Journal of Mathematical Sciences 2 (2015) 1-11 **Betty Jones & Sisters Publishing**

On Solving the Condensed KKT System with Application to Design Optimization

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Abstract: We consider a general nonlinear optimization problem subject to equality and inequality constraints. Suppose that the first and second derivatives of the objective and constraint functions are available. The optimization problem is solved by the Lagrange multiplier approach and the interior-point method. The inequality constraints are introduced as logarithmic terms in a family of optimization problems depending on a positive barrier parameter that asymptotically goes to zero. Applying the Karush-Kuhn-Tucker (KKT) first-order necessary optimality conditions we are faced with a nonlinear equation for which the Newton method is used. The resulting primal-dual system of linear equations can be symmetrized and transformed into a problem of smaller dimension. The condensed KKT matrix is symmetric but indefinite and increasingly ill-conditioned as the optimization proceeds. To find an optimal solution satisfying the perturbed optimality conditions we apply an iterative solver based on the null space approach in conjunction with suitable preconditioners. For the stepsize selection we use an augmented Lagrangian merit function. The method is illustrated on a PDE-constrained shape optimization problem with box constraints for the design parameters.

Key words: Nonlinear programming, constraint functions, interior-point method, condensed KKT system, preconditioning, design optimization.

1. Introduction

Many areas of the sciences and engineering, especially applications in structural design, lead to optimization problems with constraints which require the solution of partial differential equations (PDEs). The solution of such PDEs-constrained optimization problem is a major computational task. It needs proper discretization techniques, reliable iterative procedures and variety of merit functions to insure a convergence of the optimization algorithms. In the last two decades, a great deal of interest has been devoted to the development of interior-point (IP) approach for large scale nonlinear programming [1, 2, 3, 4, 5]. The IP (also called barrier) methods define a sequence of Karush-Kuhn-Tucker (KKT) equations in so-called saddle point form. By using the Newton method, we get a linear system which can be symmetrized and transformed into a problem of smaller dimension. The resulting condensed KKT matrix is symmetric (but indefinite) and increasingly ill-conditioned as the optimization proceeds. Various iterative procedures for the solution of the condensed KKT system have been recently proposed [6, 7, 8]. For the numerical solution of saddle point systems arising in a wide variety of technical and scientific applications we refer the reader to [9].

The aim of this paper is to discuss the effectiveness of a kind of null-space iterative algorithm for solving the condensed KKT system which arises in a PDE-constrained optimization problem with application to structural design. Section 2 presents the

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design optimization task. Right-transforming iterations method is studied in Section 3. In Section 4, two types of merit functions for convergence of the algorithm are discussed. To update the iterates, the line-search approach is applied. Some numerical results are given in the last Section.

We consider first a nonlinear programming problem in a general setting of the form

$$\min_{x \in R^n} f(x) \quad , \tag{1}$$

subject to

$$h(x) = 0\,, \qquad g(x) \geq 0\,, \tag{2}$$

where $f : R^n \to R, h : R^n \to R^\ell, \ell < n$, and $g : R^n \to R^m$. Assume that the objective and constraint functions are smooth, nonlinear, and not necessarily convex. Denote the *feasible set* by $F := \{x \in R^n \mid h(x) = 0, g(x) \geq 0\}$ and by $A(x) := \{1 \leq j \leq m \mid g_j(x) = 0\}$ the so-called *active set*, i.e., the set of indices for which the inequalities become equalities in point $x \in F$. Consider the set

$$G(x) := \bigcup_{j=1}^{\ell} \{\nabla_x h_j(x)\} \cup \bigcup_{j \in A(x)} \{\nabla_x g_j(x)\} \quad , \tag{3}$$

referred to as the set of gradients of the equality constraints and the active inequality constraints. The introduction of Lagrange multipliers $y \in R^\ell$ and $z \in R_+^m := [0, \infty)^m$ to the constraints (2) leads to the saddle point problem

$$\min_{x \in R^n} \quad \max_{y \in R^l, z \in R_+^m} L(x, y, z) \tag{4}$$

for the Lagrangian

$$L(x, y, z) := f(x) + y^T h(x) - z^T g(x) \tag{5}$$

The first-order KKT conditions are given by

$$\nabla_x L(x, y, z) = \nabla_x f(x) + \nabla_x h(x) y - \nabla_x g(x) z = 0 \tag{6}$$

$$h(x) = 0 \tag{7}$$

$$g(x) \geq 0, z \geq 0, z_j g_j(x) = 0, \quad 1 \leq j \leq m\,. \tag{8}$$

For a feasible point $x \in F$ a strict complementarity holds true if $z_j > 0$ for $j \in A(x)$. Furthermore, consider the Hessian of the Lagrangian

$$\nabla_x^2 L := \nabla_x^2 L(x, y, z) = \nabla_x^2 f(x) + \nabla_x^2 h(x) y - \nabla_x^2 g(x) z. \tag{9}$$

Denote by $J(x)$ the Jacobian of all constraints that are equal to zero at $x \in R^n$ and by $N_J = N_J(x)$ a basis of the kernel of $J(x)$. Then, the second-order KKT condition requires a positive definiteness of the reduced Hessian (9) on the kernel of $J(x)$, i.e., $w^T \nabla_x^2 L w > 0$ for $w \in N_J(x)$. For more details we refer to [10].

