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Kocvara, Michal; Loghin, Daniel; Turner, James

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CONSTRAINT INTERFACE PRECONDITIONING FOR TOPOLOGY OPTIMIZATION PROBLEMS*

M. KOČVARA[†], D. LOGHIN[‡], AND J. TURNER[‡]

Abstract. The discretization of constrained nonlinear optimization problems arising in the field of topology optimization yields algebraic systems which are challenging to solve in practice, due to pathological ill-conditioning, strong nonlinearity, and size. In this work we propose a methodology which brings together existing fast algorithms, namely, interior point for the optimization problem and a novel substructuring domain decomposition method for the ensuing large-scale linear systems. The main contribution is the choice of interface preconditioner which allows for the acceleration of the domain decomposition method, leading to performance independent of problem size.

Key words. topology optimization, domain decomposition, Newton–Krylov, preconditioning, interior point

AMS subject classifications. 65K10, 65N55, 65F10, 90C51, 49N90

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1. Introduction. The aim of topology optimization is to determine the optimal distribution of a certain amount of material within a prescribed value in order to minimize the strain energy (or compliance) of a given structure. The distinguishing feature separating this approach from shape optimization involves the introduction of new boundaries, allowing for the consideration of a broader range of feasible solutions. The main problem when pursuing such an approach is that a large number of design variables are required in the discrete formulation in order to maintain the quality of the contours in the final design. Solutions are typically obtained through the use of iterative optimization techniques, requiring repeated discretizations via the finite element method, corresponding to a sequence of linearized problems. As a result, even problems resulting from using relatively coarse discretization parameters can be computationally demanding. Our aim in this paper is to introduce solution methods adapted to the complex nature of this class of problems.

Attempts to alleviate such difficulties can involve the application of a faster finite element solver, or the use of efficient discretization techniques [9]. Standard approaches based around Picard iterations target the ill-conditioned equilibrium equations, from which the bulk of computational effort resides. In [31], MINRES coupled with recycling is explored based on the observation that the densities are only expected to undergo minor changes after a relatively small number of iterative steps. The ill-conditioning is dealt with through a preconditioning strategy involving both rescaling and an incomplete Cholesky decomposition.

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[†]School of Mathematics, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK, and Institute of Information Theory and Automation, Czech Academy of Sciences, Pod vodárenskou věží 4, 18208 Praha 8, Czech Republic (m.kocvara@bham.ac.uk). The work of this author has been partly supported by the EU FP7 project AMAZE and by grant A100750802 of the Czech Academy of Sciences.

[‡]School of Mathematics, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK (d.loghin@bham.ac.uk, turnerj777@yahoo.co.uk).

In terms of parallel computing, the application of the preconditioned conjugate gradient method coupled with Jacobi preconditioning has been considered in a number of references, including [7, 11, 18, 22, 30]. Two additional approaches are considered in [30], namely, preconditioning based on an ILU factorization, as well as condensation through substructuring coupled with a diagonal preconditioner for the resulting interface problem.

Alternatively, primal-dual Newton methods can be considered, with particular focus on interior point approaches. Examples illustrating the application of such approaches for solving large scale topology optimization problems can be found in [3, 14, 21]. The KKT conditions from the resulting nonlinear equality constrained optimization problem are then solved using Newton's method. Evidently, for large scale problems, obtaining solutions to the resulting system of equations will become expensive and even prohibitive in certain cases. In [21], Maar and Schulz applied multigrid to the resulting system, and from their results were able to witness an approximately linear overall complexity with respect to the number of unknowns used in the problem.

In this paper, we propose to apply domain decomposition to the resulting Newton system described above, which will then be solved using GMRES coupled with an appropriate preconditioning strategy. An important component within our preconditioner is based on targeting the resulting interface problem, which will be achieved through the consideration of an appropriate fractional Sobolev norm. Our paper will conclude by illustrating that results can be obtained without dependence on the chosen mesh parameter.

2. Problem description. Consider a material occupying an open and connected domain $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$. We assume that the elasticity tensor for the material can be modeled as $E(\mathbf{x}) = \rho(\mathbf{x})^\mu \bar{E}$, where $\rho(\mathbf{x})$ is the density, $\mu \in [1, 3]$, and \bar{E} is a prescribed constant tensor. This expression describes a common approximation of the material properties known as the solid isotropic material with penalization (SIMP) model. In this paper we will be interested in the variable thickness sheet (VTS) problem, corresponding to the choice $\mu = 1$, for which existence of solutions holds (see, e.g., [4, pp. 272–274]). We assume that the material is clamped (i.e., we assume Dirichlet conditions) along the subset $\partial\Omega_D$ of the boundary and that both body forces $f : \Omega \rightarrow \mathbb{R}^2$ and boundary tractions $g : \partial\Omega_N \rightarrow \mathbb{R}^2$ act on the material, resulting in a displacement u which satisfies the following equilibrium equations in Ω :

$$-\operatorname{div}\sigma(u) = f,$$

where, by Hooke's law, the stress tensor is $\sigma(u) = E : \varepsilon(u)$.

