Megiddo (Ref. 5). The main idea of the algorithm is to work simultaneously on primal and dual linear programming problems and generate a sequence of pairs of their interior feasible solutions. In the last decade, primal-dual algorithms have emerged as the most useful algorithms from the interior-point class in linear programming applications; see also Refs. 6–8.

The primal-dual method has been extended recently to nonlinear programming by El-Bakry, Tapia, Tsuchiya, and Zhang (Ref. 9) and has

started to prove its impressive computational performance for nonlinear and semidefinite programming; see e.g. Refs. 10–13. The results in the cited studies indicate that primal-dual methods are very promising, although many theoretical and practical difficulties remain to be solved.

The paper is organized as follows. In Section 2, we describe the eddy current equations and give an expression for the energy dissipation used as objective function in our considerations. In Section 3, we introduce the primal-dual formulation of our nonlinear nonconvex optimization problem based on the classical logarithmic barrier functions. The Karush–Kuhn–Tucker first-order necessary conditions for optimality result in a nonlinear equation for the unknown variables. Perturbed complementarity conditions with a decreasing barrier parameter at each optimization step are used. Transforming iterations for null space formulations, proposed as smoothers for multigrid methods in Ref. 3, are applied in Section 4 for the iterative solution of linear-quadratic subproblems. In Section 5, we discuss the choice of the merit function, steplength strategy, barrier parameter, and watchdog technique. In Section 6, we include some numerical experiments applying the primal-dual interior-point method to the nonlinear problem and present the respective material distributions for a two-dimensional isotropic conductor. Finally, in Section 7, we give some concluding remarks.

2. Eddy Current Equations

We consider electromagnetic fields in the low frequency regime which can be described by the quasistationary limit of the Maxwell equations, also known as the eddy current equations,

$$\partial B/\partial t + \operatorname{curl} E = 0, \qquad \operatorname{div} B = 0, \qquad \operatorname{curl} H = J, \tag{1}$$

$$B = \mu H, \qquad J = \sigma E. \tag{2}$$

Here, E and H stand for the electric and magnetic field, B and J denote the magnetic induction and current density; μ and σ refer to the magnetic permeability and electric conductivity, respectively [for a justification of the eddy current equations, see e.g. Ammari, Buffa, and Nédélec (Ref. 14)].

In the 2D case, assuming that the current density is given by

$$J = (J_1(x_1, x_2, t), J_2(x_1, x_2, t), 0),$$

the electric and magnetic fields take the form

$$E = (E_1(x_1, x_2, t), E_2(x_1, x_2, t), 0), \qquad H = (0, 0, H(x_1, x_2, t)).$$

We use a potential formulation by introducing a scalar electric potential φ and a magnetic vector potential A according to

$$E = -\text{grad}\,\varphi - \partial A/\partial t, \qquad B = \text{curl}\,A,$$

where curl is the two-dimensional scalar operator

$$\text{curl}\,(A_1, A_2) = \partial A_1/\partial x_2 - \partial A_2/\partial x_1;$$

see e.g. Biro and Preis (Ref. 15). Then, (1)–(2) give rise to the following coupled system of PDEs for the electromagnetic potentials φ and A,

$$\text{div}(\sigma\,\text{grad}\,\varphi) = 0, \qquad \text{in } \Omega, \tag{3}$$

$$\sigma n \cdot \text{grad}\,\varphi = \begin{cases} I_\nu, & \text{on } \Gamma_\nu \subset \partial\Omega, \\ 0, & \text{elsewhere}, \end{cases} \tag{4}$$

$$\sigma(\partial A/\partial t) + \text{curl}\,\mu^{-1}\,\text{curl}\,A = \begin{cases} -\sigma\,\text{grad}\,\varphi, & \text{in } \Omega, \\ 0, & \text{in } R^3 \backslash \bar{\Omega}, \end{cases} \tag{5}$$

the latter with appropriate initial and boundary conditions. Note that, in (4), we refer to I_ν as the fluxes associated with the contacts $\Gamma_\nu \subset \partial\Omega$, $1 \leq \nu \leq N_c$, satisfying the compatibility conditions

$$\sum_{\nu=1}^{N_c} I_\nu = 0.$$

The electric energy dissipation given by the Joule–Lenz law reads as follows:

$$f(\varphi, \sigma, A) := \int_\Omega J \cdot E\,dx. \tag{6}$$

In particular, in the stationary regime, this reduces to

$$f(\varphi, \sigma) = -\int_\Omega J \cdot \text{grad}\,\varphi\,dx = -\int_\Omega \text{div}(\varphi J)\,dx. \tag{7}$$

The last equality in (7) follows from

$$\text{div}(\varphi J) = J \cdot \text{grad}\,\varphi + \varphi\,\text{div}\,J,$$

taking into account the fact that

$$\text{div}\,J = 0$$

in view of (1). Using the Gauss theorem and the Neumann boundary conditions from (4), we get

$$f(\varphi, \sigma) = -\int_{\partial\Omega} n \cdot J\, \varphi \, ds = \sum_{\nu=1}^{N_c} \int_{\Gamma_\nu} I_\nu \varphi \, ds. \tag{8}$$

3. Primal-Dual Interior-Point Method

We solve the optimization problem for the energy dissipation given by (8),

$$\min_{\varphi, \sigma} \quad f(\varphi, \sigma) = \min_{\varphi, \sigma} \sum_{\nu} \int_{\Gamma_\nu} I_\nu \varphi \, ds, \tag{9}$$

$$\text{s.t.} \quad \varphi \text{ satisfies (3)–(4)}, \tag{10a}$$

$$\int_\Omega \sigma \, dx = C \qquad \text{(mass constraint)}, \tag{10b}$$

$$\sigma_{\min} \le \sigma \le \sigma_{\max} \qquad \text{(conductivity box constraint)}. \tag{10c}$$

Here, $\sigma_{\min}$ and $\sigma_{\max}$ are a priori given positive limits for the conductivity and C is a fixed given value. In general formulations of nonlinear programming problems, the objective function f and the inequality constraints are supposed to be twice continuously differentiable. In our case, this requirement is obviously satisfied.

Note that we formulate a constrained optimization problem, where the differential equation (10a) for φ is part of the constraints. This is in contrast to many standard optimization approaches, which consider φ as a function of the independent variable σ via the differential equation. However, this simultaneous optimization approach reduces the overall computational complexity of the resulting optimization algorithm.

After a finite-element discretization of the domain with discretization parameter h, we get the following finite-dimensional nonlinear programming problem:

$$\min_{\varphi_h, \sigma_h} \quad f(\varphi_h, \sigma_h), \tag{11}$$

$$\text{s.t.} \quad A_h(\sigma_h)\, \varphi_h = b_h, \tag{12a}$$

$$g(\sigma_h) := \int_\Omega \sigma \, dx = C, \tag{12b}$$

$$\sigma_{\min} \le \sigma_i \le \sigma_{\max}, \qquad 1 \le i \le N, \tag{12c}$$

where A_h is the finite–element stiffness matrix, b_h is the discrete load vector, and $\sigma_h = (\sigma_i)_{i=1}^N$ is the discrete conductivity vector. The discretization parameter is of order $h = O(N^{-1})$, where N is the number of finite elements. We suppose that the conductivity is a constant on each element; i.e., σ_i is the value of σ on the ith element. Note that the lower bound $\sigma_{\min}$ plays a crucial role in keeping the ellipticity of the discrete problem.