We use further the idea of the interior-point approach by transforming the original optimization problem to a sequence of problems with logarithmic barrier functions, depending on a positive barrier parameter ρ which asymptotically goes to zero. Under some additional restrictions, the theoretical result for the existence and uniqueness of a local minimizer for (1)-(2) when $\rho \to 0$ can be found in [10]. As a function of ρ, the set of all solutions $x(\rho)$ defines a continuously differentiable path known as *barrier trajectory*. The family of equality constrained sub-problems has the form

$$\min_{x \in R^n} \beta^{(\rho)}(x) := \min_{x \in R^n} \left(f(x) - \rho \sum_{j=1}^{m} \log g_j(x) \right),$$

subject to $h(x) = 0$. (10)

We denote the Lagrangian of (10) by $L^{(\rho)}(x,y) := \beta^{(\rho)}(x) + y^T h(x)$ and obtain the following saddle point problem:

$$\min_{x \in R^n} \max_{y \in R^\ell} L^{(\rho)}(x,y).$$

Then the first-order KKT conditions read

$$\begin{pmatrix} \nabla_x L^{(\rho)}(x,y) \\ \nabla_y L^{(\rho)}(x,y) \end{pmatrix} = \begin{pmatrix} \nabla f(x) + \nabla h(x) y - \sum_{j=1}^{m} \frac{\rho}{g_j(x)} \nabla g_j(x) \\ h(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (11)$$

By using perturbed complementarity variables $z_j = z_j^{(\rho)} := \frac{\rho}{g_j\left(x^{(\rho)}\right)}, 1 \le j \le m$, we get from (11) the following equations:

$$F^{(\rho)}(x,y,z) := \nabla L^{(\rho)}(x,y,z) = \begin{pmatrix} \nabla f(x) + J_E^T y - J_I^T z \\ h(x) \\ Dg(x) z - \rho e \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (12)$$

where J_E and J_I are the $\ell \times n$ and $m \times n$ Jacobians with respect to the equality and inequality constraints (2), $D_g := diag(g_j(x))_{j=1}^m$ is a diagonal matrix, and $e := (1,...,1)^T \in R^m$ is the vector of all ones. Note that $J_E^T = \nabla h(x)$ and $J_I^T = \nabla g(x)$

Thus, the first component of $\nabla L^{(\rho)}$ can be written as

$$\nabla x L^{(\rho)}(x,y,z) := \nabla f(x) + \nabla h(x) y - \nabla g(x) z. \quad (13)$$

The nonlinear system (12) is solved by Newton's method. Denoting the solution vector by $\varphi = (x,y,z)^T$ and the increments by $\Delta\varphi = (x,y,z)^T$, we achieve the so-called *primal-dual system*

$$K \Delta\varphi = -F^{(p)}(\varphi) \quad (14)$$

with the *primal-dual matrix*

$$K = \begin{pmatrix} \nabla_x^2 L^{(\rho)} & J_E^T & -J_I^T \\ J_E & 0 & 0 \\ J_I & 0 & D_z^{-1} D_g \end{pmatrix}, \quad (15)$$

where $D_z := diag(z_j(x))_{j=1}^m$ is a diagonal matrix. Taking into account that D_g is diagonal and invertible, we eliminate Δz to obtain the so-called *condensed primal-dual system*

$$\tilde{K} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = -\begin{pmatrix} \nabla f(x) + J_E^T y - \rho J_I^T D_g^{-1} e \\ h(x) \end{pmatrix}, \quad (16)$$

$$\tilde{K} = \begin{pmatrix} \tilde{\nabla}_x^2 L^{(\rho)} & J_E^T \\ J_E & 0 \end{pmatrix}$$

with $n \times n$ matrix $\tilde{\nabla}_x^2 L^{(\rho)} := \nabla_x^2 L^{(\rho)} + J_I^T D_g^{-1} D_z J_I$, called the condensed primal-dual Hessian. Note that J_E is a real $l \times n$ matrix of full rank l ($l < n$) and $\tilde{\nabla}_x^2 L^{(\rho)}$ is symmetric and positive definite on the kernel of J_E.

The condensed primal-dual saddle point system (16) is symmetric, indefinite, and ill-conditioned with some diagonal elements becoming unbounded as $\rho \to 0$.

It was shown in [2] that this poor conditioning is benign in the sense that by using certain indefinite factorization of the primal-dual system, the solution can be well determined.