We employ next a weak formulation in order to define our topology optimization problem. The natural spaces arising in this context are the standard spaces $L^2(\Omega)$, $H^1(\Omega)$, and

$$H_D^1(\Omega) = \{v \in H^1(\Omega) : v|_{\partial\Omega_D} = 0\}.$$

For the description of the preconditioners associated with a domain decomposition approach with corresponding interface Γ between subdomains, we will require the fractional Sobolev space

$$\Lambda := [H_D^1(\Gamma), L^2(\Gamma)]_{1/2},$$

which is an interpolation space of index $1/2$ (see [19] for details).

2.1. Weak formulation. Let $\mathcal{V} = [H_D^1(\Omega)]^2$ and let $a_\rho(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R}$ and $F(\cdot) : \mathcal{V} \rightarrow \mathbb{R}$ be defined below,

$$a_\rho(w, v) = \int_{\Omega} \rho(\mathbf{x}) (\varepsilon(w) : \bar{E} : \varepsilon(v)) \, d\mathbf{x},$$

where $\varepsilon(v)$ is the strain tensor corresponding to a displacement v and

$$F(v) := \int_{\Omega} f \cdot v \, d\mathbf{x} + \int_{\partial\Omega_N} g \cdot v \, ds.$$

We seek $u \in \mathcal{V}$ such that for all $v \in \mathcal{V}$

$$a_\rho(u, v) = F(v).$$

In order to formulate our topology optimization problem, we define the following admissible set for our design variable ρ :

$$\mathcal{Q}^c = \left\{ \rho \in \mathcal{Q} \equiv L^\infty(\Omega) \mid 0 < \underline{\rho} \leq \rho(\mathbf{x}) \leq \bar{\rho} \text{ a.e. in } \Omega, \int_{\Omega} \rho(\mathbf{x}) \, d\mathbf{x} = \mathcal{M}_\Omega \right\},$$

where \mathcal{M}_Ω denotes the amount of material available, and $\bar{\rho}$ and $\underline{\rho}$ denote upper and lower limits on the density function, respectively.

Consider now the following nonlinear minimization problem

$$(2.1) \quad \min_{(u, \rho) \in \mathcal{V} \times \mathcal{Q}^c} \quad \frac{1}{2} a_\rho(u, u) \quad \left[= \frac{1}{2} F(u) \right]$$

$$(2.2) \quad \text{subject to:} \quad a_\rho(u, v) = F(v) \quad \forall v \in \mathcal{V}.$$

The state variable corresponds to the displacement of the material u , while the design variable is the density function $\rho(\mathbf{x}) : \Omega \rightarrow \mathbb{R}_+$.

Let now $\mathcal{V}_h, \mathcal{Q}_h^c$ denote finite-dimensional subspaces of \mathcal{V} and \mathcal{Q}^c , respectively, and consider the following discrete weak formulation of our minimization problem:

$$(2.3) \quad \min_{(u_h, \rho_h) \in \mathcal{V}_h \times \mathcal{Q}_h^c} \quad \frac{1}{2} a_\rho(u_h, u_h) \quad \left[= \frac{1}{2} F(u_h) \right]$$

$$(2.4) \quad \text{subject to:} \quad a_\rho(u_h, v_h) = F(v_h) \quad \forall v_h \in \mathcal{V}_h.$$

Using finite element bases for \mathcal{V}_h and \mathcal{Q}_h , the minimization problem (2.3)–(2.4) yields the following discrete constrained minimization problem:

$$(2.5) \quad \min_{(\mathbf{u}, \boldsymbol{\rho}) \in \mathbb{R}^n \times \mathbb{R}^m} \quad \frac{1}{2} \mathbf{u}^T A(\boldsymbol{\rho}) \mathbf{u} \quad \left[= \frac{1}{2} \mathbf{f}^T \mathbf{u} \right]$$

$$(2.6) \quad \text{subject to:} \quad A(\boldsymbol{\rho}) \mathbf{u} = \mathbf{f},$$

$$(2.7) \quad \mathbf{q}^T \boldsymbol{\rho} = \mathbf{q}^T \mathbf{1},$$

$$(2.8) \quad \underline{\rho} \mathbf{1} \leq \boldsymbol{\rho} \leq \bar{\rho} \mathbf{1},$$

where $q_i := [\mathbf{q}]_i = |T_i|$. Working with a piecewise constant approximation ρ_h , we can write the assembly process of the stiffness matrix as follows:

$$A(\boldsymbol{\rho}) = \sum_{i=1}^m \rho_i A_i,$$

where A_i is global representation of the elemental matrix corresponding to simplex T_i . This will allow for a certain simplified expression for the Jacobian matrix when considering the first-order conditions for our minimization problem.