For simplicity of presentation, until the end of this section we omit the index h for the discretization parameter. Our optimization problem has the following form:

$$\min_{\varphi,\,\sigma} \quad f(\varphi, \sigma), \tag{13}$$

$$\text{s.t.} \quad A(\sigma)\,\varphi - b = 0, \qquad g(\sigma) - C = 0, \tag{14a}$$

$$\sigma - \sigma_{\min} e \geq 0, \qquad \sigma_{\max} e - \sigma \geq 0, \tag{14b}$$

where

$$e \in R^N, \qquad e = (e_1, \ldots, e_N)^T, \qquad e_i = 1, \qquad 1 \leq i \leq N.$$

The Lagrangian function associated with problem (13)–(14) is

$$\begin{aligned} &L(\varphi, \sigma, \lambda, \eta, z, w) \\ &:= f(\varphi, \sigma) + \lambda^T [A(\sigma)\varphi - b] + \eta[g(\sigma) - C] \\ &- z^T(\sigma - \sigma_{\min} e) - w^T(\sigma_{\max} e - \sigma). \end{aligned} \tag{15}$$

Here λ, η and $z \geq 0$, $w \geq 0$ are the Lagrange multipliers for the equality and inequality constraints in (14). The necessary first-order Karush–Kuhn–Tucker (KKT) optimality conditions read as follows:

$$\nabla_\varphi L = \nabla_\varphi f + A(\sigma)^T \lambda = 0, \tag{16a}$$

$$\nabla_\sigma L = \partial_\sigma(\lambda^T A(\sigma)\varphi) + \eta \nabla g(\sigma) - z + w = 0, \tag{16b}$$

$$\nabla_\lambda L = A(\sigma)\varphi - b = 0, \tag{16c}$$

$$\nabla_\eta L = g(\sigma) - C = 0, \tag{16d}$$

$$D_1 z = 0, \qquad D_2 w = 0, \tag{16e}$$

$$z \geq 0, \qquad w \geq 0, \tag{16f}$$

where

$$D_1 = \operatorname{diag}(\sigma_i - \sigma_{\min}), \qquad D_2 = \operatorname{diag}(\sigma_{\max} - \sigma_i)$$

denote diagonal matrices in the complementarity conditions.

The Hessian of the Lagrangian with respect to (φ, σ) is denoted by

$$H = H(\varphi, \sigma, \lambda) = \begin{bmatrix} 0 & L_{\varphi\sigma} \\ L_{\sigma\varphi} & L_{\sigma\sigma} \end{bmatrix}, \tag{17}$$

where

$$L_{\sigma\varphi} = L_{\varphi\sigma}^T = \partial_\sigma(\lambda^T A(\sigma)), \tag{18a}$$

$$L_{\sigma\sigma} = \partial_{\sigma\sigma}^2(\lambda^T A(\sigma)\varphi). \tag{18b}$$

Our purpose is to find an isolated (locally unique) local minimum of problem (13)–(14). Assume that at least one such point exists, and denote the solution by

$$\Phi^* := (\varphi^*, \sigma^*, \lambda^*, \eta^*, z^*, w^*).$$

Following the theory in Fiacco and McCormick (Ref. 16), the standard assumptions for the application of the Newton method to our optimization problem are these:

(A1) Existence. There exists Φ^*, solution of problem (13)–(14), satisfying the first-order KKT conditions (16).

(A2) Smoothness. The Hessian matrices, corresponding to the objective function, equalities, and inequalities exist and are locally Lipschitz continuous at (φ^*, σ^*).

(A3) Regularity. The gradients of the constraints whose right-hand side is zero (i.e., all the equalities and the active inequality constraints) at (φ^*, σ^*) are linearly independent.

(A4) Strict Complementarity. $z^* + \sigma^* - \sigma_{\min} e > 0$ and $w^* + \sigma_{\max} e - \sigma^* > 0$.

(A5) Second-Order Sufficiency Conditions. $\eta^T H^* \eta > 0$, for all vectors $\eta \in \mathrm{Ker}\,(J)$, $\eta \neq 0$, where J is the Jacobian of all constraints whose right-hand side is zero at (φ^*, σ^*) and $H^* := H(\varphi^*, \sigma^*, \lambda^*)$.

In the last few years, various primal-dual approaches have been suggested. Some authors deal with the corresponding inequality constraints adding nonnegative slack variables directly to the optimization problem; see e.g. Refs. 3 and 9. Another approach is to apply primal-dual Newton-type interior-point methods, based on the logarithmic barrier function method, which was introduced by Frisch implicitly (Ref. 17) and popularized by Fiacco and McCormick (Ref. 16) in the late 1960s. Recent studies in this area have been reported in Refs. 11, 18, 19.

The logarithmic barrier function associated with the optimization problem (13)–(14) consists of solving a sequence of minimization subproblems of the form

$$\min_{\varphi,\sigma} \quad \beta(\varphi, \sigma, p),$$

$$\beta(\varphi, \sigma, p) := f(\varphi, \sigma) - p\,[\log(\sigma - \sigma_{\min} e) + \log(\sigma_{\max} e - \sigma)], \tag{19}$$

$$\text{s.t.} \quad A(\sigma)\varphi - b = 0, \qquad g(\sigma) - C = 0, \tag{20}$$

where $\beta(\varphi, \sigma, p)$ is the barrier function and $p > 0$ is the barrier parameter. We suppose here that

$$\sigma > \sigma_{\min} e, \qquad \sigma_{\max} e > \sigma,$$

so that the logarithmic terms serve as a barrier. Obviously, this method is an interior-point method, in the sense that it keeps the iterates strictly feasible with respect to the inequality constraints. The subproblems (19)–(20) are solved for decreasing values of p and have the following Lagrangian:

$$L_p(\varphi, \sigma, \lambda, \eta) := \beta(\varphi, \sigma, p) + \lambda^T[A(\sigma)\varphi - b\,] + \eta[g(\sigma) - C].$$

The first-order KKT conditions for the logarithmic barrier optimization subproblems result in

$$\nabla_\varphi L_p = \nabla_\varphi f + A\,(\sigma)^T\lambda = 0, \tag{21a}$$

$$\nabla_\sigma L_p = \partial_\sigma(\lambda^T A(\sigma)\varphi) + \eta\nabla g(\sigma) - pD_1^{-1}e + pD_2^{-1}e = 0, \tag{21b}$$

$$\nabla_\lambda L_p = A(\sigma)\varphi - b = 0, \tag{21c}$$

$$\nabla_\eta L_p = g(\sigma) - C = 0. \tag{21d}$$

Comparison of (16b) and (21b) reveals that the terms $pD_1^{-1}e$ and $pD_2^{-1}e$ may serve as the Lagrange multipliers z and w for the inequality constraints. The interior-point method is now characterized by substituting the last two complementarity conditions (16e)–(16f) by the perturbed complementarity conditions

$$D_1 z = pe, \qquad D_2 w = pe. \tag{22}$$

Our primal-dual interior-point algorithm is based on the Newton-type method applied to three sets of equations: primal feasibility (φ, σ), dual feasibility (λ, η) and perturbed complementarity conditions, related to (z, w). We denote by

$$\Phi := (\varphi, \sigma, \lambda, \eta, z, w)$$

the solution of the optimization subproblem. The KKT conditions (16) lead to the following nonlinear equation:

$$F_p(\Phi) := \begin{bmatrix} \nabla_\varphi L \\ \nabla_\sigma L \\ \nabla_\lambda L \\ \nabla_\eta L \\ \nabla_z L \\ \nabla_w L \end{bmatrix} = \begin{bmatrix} \nabla_\varphi f + A(\sigma)^T \lambda \\ \partial_\sigma(\lambda^T A(\sigma)\varphi) + \eta \nabla g(\sigma) - z + w \\ A(\sigma)\varphi - b \\ g(\sigma) - C \\ D_1 z - pe \\ D_2 w - pe \end{bmatrix} = 0, \qquad (23)$$

where

$$\nabla_z L = D_1 z - pe, \qquad \nabla_w L = D_2 w - pe.$$

The search direction is given by

$$\Delta\Phi := (\Delta\varphi, \Delta\sigma, \Delta\lambda, \Delta\eta, \Delta z, \Delta w).$$