2. Design Optimization

In this section, we consider the problem of optimal structural design of novel micro-structural biomorphic Silicon Carbide (SiC) ceramic materials described in details in [11]. We compute the optimal material distribution in a given domain $\Omega \subset R^d, d = 2,3$ where a surface traction **t** is applied to a part of the boundary $\Gamma_T \subset \partial\Omega$ and given displacements q are specified on the remaining portion $\Gamma_D (\Gamma_D \cup \Gamma_T = \partial\Omega)$. A macroscopic scale model has been provided by the periodic homogenization theory [12]. Homogenization is possible if the macro- and microscales are well separated, i.e., we assume that the periodic cells in the macrostructures are infinitely many but infinitely small and periodically distributed throughout the medium. The unit microcell $Y = [0,1]^d$ consisting of an interior part treated as a weak material or void surrounded by a layer of SiC and an outer layer of carbon (C) serves in our application as a representative volume element (RVE). We suppose that in the microscale our design composite has a square (when d = 2) or cubic (when d = 3) hole located at the center of Y. For isotropic linear elastic constituents of the material in the microcell, the fourth-order homogenized elasticity tensor $E^H = \left(E^H_{ijkl}\right), i, j, k, l = 1,..., d,$ can be computed (see [12]) by

$$E^H_{ijkl} = \frac{1}{|Y|}\int_Y \left(E_{ijkl}(y) - E_{ijpq}(y)\frac{\partial \xi^{kl}_p}{\partial y_q}\right) dy, \quad (17)$$

where the Einstein convention of a summation on repeated indices is applied. Note that $E_{ijkl}(y)$ are piecewise constants in Y and the characteristic displacements $\left\{\xi^{kl}_p\right\} \in H^1(Y)$ are periodic functions in Y which satisfy the equations

$$\int_y \left(E_{ijpq}(y)\frac{\partial \xi^{kl}_p}{\partial y_q}\right)\frac{\partial \phi_i}{\partial y_j} dy = \int_y E_{ijkl}(y)\frac{\partial \phi_i}{\partial y_j} dy, \forall \phi \in V_Y . \quad (18)$$

Here, V_Y is the set of all admissible Y-periodic virtual displacement fields.

Denote by $J(\mathbf{u},\mu)$ the objective (cost) function which has to be minimized. The displacement vector $u = (u_1,...,u_d)^T$ represents the *state variables* and the vector $\mu = (\mu_1, \mu_2)^T$ stands for the *design parameters.*

In our practical application μ_1 and μ_2 are respectively the widths of the carbon and silicon carbide layers in the microstructure. The dependence of the homogenized elasticity tensor on these quantities has been determined by linear conforming discretization and multivariational splines. The choice of the objective is discussed in Section 4.

Our nonlinear constrained optimization problem has the form $J(u,\mu) = \inf_{v,\sigma} J(v,\sigma)$, subject to the following equality and inequality constraints

$$\sum_{i,j,k,l=1}^{d} \int_\Omega E^H_{ijkl}(x)\frac{\partial u_k}{\partial x_l}\frac{\partial \phi_i}{\partial x_j} dx = \int_\Omega f.\phi dx + \int_{\Gamma_T} t.\phi ds, \forall \phi \in V_0. \quad (19)$$

$$c(\mu) := \sum_{i=1}^{2} \mu_i = C, \mu_{\min} e \le \mu \le \mu_{\max} e \quad (20)$$

for given parameters $\mu_{\min} = 0, \mu_{\max} = 0.5$ and a given constant C. Note that (19) is the weak form of the homogenized equilibrium equation. Here,

$u \in V_D = \{v \in H^1(\Omega) \mid v = q \text{ on } \Gamma_D\}$ and

$V_0 = \{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_D\}$.

The state variables are discretized by conforming P1 elements with respect to a simplicial triangulation of Ω whereas the design variables are approximated by elementwise constants. The discrete analogs of the constraints (19)-(20) read as follows:

$$\begin{aligned} &A(\mu)u - b = 0, \quad \mu - \mu_{\min} e \geq 0, \\ &c(\mu) - C = 0, \quad \mu_{\max} e - \mu \geq 0, \end{aligned} \tag{21}$$

where $e = (1,1)^T$, $A(\mu)$ is the stiffness matrix corresponding to (19), and **b** is the discrete load vector. Note that $\mu_i = 0, i = 1,2$, corresponds to a complete void, $\mu_1 + \mu_2 = 0.5$ corresponds to a complete solid material, and $0 < \mu_1, \mu_2 < 0.5$ and $0 < \mu_1 + \mu_2 < 0.5$ to the porous composite with a hole centered in the microcell.