3. Interior point method. Traditional and popular approaches for solving optimization problems such as (2.5)–(2.8) involve separate treatment of both the design objective and the equilibrium equations. Typically, for an initial given design the stiffness matrix is assembled and used to solve the equilibrium equations for the displacement \mathbf{u} . This \mathbf{u} is then used to obtain an appropriate update to the design variables, which is then checked for suitability based on previous values. If an appropriate solution has yet to be found, the process is repeated. Typical approaches used to obtain an update to the design variables include both the optimality criteria method [4, p. 308] and the method of moving asymptotes [26], usually followed by both sensitivity and filtering analyses to cater for the general SIMP setting [25].

More recently, fully coupled approaches have been receiving considerable attention within the PDE constrained optimization community. In these approaches, all constraints are included and no subproblems are being solved separately. An important feature within these methods is that the equilibrium equations are embedded within the optimization routine, allowing for the simultaneous treatment of all constraints within the problem. Examples highlighting the benefits, and in particular the savings in computational time for such methods, can be found in a number of sources, including [5, 6, 14]. We describe below an interior point method as applied to the topology optimization problem introduced in (2.5)–(2.8).

Interior point methods are used to solve both convex linear and nonlinear optimization problems iteratively by considering updates confined to the feasible region (cf. [8, 10, 33]). As well as obtaining solutions in polynomial time, these methods have been used to determine solutions to previously intractable problems, meaning that they are useful from both a theoretical as well as a practical viewpoint. We begin by rewriting the formulation (2.5) slightly to incorporate the inequality constraints within the objective function. This will be achieved through the use of logarithmic barrier terms as illustrated below:

$$(3.1) \quad \min_{(\mathbf{u}, \boldsymbol{\rho}) \in \mathbb{R}^n \times \mathbb{R}^m} \frac{1}{2} \mathbf{u}^T A(\boldsymbol{\rho}) \mathbf{u} - r \sum_{i=1}^m \log(\rho_i - \underline{\rho}) - s \sum_{i=1}^m \log(\bar{\rho} - \rho_i)$$

$$(3.2) \quad \text{subject to: } A(\boldsymbol{\rho}) \mathbf{u} = \mathbf{f},$$

$$(3.3) \quad \mathbf{q}^T \boldsymbol{\rho} = \mathbf{q}^T \mathbf{1}$$

with $r, s > 0$ and where $[\boldsymbol{\rho}]_i = \rho_i$.

The Lagrangian associated with the problem (3.1)–(3.3) is

$$(3.4) \quad \mathcal{L}^{(r,s)}(\mathbf{v}, \lambda, \mathbf{u}, \boldsymbol{\rho}) := \frac{1}{2} \mathbf{u}^T A(\boldsymbol{\rho}) \mathbf{u} - r \sum_{i=1}^m \log(\rho_i - \underline{\rho}) - s \sum_{i=1}^m \log(\bar{\rho} - \rho_i) \\ + \mathbf{v}^T (\mathbf{f} - A(\boldsymbol{\rho}) \mathbf{u}) + \lambda (\mathbf{q}^T \mathbf{1} - \mathbf{q}^T \boldsymbol{\rho}).$$

The stationary points are defined by setting to zero the relevant partial derivatives of the Lagrangian (3.4):

$$(3.5) \quad \nabla_{\mathbf{v}} \mathcal{L} = \mathbf{f} - A(\boldsymbol{\rho}) \mathbf{u} = \mathbf{0},$$

$$(3.6) \quad \nabla_{\lambda} \mathcal{L} = \mathbf{q}^T \boldsymbol{\rho} - \mathbf{q}^T \mathbf{1} = 0,$$

$$(3.7) \quad \nabla_{\mathbf{u}} \mathcal{L} = A(\boldsymbol{\rho}) \mathbf{u} - A(\boldsymbol{\rho}) \mathbf{v} = \mathbf{0},$$

$$(3.8) \quad \nabla_{\boldsymbol{\rho}} \mathcal{L} = \frac{1}{2} B(\mathbf{u})^T \mathbf{u} - B(\mathbf{u})^T \mathbf{v} - \lambda \mathbf{q} - r X^{-1} \mathbf{1} + s \tilde{X}^{-1} \mathbf{1} = \mathbf{0}.$$

In the above, $B(\mathbf{u}) := [A_1\mathbf{u}, A_2\mathbf{u}, \dots, A_m\mathbf{u}] \in \mathbb{R}^{n \times m}$ and

$$X := \text{diag}(\boldsymbol{\rho} - \underline{\rho}\mathbf{1}), \quad \tilde{X} := \text{diag}(\bar{\rho}\mathbf{1} - \boldsymbol{\rho}).$$