The update $\Phi \leftarrow \Phi + \Delta\Phi$ is determined by the increment $\Delta\Phi$ computed by using the Newton method for the following p-dependent system of equations:

$$K_p \Delta\Phi = -F_p(\Phi), \qquad (24)$$

where (24) is often referred to as the primal-dual system and is solved at each iteration with a decreasing positive parameter p. More precisely, (24) is equivalent to

$$\begin{bmatrix} 0 & L_{\varphi\sigma} & L_{\varphi\lambda} & 0 & 0 & 0 \\ L_{\sigma\varphi} & L_{\sigma\sigma} & L_{\sigma\lambda} & L_{\sigma\eta} & -I & I \\ L_{\lambda\varphi} & L_{\lambda\sigma} & 0 & 0 & 0 & 0 \\ 0 & L_{\eta\sigma} & 0 & 0 & 0 & 0 \\ 0 & Z & 0 & 0 & D_1 & 0 \\ 0 & -W & 0 & 0 & 0 & D_2 \end{bmatrix} \begin{bmatrix} \Delta\varphi \\ \Delta\sigma \\ \Delta\lambda \\ \Delta\eta \\ \Delta z \\ \Delta w \end{bmatrix} = - \begin{bmatrix} \nabla_\varphi L \\ \nabla_\sigma L \\ \nabla_\lambda L \\ \nabla_\eta L \\ \nabla_z L \\ \nabla_w L \end{bmatrix}, \qquad (25)$$

where I stands for the identity matrix and

$$Z = \mathrm{diag}(z_i), \qquad W = \mathrm{diag}(w_i)$$

are diagonal matrices. The remaining nonzero entries of K_p are given by (18) and the following expressions:

$$L_{\lambda\varphi} = L_{\varphi\lambda}^T = A(\sigma), \qquad (26a)$$

$$L_{\lambda\sigma} = L_{\sigma\lambda}^T = \partial_\sigma(\varphi^T A(\sigma)), \qquad (26b)$$

$$L_{\eta\sigma} = L_{\sigma\eta}^T = \nabla^T g(\sigma). \qquad (26c)$$

Note that $L_{\lambda\varphi} = A(\sigma)$ is the stiffness matrix of the electric potential equation, $L_{\sigma\sigma}$ is a diagonal matrix, and $L_{\eta\sigma} = \nabla^T g(\sigma)$ is just one row vector.

The primal-dual matrix K_p from (24) is sparse, nonsymmetric, indefinite, and usually well-conditioned; i.e., it has a bounded condition number as $p \to 0$. Recently, several ideas have been described as how to solve the primal-dual equations, and thus compute accurate increments (search direction). For example, one can take advantage essentially of the fact that Z and W are diagonal matrices, and hence the primal-dual matrix can be symmetrized easily. This approach has been proposed recently by Forsgen, Gill, and Shinnerl (Ref.20), who have shown that the symmetric full primal-dual matrix produced is asymptotically ill-conditioned, but that this ill-conditioning is benign, in the sense that the solution of the symmetrized system is well determined. Another approach is to transform K_p to a smaller (so-called condensed) matrix, which is inherently ill-conditioned, but the ill-conditioning should not necessarily be avoided and has no negative consequences. For detailed discussion, see e.g. Wright (Ref. 19).

Now, our approach is to eliminate the increments for z and w from the 5th and 6th rows of (25), namely,

$$\Delta z = D_1^{-1}(-\nabla_z L - Z\Delta\sigma), \tag{27a}$$

$$\Delta w = D_2^{-1}(-\nabla_w L + W\Delta\sigma). \tag{27b}$$

Substituting (27) into the second row of (25), we get the following linear system for the increments of $\psi := (\varphi, \sigma, \lambda, \eta)$:

$$\tilde{K}_p \Delta\psi = -\tilde{\xi}_p(\psi), \tag{28a}$$

$$\Delta\psi := (\Delta\varphi, \Delta\sigma, \Delta\lambda, \Delta\eta), \tag{28b}$$

where $\tilde{K}_p$ is the matrix and $\tilde{\xi}_p(\psi)$ is the right-hand side of the following system:

$$\begin{bmatrix} 0 & L_{\varphi\sigma} & L_{\varphi\lambda} & 0 \\ L_{\sigma\varphi} & \tilde{L}_{\sigma\sigma} & L_{\sigma\lambda} & L_{\sigma\eta} \\ L_{\lambda\varphi} & L_{\lambda\sigma} & 0 & 0 \\ 0 & L_{\eta\sigma} & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta\varphi \\ \Delta\sigma \\ \Delta\lambda \\ \Delta\eta \end{bmatrix} = - \begin{bmatrix} \nabla_\varphi L \\ \tilde{\nabla}_\sigma L \\ \nabla_\lambda L \\ \nabla_\eta L \end{bmatrix}. \tag{29}$$

The $\sigma\sigma$-entry of $\tilde{K}_p$ is now replaced by

$$\tilde{L}_{\sigma\sigma} = L_{\sigma\sigma} + D_1^{-1} Z + D_2^{-1} W,$$

and the modified entry for the right-hand side is

$$\tilde{\nabla}_\sigma L = \nabla_\sigma L + D_1^{-1}\nabla_z L - D_2^{-1}\nabla_w L.$$

4. Transforming Null Space Iterations

In this section, we explain the way in which we solve the condensed primal-dual system (29) to compute the search direction $\Delta\psi$. As discussed in Section 3, the matrix K_p (in this section, we omit the subscript p and denote the matrix by K) is typically indefinite. Similar indefinite systems of linear equations arise in the computation of saddle points when solving Stokes equations and Navier–Stokes equations. Iterative methods based e.g., on the Uzawa algorithm for solving saddle-point problems have been proposed by Bank, Welfert, and Yserentant (Ref. 21). Direct methods for the solution can also be applied, where direct range space and null space methods are distinguished. In Schulz and Wittum (Ref. 22), this distinction has been transferred to iterative methods.

First, let us consider the following range space formulation of K:

$$K = \begin{bmatrix} A & B^T \\ B & D \end{bmatrix} = \begin{bmatrix} 0 & L_{\varphi\sigma} & L_{\varphi\lambda} & 0 \\ L_{\sigma\varphi} & \tilde{L}_{\sigma\sigma} & L_{\sigma\lambda} & L_{\sigma\eta} \\ L_{\lambda\varphi} & L_{\lambda\sigma} & 0 & 0 \\ 0 & L_{\eta\sigma} & 0 & 0 \end{bmatrix}. \tag{30}$$

Here,

$$A = \begin{bmatrix} 0 & L_{\varphi\sigma} \\ L_{\sigma\varphi} & \tilde{L}_{\sigma\sigma} \end{bmatrix}, \qquad D = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

so that, in the Schur complement

$$S := D - BA^{-1}B^T,$$

the first block A of K is taken as a pivot block and its definiteness plays a crucial role. In many practical applications such as (i) solving discrete saddle-point problems arising in Stokes equations and Navier–Stokes equations or (ii) linear programming problems, the block A is positive definite. For nonlinear convex problems (i.e., convex objective function, linear equality constraints, and concave inequality constraints), the Hessian of the Lagrangian function is positive semidefinite. Preconditioned iterative solvers for the corresponding saddle-point problems have been proposed, for example, by Rusten and Winther (Ref. 23) and, in the context of multigrid methods, by Wittum (Ref. 24).