The discretized constrained minimization problem is solved by primal-dual interior-point method substituting the inequality constraints in (21) by logarithmic barrier functions. Assuming that $\mu > \mu_{\min} e$ and $\mu_{\max} e > \mu$ this substitution results in the following parameterized family of optimization subproblems

$$\beta^{(\rho)}(u,\mu) = \inf_{v,\sigma} \begin{bmatrix} J(v,\sigma) - \rho(\log(\sigma - \mu_{\min} e) \\ + \log(\mu_{\max} e - \sigma)) \end{bmatrix} \tag{22}$$

subject to the equality constraints

$$A(\mu)u - b = 0, c(\mu) - C = 0 \tag{23}$$

where $\rho > 0$ is a suitably chosen barrier parameter. Coupling the equality constraints by Lagrangian multipliers we have the following Lagrangian function associated with the problem (22)-(23)

$$\begin{aligned} L^{(\rho)}(u,\mu,\lambda,\eta) &:= J(u,\mu) - \rho(\log(\mu - \mu_{\min} e) \\ &+ \log(\mu_{\max} e - \mu)) \\ &+ \lambda^T (A(\mu)u - b) + \eta(c(\mu) - C). \end{aligned}$$

The first-order KKT conditions are given by

$$F^{(\rho)}(u,\mu,\lambda,\eta) = 0 \tag{24}$$

where $F^{(\rho)}(u,\mu,\lambda,\eta)$ reads componentwise as follows:

$$F_1^{(\rho)} := \nabla u L^{(\rho)} = \nabla u J + A(\mu)^T \lambda,$$

$$F_2^{(\rho)} := \nabla \mu L^{(\rho)} = \partial \mu(\lambda^T A(\mu)u + \eta \nabla c(\mu) - \rho D_1^{-1} e + \rho D_2^{-1} e),$$

$$F_3^{(\rho)} := \nabla_\lambda L^{(\rho)} = A(\mu)u - b,$$

$$F_4^{(\rho)} := \nabla_\eta L^{(\rho)} = c(\mu) - C$$

with

$$D_1 := diag(\mu_i - \mu_{\min}) \text{ and } D_2 := diag(\mu_{\max} - \mu_i),$$

i=1, 2. Since for $\rho \to 0$ the expressions $\rho D_1^{-1} e$ and $\rho D_2^{-1} e$ approximate the complementarity conditions associated with the inequalities in (21), we introduce $z := \rho D_1^{-1} e \geq 0$ and $w = \rho D_2^{-1} e \geq 0$ serving as perturbed complementarity variables. Then, the primal-dual Newton-type interior-point method is applied to three sets of variables: primal feasibility (u, μ), dual feasibility (λ, η), and perturbed complementarity related to (z, w).

Denote the Lagrangian function of our discrete optimization problem by

$$\begin{aligned} L(u,\mu,\lambda,\eta,z,w) &:= J(u,\mu) \\ &+ \lambda^T (A(\mu)u - b) + \eta(c(\mu) - C) \\ &- z^T (\mu - \mu_{\min} e) - w^T (\mu_{\max} e - \mu) \end{aligned} \tag{25}$$

The Newton method applied to the KKT conditions results in

$$\begin{pmatrix} 0 & L_{u\mu} & L_{u\lambda} & 0 & 0 & 0 \\ L_{\mu u} & L_{\mu\mu} & L_{\mu\lambda} & L_{\mu\eta} - I & I & \\ L_{\lambda u} & L_{\lambda\mu} & 0 & 0 & 0 & 0 \\ 0 & L_{\eta\mu} & 0 & 0 & 0 & 0 \\ 0 & Z & 0 & 0 & D_1 & 0 \\ 0 & -W & 0 & 0 & 0 & D_2 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta \mu \\ \Delta \lambda \\ \Delta \eta \\ \Delta z \\ \Delta w \end{pmatrix} = - \begin{pmatrix} \nabla u L \\ \nabla \mu L \\ \nabla \lambda L \\ \nabla \eta L \\ \nabla z L \\ \nabla w L \end{pmatrix}, \tag{26}$$

where I stands for the identity matrix, $Z = diag(z_i)$ and $W = diag(w_i), i = 1,2$ are diagonal matrices. The coefficient matrix (26) is the primal-dual system in our real-life application. It can be easily symmetrized since the matrices Z and W are diagonal. We do not use this approach here but instead perform a block elimination of the increments Δz and Δw yielding the condensed *primal-dual system*

$$\begin{pmatrix} 0 & L_{u\mu} & L_{u\lambda} & 0 \\ L_{\mu u} & \tilde{L}_{\mu\mu} & L_{\mu\lambda} & L_{\mu\eta} \\ L_{\lambda u} & L_{\lambda\mu} & 0 & 0 \\ 0 & L_{\eta\mu} & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta u \\ \Delta\mu \\ \Delta\lambda \\ \Delta\eta \end{pmatrix} = - \begin{pmatrix} \nabla_u L \\ \tilde{\nabla}_\mu L \\ \nabla_\lambda L \\ \nabla_\eta L \end{pmatrix}, \quad (27)$$

where $\tilde{L}_{\mu\mu} := L_{\mu\mu} + D_1^{-1} Z + D_2^{-1} W$ and the modified entry for the right-hand side is

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

Some preliminary results for solving the condensed primal-dual system by primal-dual interior-point method using damped Newton iterations can be found in [13].