We consider also the null space formulation of K,

$$K = \begin{bmatrix} A & B^T \\ B & D \end{bmatrix} = \begin{bmatrix} 0 & L_{\varphi\lambda} & L_{\varphi\sigma} & 0 \\ L_{\lambda\varphi} & 0 & L_{\lambda\sigma} & 0 \\ L_{\sigma\varphi} & L_{\sigma\lambda} & \tilde{L}_{\sigma\sigma} & L_{\sigma\eta} \\ 0 & 0 & L_{\eta\sigma} & 0 \end{bmatrix}, \tag{31}$$

where

$$A = \begin{bmatrix} 0 & L_{\varphi\lambda} \\ L_{\lambda\varphi} & 0 \end{bmatrix}$$

is now an indefinite, but nonsingular matrix. Moreover, we recall that

$$L_{\lambda\varphi} = A(\sigma)$$

is exactly the stiffness matrix corresponding to the electric potential equation (3); hence, A^{-1} exists and the Schur complement, in this case

$$S = D - BA^{-1}B^T,$$

is correctly defined. Furthermore, iterative solvers implementing A^{-1} are already available, which is a typical situation for optimization problems, where discretized differential equations form the bulk of the constraints. Therefore, the null space formulation turns out to be a more natural and attractive approach for solving the condensed primal-dual system; see e.g. Refs. 3,11,19.

We use transforming null space iterations for our problem (29), as proposed by Maar and Schulz (Ref. 3) in the context of multigrid methods. Transforming iterations have been introduced earlier as smoothers for multigrid methods in range space formulations by Wittum (Ref. 24). Here, these null-space iterations are used directly as iterative solvers.

The main effort is concentrated on constructing auxiliary matrices K^L and K^R, respectively called, left and right transformations, so that the following regular splitting is possible:

$$K^L K K^R = M_1 - M_2, \tag{32}$$

with reasonable matrix M_1 and $M_2 \sim 0$. The left-transforming iteration corresponds to preconditioning, whereas the right-transforming iteration is identical with the distributive iteration; see Wittum (Ref. 24), where also a complete convergence theory of the proposed method can be found.

For solving the system

$$K\Delta\psi = b,$$

starting with an initial guess for $\Delta\psi$, the transforming iteration is given by

$$\Delta\psi^{\text{new}} := \Delta\psi^{\text{old}} + K^R M_1^{-1} K^L (b - K\Delta\psi^{\text{old}}).$$

Let $\tilde{L}_{\lambda\varphi}$ be a preconditioner for the stiffness matrix (e.g., pointwise or blockwise ILU decomposition; Jacobi, Gauss–Seidel, or SSOR iteration). We approximate the block A as follows:

$$A = \begin{bmatrix} 0 & L_{\varphi\lambda} \\ L_{\lambda\varphi} & 0 \end{bmatrix} \sim \begin{bmatrix} 0 & \tilde{L}_{\varphi\lambda} \\ \tilde{L}_{\lambda\varphi} & 0 \end{bmatrix}. \tag{33}$$

Typical left and right transformations are of the form

$$K^L = I, \qquad K^R = \begin{bmatrix} I & -\tilde{A}^{-1}B^T \\ 0 & I \end{bmatrix} = \begin{bmatrix} I & 0 & -\tilde{L}_{\lambda\varphi}^{-1}L_{\lambda\sigma} & 0 \\ 0 & I & -\tilde{L}_{\varphi\lambda}^{-1}L_{\varphi\sigma} & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}.$$

For the regular splitting

$$KK^R = M_1 - M_2,$$

from (32) we obtain

$$KK^R = \begin{bmatrix} 0 & L_{\varphi\lambda} & 0 & 0 \\ L_{\lambda\varphi} & 0 & 0 & 0 \\ L_{\sigma\varphi} & L_{\sigma\lambda} & \tilde{S} & L_{\sigma\eta} \\ 0 & 0 & L_{\eta\sigma} & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & L_{\varphi\sigma} - L_{\varphi\lambda}\tilde{L}_{\varphi\lambda}^{-1}L_{\varphi\sigma} & 0 \\ 0 & 0 & L_{\lambda\sigma} - L_{\lambda\varphi}\tilde{L}_{\lambda\varphi}^{-1}L_{\lambda\sigma} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where

$$M_1 = \begin{bmatrix} 0 & L_{\varphi\lambda} & 0 & 0 \\ L_{\lambda\varphi} & 0 & 0 & 0 \\ L_{\sigma\varphi} & L_{\sigma\lambda} & \tilde{S} & L_{\sigma\eta} \\ 0 & 0 & L_{\eta\sigma} & 0 \end{bmatrix} = \begin{bmatrix} A & 0 \\ B & S \end{bmatrix}, \tag{34}$$

with

$$S := \begin{bmatrix} \tilde{S} & L_{\sigma\eta} \\ L_{\eta\sigma} & 0 \end{bmatrix},$$

$$\tilde{S} := \tilde{L}_{\sigma\sigma} - L_{\sigma\varphi}\tilde{L}_{\lambda\varphi}^{-1}L_{\lambda\sigma} - L_{\sigma\lambda}\tilde{L}_{\varphi\lambda}^{-1}L_{\varphi\sigma}.$$

The matrix M_2 is close to 0, if a good preconditioner for the stiffness matrix has been chosen. We solve the system (28) with

$$\Delta\psi^{\text{new}} = \Delta\psi^{\text{old}} + K^R M_1^{-1}(-\tilde{\xi}_p - \tilde{K}_p\Delta\psi^{\text{old}}). \tag{35}$$

We denote the defect by

$$d = -\tilde{\xi}_p - \tilde{K}_p\Delta\psi^{\text{old}}$$

and solve systems of the form

$$\delta = M_1^{-1}d, \qquad \text{i.e.,} \qquad M_1\delta = d.$$

Using the approximation (33) in (34), we obtain

$$\begin{bmatrix} 0 & \tilde{L}_{\varphi\lambda} & 0 & 0 \\ \tilde{L}_{\lambda\varphi} & 0 & 0 & 0 \\ L_{\sigma\varphi} & L_{\sigma\lambda} & \tilde{S} & L_{\sigma\eta} \\ 0 & 0 & L_{\eta\sigma} & 0 \end{bmatrix} \begin{bmatrix} \delta_\varphi \\ \delta_\lambda \\ \delta_\sigma \\ \delta_\eta \end{bmatrix} = \begin{bmatrix} d_\varphi \\ d_\lambda \\ d_\sigma \\ d_\eta \end{bmatrix}.$$

After finding

$$\delta_\lambda = +\tilde{L}_{\varphi\lambda}^{-1} d_\varphi, \qquad \delta_\varphi = +\tilde{L}_{\lambda\varphi}^{-1} d_\lambda,$$

we have to solve the following problem:

$$\begin{bmatrix} \tilde{S} & L_{\sigma\eta} \\ L_{\eta\sigma} & 0 \end{bmatrix} \begin{bmatrix} \delta_\sigma \\ \delta_\eta \end{bmatrix} = \begin{bmatrix} d_\sigma \\ d_\eta \end{bmatrix} - \begin{bmatrix} L_{\sigma\varphi} & L_{\sigma\lambda} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \delta_\varphi \\ \delta_\lambda \end{bmatrix}. \tag{36}$$

Note that $\tilde{S}$ is a symmetric and nonsingular matrix and that $L_{\sigma\eta}$ is a column vector. The global matrix in (36) is symmetric and indefinite. One can also take advantage of the LU decomposition of this matrix, namely,

$$\begin{bmatrix} \tilde{S} & L_{\sigma\eta} \\ L_{\eta\sigma} & 0 \end{bmatrix} = \begin{bmatrix} \tilde{S} & 0 \\ L_{\eta\sigma} & -L_{\eta\sigma}\tilde{S}^{-1}L_{\sigma\eta} \end{bmatrix} \begin{bmatrix} I & \tilde{S}^{-1}L_{\sigma\eta} \\ 0 & I \end{bmatrix}. \tag{37}$$

In this case, solving systems with (37) requires two actions of $\tilde{S}^{-1}$.

Compute now $K^R\delta$ and find the increments from (35) as follows:

$$\Delta\sigma^{\text{new}} = \Delta\sigma^{\text{old}} + \delta_\sigma, \tag{38a}$$

$$\Delta\eta^{\text{new}} = \Delta\eta^{\text{old}} + \delta_\eta, \tag{38b}$$

$$\Delta\varphi^{\text{new}} = \Delta\varphi^{\text{old}} + \delta_\varphi - \tilde{L}_{\lambda\varphi}^{-1} L_{\lambda\sigma}\delta_\sigma, \tag{38c}$$

$$\Delta\lambda^{\text{new}} = \Delta\lambda^{\text{old}} + \delta_\lambda - \tilde{L}_{\varphi\lambda}^{-1} L_{\varphi\sigma}\delta_\sigma. \tag{38d}$$

We apply the algorithm above (with a fixed number of iterations) to find the increments of the primal and dual variables $\Delta\varphi$, $\Delta\sigma$, $\Delta\lambda$, $\Delta\eta$ and then use (27) to find the global search direction $\Delta\Phi$.

5. Choice of Merit Function, Steplength, and Barrier Parameter. Watchdog Technique

In this section, we explain how to apply the Newton method to solve the nonlinear Eq. (23), i.e.,

$$F_p(\Phi) = 0.$$

This problem comes from the KKT conditions, which are necessary optimality conditions, so that the minimization problem (13) and the nonlinear problem (23) are not equivalent. The Newton method may find solutions of (23) that are not minimizers of the objective function f. These extraneous solutions may correspond to maximizers or saddle points of f. Therefore, the ideal variant $\Phi \leftarrow \Phi + \Delta\Phi$ may not always happen, so that various modifications to the basic Newton method have to be implemented to avoid convergence to such extraneous solutions.

Two versions of the Newton method are possible, namely, trust-region and line-search methods. Our method uses a variation of the line-search approach; i.e., after computation of the search direction $\Delta\Phi$, we try to choose a positive scalar α to update the solution $\Phi \leftarrow \Phi + \alpha\Delta\Phi$ measuring the progress in minimization at each iteration.

Several different ideas have been suggested recently to define a merit function, to control the barrier parameter p, to select the steplength α, and to choose an appropriate convergence criterion; see e.g. Refs. 3, 9, 11, 18. We follow mainly the strategy proposed in Ref. 11, where two merit functions have been considered. Our purpose is to find simultaneously solutions of the minimization subproblem (19)–(20) and the nonlinear primal-dual equation (23).

To simplify the notation, we denote the primal variables by

$$x = (\varphi, \sigma),$$

the dual variables by

$$y = (\lambda, \eta),$$

and the complementarity variables by

$$v = (z, w).$$

Let the equality and inequality constraints be

$$c_1(x) = c_1(\varphi, \sigma) = A(\sigma)\varphi - b, \tag{39a}$$

$$c_2(x) = c_2(\sigma) = g(\sigma) - C, \tag{39b}$$

$$d_1(x) = d_1(\sigma) = \sigma - \sigma_{\min} e, \tag{39c}$$

$$d_2(x) = d_2(\sigma) = \sigma_{\max} e - \sigma. \tag{39d}$$

Our primary merit function is based on the logarithmic barrier function and the augmented Lagrangian term, concerning only the equality constraints,

$$\begin{aligned} M &:= M(x, y, p, p_A) \\ &= f(x) - p \sum_{i=1}^{2} \log d_i(x) + y^T c(x) + (1/2)\, p_A\, c(x)^T c(x), \end{aligned} \tag{40}$$

where

$$c(x) = (c_1(x), c_2(x)).$$

The parameter p_A is a fixed positive scalar, which can be changed during the iteration in the case when

$$\Delta x = (\Delta\varphi, \Delta\sigma)$$

is not a descent direction for the primary merit function. It is easy to show that Δx can be guaranteed to be a descent direction for M; i.e.,

$$\Delta x^T \nabla_x M < 0,$$

if p_A is sufficiently large. The gradient of M with respect to x is

$$\begin{aligned}\nabla_x M &:= \nabla_x M(x, y, p, p_A) \\ &= \nabla f(x) - pJ_{\text{in}}^T D^{-1} e + J_{\text{eq}}^T y + p_A J_{\text{eq}}^T c(x),\end{aligned} \tag{41}$$

where

$$J_{\text{eq}} = \begin{bmatrix} L_{\lambda\varphi} & L_{\lambda\sigma} \\ 0 & L_{\eta\sigma} \end{bmatrix}, \qquad J_{\text{in}} = \begin{bmatrix} 0 & I \\ 0 & -I \end{bmatrix},$$

and J_{eq} and J_{in} are the Jacobian matrices corresponding to the equality and inequality constraints, respectively. The nonzero entries are given by (26). Then, we have

$$\begin{aligned}\Delta x^T \nabla_x M &= \Delta x^T (\nabla f - pJ_{\text{in}}^T D^{-1} e) + \Delta x^T J_{\text{eq}}^T y + p_A \Delta x^T J_{\text{eq}}^T c(x) \\ &= \Delta x^T (\nabla f - pJ_{\text{in}}^T D^{-1} e) - c(x)^T y - p_A c(x)^T c(x),\end{aligned} \tag{42}$$

taking into account that

$$J_{\text{eq}} \Delta x = -c(x),$$

which is equivalent to the third and fourth rows of the system (25). Hence,

$$\Delta x^T \nabla_x M < 0,$$

if

$$p_A > [\Delta x^T (\nabla f - pJ_{\text{in}}^T D^{-1} e) - c(x)^T y] / c(x)^T c(x).$$

Since p_A can become unacceptably large as $\|c\|$ is small, in our practical implementation we choose

$$p_A = \min \{(5/c^T c)[\Delta x^T (\nabla f - pJ_{\text{in}}^T D^{-1} e) - c(x)^T y], 100\} \tag{43}$$

only in the case when

$$\Delta x^T \nabla_x M \geq 0.$$

If Δx is a descent direction for M, then p_A does not change and its value is stored as chosen at each iteration.

Our secondary merit function used for the line-search procedure is the l_2-norm of the residual, given by (23). The stopping criterion $\|F_p\| < \mathsf{tol}$ for a given tolerance is considered in recent studies; see e.g. Refs. 3 and 9. Similarly to the implementation done in Gay, Overton, and Wright (Ref. 11), we apply the watchdog technique, originally proposed by Chamberlain, Lemaréchal, Pedersen, and Powell (Ref. 25). The main idea is to allow some iterations to choose steplengths that are much larger than those that would be allowed normally. More precisely, for an a priori given integer positive parameter watchdog, we allow the primary merit function not to decrease. However, if after watchdog iterations the primary merit function has not been decreased, the watchdog barks, and the algorithm ensures the progress of M with a parameter p_A, as chosen in (43).