3. Right-Transforming Iterations

In this section, we consider the *null-space* decomposition of the condensed primal-dual system (27) interchanging the second and the fourth rows and columns. The resulting matrix can be written according to

$$K = \begin{pmatrix} A & B^T \\ B & D \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & L_{u\lambda} & L_{u\mu} & 0 \\ L_{\lambda u} & 0 & L_{\lambda\mu} & 0 \\ L_{\mu u} & L_{\mu\lambda} & \tilde{L}_{\mu\mu} & L_{\mu\eta} \\ 0 & 0 & L_{\eta\mu} & 0 \end{array}\right), \quad (28)$$

where the first diagonal block

$$A = \begin{pmatrix} 0 & L_{u\lambda} \\ L_{\lambda u} & 0 \end{pmatrix} \quad (29)$$

is now symmetric (but indefinite) nonsingular matrix. We remind that $L_{\lambda u} = A(\mu)$ is exactly the stiffness matrix corresponding to the homogenized state equation. Hence, A^{-1} exists, and the Schur complement $S := D - BA^{-1}B^T$ is correctly defined.

The idea of the right-transforming iterations, proposed in [14], for the solution of the condensed KKT system is based on the availability of an appropriate "right matrix" K_R, which is multiplied to K from the right to get the following regular splitting of K

$$KK^R = M_1 - M_2 \quad (30)$$

with a right factor K_R given below. For the regular splitting one requires relatively easily invertible matrix M_1 and $M_2 \sim 0$. For solving a linear system of the form $K\Delta\varphi = \xi$, starting with an initial guess for $\Delta\varphi := (\Delta u, \Delta\lambda, \Delta\mu, \Delta\eta)^T$, the transforming iteration proposed in [14] is described by

$$\Delta\varphi := \Delta\varphi + K^R M_1^{-1} (\xi - K\Delta\varphi). \quad (31)$$

Furthermore, the new iterate φ^{new} is obtained by a line-search in the direction $\Delta\varphi$, namely

$$\varphi_i^{new} = \varphi_i^{old} + s_i (\Delta\varphi)_i, 1 \le i \le 4.$$

The line-search approach and the choice of the steplengths parameters s_i is discussed in detail in Section 4. Using an appropriate preconditioner $\tilde{L}_{u\lambda}$ for the stiffness matrix $L_{u\lambda}$, we approximate the first diagonal block (29) as follows:

$$A = \begin{pmatrix} 0 & L_{u\lambda} \\ L_{\lambda u} & 0 \end{pmatrix} \sim \begin{pmatrix} 0 & \tilde{L}_{u\lambda} \\ \tilde{L}_{\lambda u} & 0 \end{pmatrix} =: \tilde{A}. \quad (32)$$

Then, the right transformations factor has been chosen in the form

$$K^R = \begin{pmatrix} I & -\widetilde{A}^{-1}B^T \\ 0 & I \end{pmatrix} = \begin{pmatrix} I & 0 & -\widetilde{L}_{\lambda u}^{-1}L_{\lambda\mu} & 0 \\ 0 & I & -\widetilde{L}_{u\lambda}^{-1}L_{u\mu} & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{pmatrix}$$

In this case, the regular splitting (30) becomes $KK^R = M_1 - M_2$, where

$$M_1 = \begin{pmatrix} 0 & L_{u\lambda} & 0 & 0 \\ L_{\lambda u} & 0 & 0 & 0 \\ L_{\mu u} & L_{\mu\lambda} & S & L_{\mu\eta} \\ 0 & 0 & L_{\eta\mu} & 0 \end{pmatrix} = \begin{pmatrix} A & 0 \\ R & Q \end{pmatrix} \quad (33)$$

and

$$M_2 = \begin{pmatrix} 0 & 0 & L_{u\mu} - L_{u\lambda}\widetilde{L}_{u\lambda}^{-1}L_{u\mu} & 0 \\ 0 & 0 & L_{\lambda\mu} - L_{\lambda u}\widetilde{L}_{u\lambda}^{-1}L_{\lambda\mu} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Note that $M_2 \sim 0$ if we have a good preconditioner for the stiffness matrix. In our numerical experiments we apply the incomplete Cholesky (IC) decomposition or the Algebraic Multigrid (AMG) preconditioner for $L_{u\lambda}$. The second diagonal block Q in (33) is a symmetric indefinite matrix given by

$$Q = \begin{pmatrix} S & L_{\mu\eta} \\ L_{\eta\mu} & 0 \end{pmatrix},$$

where S is the following symmetric matrix

$$S = \widetilde{L}_{\mu\mu} - L_{\mu u}\widetilde{L}_{u\lambda}^{-1}L_{\lambda\mu} - L_{\mu\lambda}\widetilde{L}_{\lambda u}^{-1}L_{u\mu}.$$