We comment now on the choice of steplengths, so that all the iterates satisfy

$$d_1(x) > 0, \qquad d_2(x) > 0, \qquad z > 0, \qquad w > 0,$$

and the updated solution lies inside the feasible region. In El-Bakry, Tapia, Tsuchiya, and Zhang (Ref. 9), the flexibility of choosing different steplengths for the various components of the solution is allowed. We consider only two separate parameters serving as steplengths for the primal variables and the complementarity conditions. For $y = (\lambda, \eta)$ and $v = (z, w)$, we use equal steplengths.

Let $\hat{\alpha}_\sigma$, $\hat{\gamma}_z$, $\hat{\gamma}_w$ be defined as

$$\hat{\alpha}_\sigma = \max\{\alpha | \sigma_{\min} e \leq \sigma + \alpha \Delta\sigma \leq \sigma_{\max} e\}, \tag{44a}$$

$$\hat{\gamma}_z = \max\{\gamma | z + \gamma \Delta z \geq 0\}, \tag{44b}$$

$$\hat{\gamma}_w = \max\{\gamma | w + \gamma \Delta w \geq 0\}. \tag{44c}$$

More precisely, we find that

$$\hat{\alpha}_\sigma = \min[\min_{\Delta\sigma_i > 0} (\sigma_{\max} - \sigma_i)/\Delta\sigma_i, \min_{\Delta\sigma_i < 0} (\sigma_{\min} - \sigma_i)/\Delta\sigma_i, 1], \qquad 1 \leq i \leq N,$$

$$\hat{\gamma}_z = -1/\min(Z^{-1}\Delta z, -1),$$

$$\hat{\gamma}_w = -1/\min(W^{-1}\Delta w, -1),$$

and we define

$$\hat{\alpha} = \hat{\alpha}_\sigma, \qquad \hat{\gamma} = \min(\hat{\gamma}_z, \hat{\gamma}_w).$$

To ensure strict feasibility, we choose a positive parameter $\tau < 1$ and define the steplengths as follows:

$$\alpha = \min(1, \tau\hat{\alpha}), \qquad \gamma = \min(1, \tau\hat{\gamma}). \tag{45}$$

Some authors consider values for τ very close to unity, for example

$$\tau = 0.99, \quad \text{or} \quad \tau = 0.999, \quad \text{or} \quad \tau = 0.9995.$$

Our choice of τ allows at each iteration a dependence on p, i.e.,

$$\tau = 1 - \min(0.01, 100p^2). \tag{46}$$

Now, we describe briefly the pseudo-code primal-dual algorithm from Gay, Overton, and Wright (Ref. 11), adding some modifications. During a given iteration, we do not require that the primary and the secondary merit functions decrease simultaneously. First, we test if the primary merit function decreases. If so, the trial steplength is accepted and a damping of the form $\alpha \leftarrow \alpha/2$; $\gamma \leftarrow \gamma/2$ is not necessary. If the primary merit function does not decrease, we check the secondary merit function. If the latter has decreased, the steplength is successful, except when watchdog iterations have occurred without a reduction in the primary merit function. Our numerical experiments show that, in almost all the tests, the watchdog does not bark, but the watchdog technique is applied to improve the reliability of the primal-dual algorithm.

Note that a descent in the primary merit function is sought only with respect to x, taking into account the original optimization problem. If the iteration is successful, x and v retain their final values, and the Lagrange multipliers for the equality constraints y are defined as the least-squares solution of

$$y = \min\|\nabla f(x) + J_{\text{eq}}^T y - J_{\text{in}}^T v\|. \tag{47}$$

Let integers itmax and lsmax are a priori given limits on the global number of iterations and the line search loop, respectively. The value tol is a given tolerance, taking part in the stopping criterion.

Algorithm PD.

Step 1. Let x be an initial primal variable satisfying $d_1(x) > 0$ and $d_2(x) > 0$. Initialize $p = 1, p_A = 10$, and set $y = 0$, $z = p/d_1$, $w = p/d_2$, iter $= 0$, watch $= 0$, lsteps $= 0$. For iter $= 0, 1, \ldots,$ do, the following steps.

Step 2. Test for convergence. Choose the following stopping criterion:

$$\|F_p(x, y, v)\| < \text{tol}, \quad \text{or} \quad p < \text{tol}^2, \quad \text{or} \quad \text{iter} > \text{itmax}, \quad \text{or} \quad \text{lsteps} > \text{lsmax}.$$

Step 3. Compute Δx and Δy from (38), $\Delta v = (\Delta z, \Delta w)$ from (27), and find the parameters α and γ from (45).

Step 4. If $\Delta x^T \nabla_x M(x, y, p, p_A) > 0$ [see (42)], update p_A by (43).

Step 5. Set $\mathsf{lsteps} = 0$.

Step 6. If $\mathsf{watch} = \mathsf{watchmax}$, restore $x, y, v, \Delta x, \Delta y, \Delta v, \alpha, \gamma, p_A$, and lsteps from saved. Set $\mathsf{watch} = \mathsf{watch} + 1$, $\alpha = \alpha/2$, $\gamma = \gamma/2$.

Step 7. If $\mathsf{lsteps} > \mathsf{lsmax}$, go to Step 12.

Step 8. If $M(x + \alpha\Delta x, y, p, p_A) < M(x, y, p, p_A)$, set $\mathsf{watch} = 0$. Go to Step 12.

Step 9. If $\mathsf{watch} < \mathsf{watchmax}$ and

$$\|F_p(x + \alpha\Delta x, y + \gamma\Delta y, v + \gamma\Delta v)\| < \|F_p(x, y, v)\|,$$

check the relation $\mathsf{watch} = 0$. If the latter is satisfied, set $\mathsf{Msave} = M(x, y, p, p_A)$ and save $x, y, v, \Delta x, \Delta y, \Delta v, \alpha, \gamma, p_A$, and lsteps as saved. Otherwise, set $\mathsf{watch} = \mathsf{watch} + 1$. Go to Step 12.

Step 10. Choose new steplengths $\alpha = \alpha/2$ and $\gamma = \gamma/2$.

Step 11. Set $\mathsf{lsteps} = \mathsf{lsteps} + 1$.

Step 12. If $\mathsf{watch} > 0$ and $M(x + \alpha\Delta x, y, p, p_A) < \mathsf{Msave}$, set $\mathsf{watch} = 0$.

Step 13. Find new iterates $x = x + \alpha\Delta x$, $v = v + \gamma\Delta v$ and define y from (47).

Step 14. Update p by either procedure ETTZ or GOW (see below) and set $\mathsf{iter} = \mathsf{iter} + 1$. Go to Step 2.

Note that the $\mathsf{restore}$ operation from Step 6 of Algorithm PD cannot take place before the save operation in the inner loop on lsteps (see Steps 7–11). We consider two different ways to decrease the barrier parameter p, namely, procedures ETTZ and GOW in accordance with Refs. 9 and 11, respectively.

Procedure ETTZ. We consider $\zeta = \min(0.2, 100\, d^T v)$ and choose a barrier parameter $p = \min(p, \zeta(d^T v)/(2N))$, where N is the number of finite elements in the discrete model.

Procedure GOW. The parameter p is allowed to remain constant for no more than 10 iterations. Otherwise, at each iteration, p decreases by a certain amount. For more details, see Ref. 11.