We denote by $d := \xi - K\Delta\varphi$ the defect in (31) and compute the corresponding entries of d as follows:

$$d_1 := -\nabla u L - L_{u\lambda}\Delta\lambda - L_{u\mu}\Delta\mu,$$

$$d_2 := -\nabla\lambda L - L_{\lambda u}\Delta u - L_{\lambda\mu}\Delta\mu,$$

$$d_3 := -\widetilde{\nabla}\mu L - L_{\mu u}\Delta u - L_{\mu\lambda}\Delta\lambda - \widetilde{L}_{\mu\mu}\Delta\mu - L_{\mu\eta}\Delta\eta,$$

$$d_4 := -\nabla\eta L - L_{\eta\mu}\Delta\mu.$$

Taking into account (31) one needs to compute $\delta = M_1^{-1}d$, i.e. to find the solution of the system $M_1\delta = d.$

Consequently, we find $\delta_1 = \widetilde{L}_{\lambda u}^{-1}d_2$ and $\delta_2 = \widetilde{L}_{u\lambda}^{-1}d_1$. To compute the remaining components of δ (namely, δ_3 and δ_4) we have to solve systems of the form

$$Qx = f \quad (34)$$

with the symmetric indefinite matrix Q and the right-hand side

$$f = (d_3 - L_{\mu u}\delta_1 - L_{\mu\lambda}\delta_2, d_4)^T.$$

For the numerical solution of the system (34) we use the iterative procedure MINRES, proposed in [15]. Convergence properties of the right-transforming iterations for PDE constrained optimization problems have been recently analysed in [16].

4. Merit Functions and Line-Search Approach

For simplicity we denote in this section the primal variables by $x = (u, \mu)^T$, the dual variables by $y = (\lambda, \eta)^T$, and the complementarity variables by $v = (z, w)^T$. A standard approach to choose a merit function for convergence is the L_2-norm $\left\| F^{(\rho)}(u, \mu, \lambda, \eta) \right\|$ of the residual resulting from the KKT conditions (24).

A more reliable approach (e.g., [3]) is to use two merit functions. Our *primary merit function* is based on the logarithmic barrier function and the augmented

Lagrangian term concerning only the equality constraints

$$M := M(x, y, \rho, \rho_A) = J(x) - \rho \sum_{i=1}^{2} \log g_i(x) + y^T h(x) + \frac{1}{2} \rho_A h(x)^T h(x) \quad (35)$$

where the equality constraints $h(x) = (h_1(x), h_2(x))$ and the inequality constraints $g(x) = (g_1(x), g_2(x))$ read as follows:

$$h_1(x) = h_1(u, \mu) = A(\mu)u - b,$$

$$h_2(x) = h_2(\mu) = c(\mu) - C,$$

$$g_1(x) = g_1(\mu) = \mu - \mu_{\min} e,$$

$$g_2(x) = g_2(\mu) = \mu_{\max} e - \mu \ . \quad (36)$$

The parameter ρ_A is a positive scalar which can be changed during the iteration in the case when $\Delta x = (\Delta u, \Delta \mu)^T$ is not a descent direction for the primary merit function, i.e., $\Delta x^T \nabla xM < 0$. The gradient of M with respect to *x* is

$$\nabla xM := \nabla xM(x, y, \rho, \rho_A) = \nabla J(x) - \rho J_I^T D^{-1} e + J_E^T y + \rho_A J_E^T h(x) \quad (37)$$

where

$$J_E = \begin{pmatrix} L_{\lambda u} & L_{\lambda \mu} \\ 0 & L_{\eta \mu} \end{pmatrix} \text{and} \quad J_I = \begin{pmatrix} 0 & I \\ 0 & -I \end{pmatrix}$$

with J_E and J_I the Jacobian matrices corresponding to the equality and inequality constraints, respectively. Then we have

$$\begin{aligned} &\Delta x^T \nabla xM \\ &= \Delta x^T (\nabla J - \rho J_I^T D^{-1} e) + \Delta x^T J_E^T y + \rho_A \Delta x^T J_E^T h(x) \\ &= \Delta x^T (\nabla J - \rho J_I^T D^{-1} e) - h(x)^T y - \rho_A h(x)^T h(x), \end{aligned} \quad (38)$$

taking into account that $J_E \Delta x = -h(x)$ according to the fourth and fifth rows of the system (26). One can see from (38) that $\Delta x^T \nabla xM < 0$ if

$$\rho_A > \frac{\Delta x^T (\nabla J - \rho J_I^T D^{-1} e) - h(x)^T y}{h(x)^T (x)}.$$

However, when $\Delta x^T \nabla xM \geq 0$, ρ_A could achieve extreme large values for $\|h\|$ being small. In this case, we rely on the following choice of ρ_A, proposed in [3]

$$\rho_A = \min\left(\frac{5}{h^T h} (\Delta x^T (\nabla J - \rho J_I^T D^{-1} e) - h(x)^T y), 100 \right). \quad (39)$$