6. Numerical Experiments

In this section, we give some details concerning our computations. We solve the optimization problem (13)–(14b) with an objective function

defined in (5). The first equality constraint is related to solving the elliptic differential equation for the electric potential φ; see (3)–(4). We allow here some modification in the conductivity; namely, we consider

$$\operatorname{div}(h(\sigma)\operatorname{grad}\varphi) = 0, \qquad \text{in } \Omega, \tag{48a}$$

$$n \cdot h(\sigma)\operatorname{grad}\varphi = \begin{cases} I_\nu, & \text{on } \Gamma_\nu \subset \partial\Omega, \\ 0, & \text{elsewhere,} \end{cases} \tag{48b}$$

where

$$h(\sigma) = [(\sigma - \sigma_{\min} + \epsilon)/(\sigma_{\max} - \sigma_{\min})]^m, \qquad 0 < \epsilon \ll 1, \tag{49}$$

with $m = 1, 2$, is treated as a conductivity. The computations were done for $\epsilon = 0.01$. Neumann boundary conditions were imposed, assuming the compatibility relation for the currents (see Section 2) on the boundary Γ_ν, $\nu = 1, \ldots, N_c$, where N_c is the number of contacts.

The computations have been carried through a rectangular domain Ω decomposed into N uniform quadrilateral finite elements. We suppose that the domain is an isotropic conductor. The rotated bilinear basis functions, proposed by Rannacher and Turek (Ref. 26), were used to construct the finite element space. The reason is that this discretization fits well with the curl-conforming edge element discretization of equation (5) for the magnetic vector potential, since in both cases the degrees of freedom are associated with the edges of the elements. In the case of rotated bilinears, for a given grid node i, $i = 1, 2, 3, 4$, the corresponding basis function

$$\{\phi_i\} \in \operatorname{span}\{1, x_1, x_2, x_1^2 - x_2^2\}$$

has a value one, vanishing on the remaining midpoints. A quadrature rule (exact for polynomials of degree three) was used to assemble the stiffness matrix. The conductivity $\sigma = (\sigma_i)_{i=1}^N$ was computed at the center points of the finite elements. Note that the diagonal matrix $L\sigma\sigma$ from (18b) is equal to zero when $m = 1$ in (49), whereas it does not vanish in the case $m = 2$.

Our primal-dual code is written in *C++* using double precision binary arithmetic. All numerical tests were run on Alpha PC164LX machine. We choose lower and upper limits for the conductivity $\sigma_{\min} = 0.01$ and $\sigma_{\max} = 1$, respectively. In all runs, an initial homogeneous distribution was proposed with $\sigma = 0.45$. The constant C in (12b) is computed in accordance with this initialization.

We apply the primal-dual Algorithm PD described in Section 5 with $\mathsf{itmax} = 200$, $\mathsf{lsmax} = 15$, $\mathsf{watchmax} = 4$, and $\mathsf{tol} = 10^{-8}$. The ETTZ procedure from Section 5 was used to define the barrier parameter p at each iteration. Tests with the GOW strategy show a similar behavior of the convergence. Both approaches may fail when p is made too small. To avoid

this difficulty, the stopping criterion in Algorithm PD includes $p < \mathrm{tol}^2$, and the parameter τ from (46) was redefined as $\tau = 0.99999$ in the case $\tau > 1 - 10^{-8}$.

The most time-consuming part of the algorithm during a given iteration is to solve the condensed primal-dual system finding the increments. Two transforming iterations were used in (35) with an initial $\Delta\psi^{\mathrm{old}} = 0$. Various iterative techniques for solving systems with symmetric and indefinite matrices of the type (36) can be implemented. We have applied the MINRES method first developed by Paige and Saunders (Ref. 27); see also Rusten and Winther (Ref. 23). The method generates at the kth iteration a new solution such that the corresponding l_2 residual norm decreases at each step. An appropriate preconditioner can be used to accelerate the rate of convergence. Note that we can also use the LU decomposition (37) and solve systems with $\tilde{S}$ twice. This variant turned out to be more expensive than the application of MINRES to the global system (36). We used a few (for example, 20) iterations as a stopping criterion in the MINRES method.

The preconditioned conjugate gradient (PCG) method was applied to solve systems with the stiffness matrix. Our stopping criterion was

$$\|r_k\|_{B^{-1}} \leq 10^{-6} \|r_0\|_{B^{-1}},$$

where r_0 and r_k are the initial and kth residuals, respectively. As a preconditioner B in the PCG method, we used the symmetric successive overrelaxation (SSOR) iteration with a relaxation parameter $\omega = 1.5$. All iterative procedures in our computations started with a zero initial guess.

The results from our numerical experiments for various numbers of contacts N_c and various number of grid points on the coordinate axes Ox and Oy, denoted by N_x and N_y, respectively, are reported in Table 1 when

Table 1. Results from applications of Algorithm PD, $m = 1$.

N_c	N_x	N_y	Iter	p	M	$\|F_p\|_2$	$\|v\|_2$
2	25	25	17	4.92E–17	4.69	9.64E–4	E–9
2	30	40	19	1.97E–17	4.47	3.49E–5	E–9
4	30	40	17	2.59E–17	26.01	6.70E–5	E–9
2	50	50	19	1.28E–18	5.10	2.99E–4	E–10
3	50	50	30	6.44E–19	3.78	2.40E–4	E–11
5	50	50	20	4.57E–17	86.08	9.52E–4	E–9
6	50	50	20	9.85E–17	85.99	1.27E–3	E–9
2	60	80	38	7.76E–17	4.79	5.62E–5	E–9
3	60	80	89	7.79E–17	3.43	4.34E–3	E–9
5	60	80	20	1.81E–17	78.58	3.59E–4	E–9
3	100	100	84	3.68E–17	4.05	3.35E–4	E–9
6	100	120	24	3.46E–17	84.30	7.62E–4	E–9

Table 2. Results from applications of Algorithm PD, $m = 2$.

N_c	N_x	N_y	Iter	p	M	$\|\|F_p\|\|_2$	$\|\|v\|\|_2$
2	25	25	19	4.29E–18	4.83	2.85E–5	E–9
2	30	40	44	1.22E–9	4.55	2.63E–2	E–6
4	30	40	26	8.36E–18	26.41	3.10E–5	E–10
2	50	50	90	1.18E–9	5.23	5.70E–3	E–6
3	50	50	75	1.07E–6	4.33	9.67E–3	E–4
5	50	50	57	1.10E–7	90.68	9.21E–2	E–5
6	50	50	45	9.64E–7	97.46	1.61E–2	E–4
2	60	80	29	1.35E–7	5.06	6.18E–3	E–5
3	60	80	59	2.66E–9	3.49	1.10E–2	E–6
5	60	80	64	1.22E–14	80.30	5.18E–2	E–8
3	100	100	24	1.78E–7	4.20	9.69E–3	E–5
6	100	120	43	4.18E–7	89.12	1.64E–2	E–5

$m = 1$ and in Table 2 when $m = 2$. The number of finite elements $N = N_x N_y$ and the dimension of the stiffness matrix (i.e., the number of grid points where the approximated electric potential is computed) is equal to $N_y(2N_x + 1) + N_x$. We report as well the global number of iterations in the main optimization loop (denoted by iter), the last value of the barrier parameter p, the final value of the primary merit function, the norm of the residual $\|F_p\|$ as a secondary merit function, and the l_2-norm $\|v\|_2$ related to the complementarity conditions at the last iteration. In all the experiments, the number of times with active watchdog mechanism, i.e., when the step was accepted without a reduction of the primary merit function, was zero.

The numerical simulation provides a material distribution that can be visualized by gray scales ranging from black ($\sigma = \sigma_{\max}$) to white ($\sigma = \sigma_{\min}$) and by corresponding height profiles. Figures 1 and 2 display the material distribution (50×50 mesh, 2 contacts) for $m = 1$ and $m = 2$, respectively.

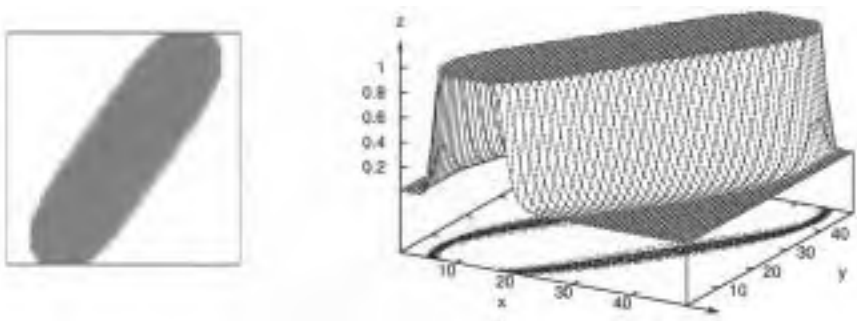

Fig. 1. Material distribution, 50×50 mesh, 2 contacts, $m = 1$.

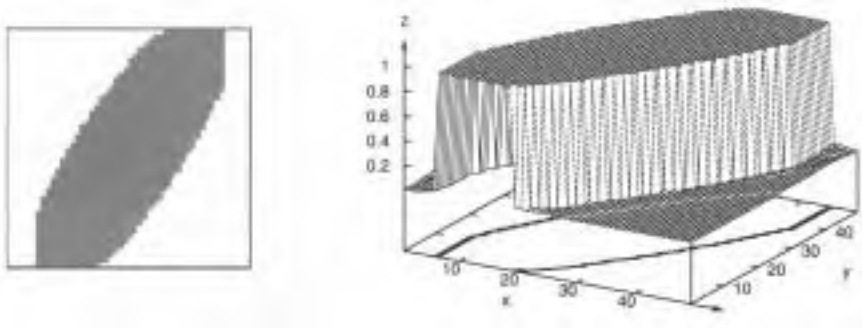

Fig. 2. Material distribution, 50×50 mesh, 2 contacts, $m = 2$.

Obviously, the observed resolution of the interface "material–no material" is sharper in the case $m = 2$. Hence, comparing both figures, one can notice easily the effect of using a higher penalty parameter $m > 1$ in the expression (49) for the modified conductivity. Figures 3–5 illustrate the corresponding material distribution (50×50 mesh, $m = 1$) for 3, 5, 6 contacts, respectively. On the axis Oz of the height profiles, one can see the resulted values of the conductivity running from $\sigma_{\min}$ up to $\sigma_{\max}$. The convergence of the solutions of the discretized problems to the solution of the infinite-dimensional optimization problem, resulting from grid refinement, is demonstrated in Figs. 5–6 where the latter shows the material distribution for a refined mesh (100×100, 6 contacts, $m = 1$) taking twice more grid points in each direction. In some experiments for $m = 2$, we reach a small decrease in the secondary merit function. However, $\|v\|_2$ was of small order and the visualized final optimal design appeared to be reasonable.

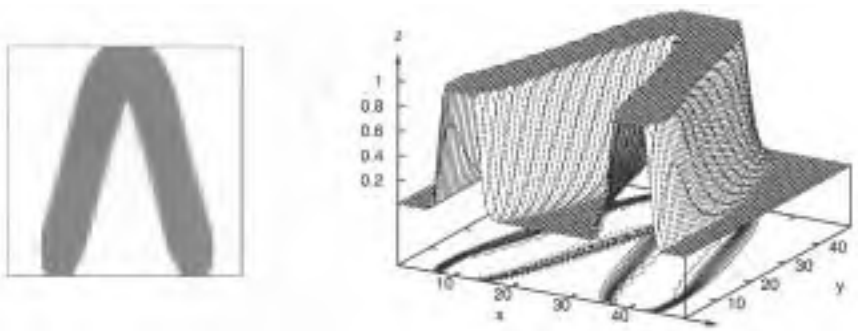

Fig. 3. Material distribution, 50×50 mesh, 3 contacts, $m = 1$.

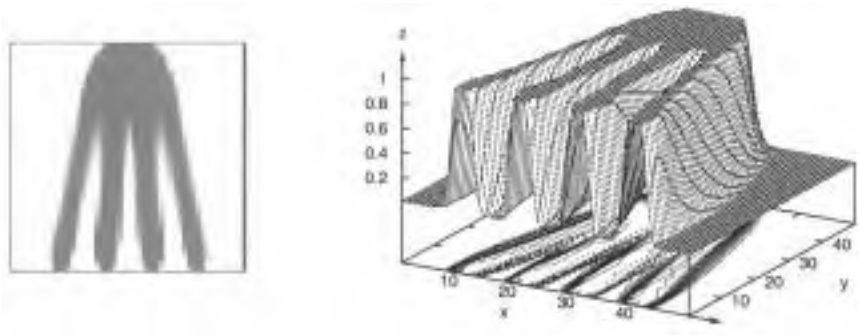

Fig. 4. Material distribution, 50×50 mesh, 5 contacts, $m = 1$.

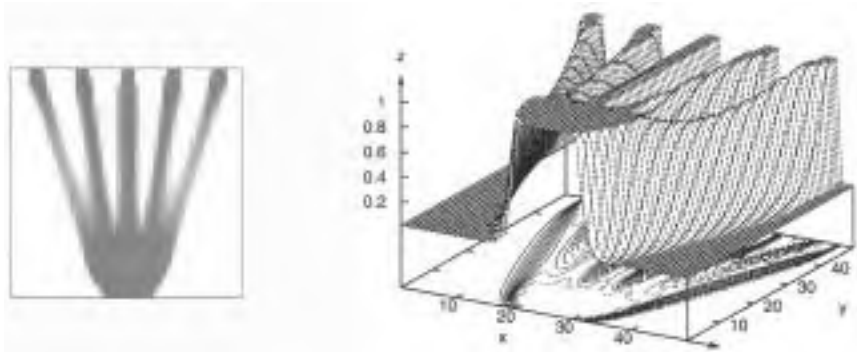

Fig. 5. Material distribution, 50×50 mesh, 6 contacts, $m = 1$.

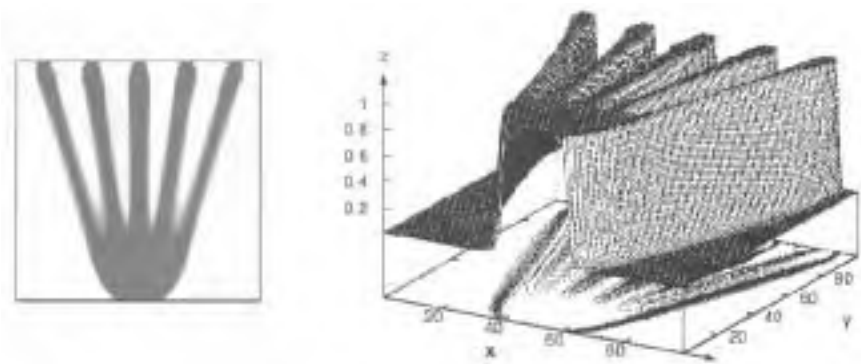

Fig. 6. Material distribution, 100×100 mesh, 6 contacts, $m = 1$.

7. Conclusions

Summarizing, we have considered problems concerning topology optimization in a conductive electromagnetic system described by the Maxwell equations which have not been studied in the literature before. The aim of our work has been to find an optimal distribution of the conductivity in a two-dimensional model with a fixed shape. Since widely used structural topology optimization algorithms are tailored to the underlying elasticity equation, a novel algorithmic approach had to be developed. We have used a primal-dual Newton interior-point method featuring simultaneous sequential quadratic programming with a hierarchy of merit functions and a watchdog strategy for convergence monitoring. The performance of the approach has been documented by several numerical results displaying both the optimal material distribution as well as the convergence history.

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