Our *secondary merit function* used for the line-search method is $\left\| F^{(\rho)}(u, \mu, \lambda, \eta) \right\|$.We consider only two parameters α and γ serving as steplengths for the primal variables and the complementarity conditions. For *y* and *v* we use equal steplengths γ. Let $\tilde{\alpha}_\mu$, $\tilde{\gamma}_z$, and $\tilde{\gamma}_w$ be defined as

$$\begin{aligned} \tilde{\alpha}_\mu &= \max\{\alpha \mid \mu_{\min} e \leq \mu + \alpha \Delta \mu \leq \mu_{\max} e\}, \\ \tilde{\gamma}_z &= \max\{\gamma \mid z + \gamma \Delta z \geq 0\}, \\ \tilde{\gamma}_w &= \max\{\gamma \mid w + \gamma \Delta w \geq 0\}. \end{aligned} \quad (40)$$

To ensure a strict feasibility, we substitute $\tilde{\alpha} = \tilde{\alpha}_\mu$, and $\tilde{\gamma} = \min\{\tilde{\gamma}_z, \tilde{\gamma}_w\}$, choose a positive parameter $\tau < 1$, and define the steplengths $\alpha = \min(1, \tau \tilde{\alpha})$ and $\gamma = \min(1, \tau \tilde{\gamma})$.

5. Numerical Results

In this section, we present some computational results concerning the microscopic problem to find the homogenized elasticity coefficients (17). The elasticity equation (18) is solved numerically by using continuous piecewise linear finite elements. In the 2D case we use triangular finite elements. In the 3D case we apply first an initial decomposition of the periodic microcell *Y* into hexahedra and then use tetrahedral shape meshes.

Due to the equal solutions $\xi^{ij} = \xi^{ji}$ of (18), $i, j = 1,\ldots, d$, $i \neq j$, one has to solve three problems ($d = 2$) and six problems ($d = 3$) in the periodic microcell Y to find the characteristic displacements.

Our numerical implementations concerning the microcells of the ceramic composites require a square hole located at the center of the unit cell (for more details we refer to [11]). Assume that the material layers in the periodicity cell have equal widths from all sides of the cell. Denote by μ_1 and μ_2 the widths of the carbon and SiC layers, respectively. The void area (e.g., for $d = 2$) can be computed as

$$A_{void} = (1-2(\mu_1+\mu_2))^2$$

and the total material density is denoted by

$$\tau(\mu) = 1 - A_{void} = 4(\mu_1+\mu_2)(1-\mu_1-\mu_2).$$

Furthermore, we briefly focus on the necessity of using adaptive mesh-refinement around the singularities in the periodic microstructure. An additional mesh-adaptivity is produced across the material interfaces in the microstructure due to the strongly varying material parameters (Young's modulus and Poisson's ratio) for both materials (SiC and C). In our numerical experiments, we use the *Zienkiewicz-Zhu* a posteriori error estimator which has been recently successfully applied to many finite element simulations and widely used in many industrial codes. The main idea of the method consists in computing a more accurate stress tensor by a post-processing and takes the difference between this so-called *recovered continuous stress* and the discrete finite element solution stress as an error estimator. In case of linear finite elements, the nodal averaging procedure or the L_2-projection technique is applied to compute the recovered stresses.

The Young modulus E (in GPa) and the Poisson ratio ν of our two materials are, respectively, $E = 10$, $\nu = 0.22$ for carbon and $E = 410$, $\nu = 0.14$ for SiC. We present some convergence results for solving linear systems with the stiffness matrix $L_{u\lambda}$ in (32) by the Preconditioned Conjugate Gradient (PCG) method. We use two preconditionetrs, incomplete Cholesky (IC) and Algebraic Multigrid (AMG) (see [17]). The latter solver used here as a preconditioner is a purely matrix-based version of the algebraic multilevel approach and can be implemented for large sparse unstructured linear systems of equations without any geometric background. For various values of the density τ (computed for the periodicity microstructure in cross section), we give in Table 1 and Table 2 numerical results, for instance, for the characteristic displacement ξ^{11} in the case $d = 3$. We report the number of degrees of freedom **d.o.f.**, the number of iterations **iter**, and the CPU-time in seconds for the first 10 adaptive refinement levels. One can see from the numerical results a better convergence and an essential efficiency of AMG-preconditioner compared to IC-factorization, especially for a larger number of unknowns.

Table 1 Convergence results with IC and AMG preconditioners, density τ=51%.

prec.	level	1	2	3	4	5	6	7	8	9	10
	d.o.f.	78	90	126	225	336	579	1185	1908	3360	5598
IC	iter	9	8	14	23	40	66	105	150	235	269
	CPU	e-16	e-16	e-16	0.1	0.2	0.2	0.9	2.4	8.2	20.9
AMG	iter	11	13	13	15	18	23	38	57	89	94
	CPU	e-16	e-16	e-16	0.2	0.3	0.5	1.5	3	7.6	14.8

Table 2 Convergence results with IC and AMG preconditioners, density τ = 84%.

prec.	level	1	2	3	4	5	6	7	8	9	10
	d.o.f.	78	93	150	261	510	1047	2103	3843	6537	10485
IC	iter	10	11	16	21	44	78	117	171	226	273
	CPU	e-16	e-16	0.1	0.1	0.1	0.6	2.4	8.4	24.3	63.7
AMG	iter	12	14	14	14	18	31	43	73	69	74
	CPU	e-16	e-16	e-16	0.2	0.4	1.1	3	7.5	15.5	25.6

Table 3 Convergence results for SiC-ceramics.

$\mu_1^{(0)}$	$\mu_2^{(0)}$	C	*iter*	μ_1	μ_2	ρ	$\left\|F^{(\rho)}\right\|_2$
0.10	0.05	0.2	11	2.5e-8	0.19	3.6e-6	7.12e-9
0.10	0.10	0.4	10	3.8e-7	0.39	3.5e-7	9.14e-9
0.15	0.05	0.3	9	7.2e-8	0.29	4.7e-7	7.29e-10
0.05	0.2	0.3	19	9.3e-7	0.29	5.6e-6	8.21e-9
0.20	0.15	0.4	11	4.6e-8	0.39	1.3e-7	9.83e-9
0.05	0.05	0.2	10	6.1e-8	0.19	9.5e-7	8.73e-10
0.10	0.15	0.3	9	7.5e-7	0.29	3.6e-6	9.06e-9
0.20	0.10	0.4	11	8.6e-8	0.39	2.7e-7	9.32e-10

As far as a design optimization is concerned, we consider as the objective functional the mean compliance of the structure defined as follows:

$$J(u,\mu)=\int_{\Omega} f.udx+\int_{\Gamma_T} t.uds, \qquad (41)$$

where **f** is the external body force applied to Ω.

For solving the optimization problem we use the primal-dual Newton-type interior-point method by means of line-search approach and two different merit functions. The primary merit function is based on the augmented Lagrangian approach. The right-transforming iterative technique is applied to the condensed KKT system (27). For the numerical solution of (34) we use MINRES, a method designed for symmetric and indefinite systems. For completeness of the presentation, we describe below this method without preconditioning. Preconditioned versions of the method are expensive and not recommended in our case, since the system with the preconditioner has to be additionally solved at each step of the iteration. As a stopping criterion we use a fixed (small) number of iterations.

MINRES method without preconditioning:

$k=0$; Compute $r_0=f-Qx_0$ for some initial guess x_0, $p_0=Qr_0$;

while ($\|\mathbf{r}_k\|$ accurate enough)

if ($k>0$) $p_k=Qr_k$;

$\alpha=r_k^T p_k / p_k^T p_k; x_{k+1}=x_k+\alpha r_k; r_{k+1}=r_k-\alpha p_k;$

check convergence; continue if necessary;

$y=Qp_k; \beta=p_k^T y / p_k^T p_k;$

If ($k=0$) $\gamma=0$;

else $\gamma=g_{k-1}^T y / p_{k-1}^T p_{k-1}$;

endif;

if ($k=0$) $r_{k+1}=p_k-\beta r_k;\ p_{k+1}=y-\beta p_k;$

else $r_{k+1}=p_k-\beta r_k-\gamma r_{k-1};$
$p_{k+1}=y-\beta p_k-\gamma p_{k-1};$

endif;

$p_{k-1} = p_k, p_k = p_{k+1};$
$r_{k-1} = r_k, r_k = r_{k+1};$
$k = k + 1;$

End;

We define initial values for the barrier parameter $\rho^{(0)} = 1$ and for the widths $\mu_1^{(0)}$ and $\mu_2^{(0)}$ of the material layers (C and SiC). Suppose that the constant *C* in (20) is given and satisfies the condition $0 < C < 0.5$. The computational results are reported in Table 3. We comment on the final number of outer iterations *iter*, the computed widths of the C- and SiC- layers (respectively, μ_1 and μ_2), the final value of the barrier parameter, and the l_2- norm of the residual $F^{(\rho)}$ from (24). We stop the iterative process when *iter* $\geq$ 12 or $\rho \leq 1.0e\text{-}8$ or $\| F^{(\rho)}\|_2 \leq tol$ with a given tolerance. The numerical results show that in all runs the width of the carbon layer μ_1 goes to zero, which is natural since SiC has a higher stiffness. Practically, this means that the microcell would be totally occupied by the SiC layer which leads to the expensive (in time) production of the so-called *pure SiC-ceramics*.

Acknowledgements

This work has been partially supported by the DAAD PPP (Project ID 57067781) within BMBF funds, FSP AMMO at the University of Applied Sciences Bielefeld, Germany, and the Bulgarian NSF Grant NumComModME2012.

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