It is important to note that the condition number of the Hessian of the Lagrangian may pose an issue for densities close to either $\underline{\rho}$ or $\bar{\rho}$ as both r and s tend to zero. To alleviate this issue, auxiliary nonnegative variables $\boldsymbol{\phi}$ and $\boldsymbol{\psi}$ are introduced in the following way:

$$(3.9) \quad \boldsymbol{\phi} = \boldsymbol{\phi}^{(r,s)} := rX^{-1}\mathbf{1} \quad \text{and} \quad \boldsymbol{\psi} = \boldsymbol{\psi}^{(r,s)} := s\tilde{X}^{-1}\mathbf{1}.$$

Using (3.9), we see that

$$\Phi X\mathbf{1} = r\mathbf{1} \quad \text{and} \quad \Psi \tilde{X}\mathbf{1} = s\mathbf{1},$$

where $\Phi := \text{diag}(\boldsymbol{\phi})$ and $\Psi := \text{diag}(\boldsymbol{\psi})$. Through this substitution, and the elimination of the Lagrange multiplier \mathbf{v} (which, by (3.5) and (3.7), is equal to $-\mathbf{u}$), the first-order optimality conditions can be written as

$$\begin{aligned} \mathcal{R}(\mathbf{u}, \lambda, \boldsymbol{\rho}, \boldsymbol{\phi}, \boldsymbol{\psi}) &:= \nabla \mathcal{L}^{(r,s)}(\mathbf{u}, \lambda, \boldsymbol{\rho}, \boldsymbol{\phi}, \boldsymbol{\psi}) \\ &= \begin{pmatrix} \mathbf{f} - A(\boldsymbol{\rho})\mathbf{u} \\ \mathbf{q}^T \boldsymbol{\rho} - \mathbf{q}^T \mathbf{1} \\ \frac{1}{2}B(\mathbf{u})^T \mathbf{u} + \lambda \mathbf{q} + \boldsymbol{\phi} - \boldsymbol{\psi} \\ r\mathbf{1} - \Phi X\mathbf{1} \\ s\mathbf{1} - \Psi \tilde{X}\mathbf{1} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \end{aligned}$$

By setting $\mathbf{y} = (\mathbf{u}, \lambda, \boldsymbol{\rho}, \boldsymbol{\phi}, \boldsymbol{\psi})^T$, Newton's method applied to the above nonlinear optimality conditions has the following form,

$$(3.10) \quad J(\mathbf{y}^{k-1}) \Delta \mathbf{y}^k = \mathcal{R}(\mathbf{y}^{k-1}),$$

where the Jacobian matrix $J(\mathbf{y})$ is given below:

$$(3.11) \quad J(\mathbf{y}) = \begin{bmatrix} A(\boldsymbol{\rho}) & B(\mathbf{u}) & & & \\ & \mathbf{q}^T & & & \\ B(\mathbf{u})^T & \mathbf{q} & I_m & -I_m & \\ & \Phi & X & & \\ & -\Psi & & \tilde{X} & \end{bmatrix}.$$

Remark 3.1. In the following, we will assume that problems of the form (3.1)–(3.3) yield Jacobian matrices $J(\mathbf{y})$ of the form (3.11), which are nonsingular for \mathbf{y} in a neighborhood of the solution. This property will be assumed to hold for both Dirichlet and mixed boundary conditions, due to the well-posedness of problem (2.1)–(2.2) for both mixed Dirichlet–Neumann and Dirichlet-only boundary conditions.

Despite J being both nonsymmetric and indefinite, its condition number is expected to be bounded under reduction of the barrier parameters r and s . Therefore, it is important to consider appropriate strategies for obtaining an accurate update through (3.10). Work by Forsgren, Gill, and Shinnerl [12] uses the diagonal structure of both Φ and Ψ to transform J into a symmetric matrix. Another possibility

is to consider appropriate techniques to condense the matrix J via block elimination or using a Schur complement approach. This approach is known to lead to ill-conditioning; however, the effect on the accuracy of the resulting solution can be benign, as discussed by Wright in [32]. Therefore, block elimination techniques remain a practical option, particularly for the situation where the original matrix J is large. The drawback in this case is the loss of sparsity and the lack of obvious (and efficient) preconditioners. For this reason, we look to exploit the sparsity present in the original unreduced system by using an iterative method coupled with an appropriate preconditioning strategy, with the original matrix shown to exhibit favorable spectral properties as shown in recent work by Greif, Moulding, and Orban [13]. The preconditioner employed for this work will be based on a decomposition of the domain Ω into subdomains, described in detail from the next section onwards. In particular, we provide a description of an interface preconditioning technique which was first introduced in [2] for solving scalar elliptic problems, and which is now adapted to the case of our constrained PDE problem.

4. Domain decomposition. In order to formulate a decomposition of our problem that is suitable for a parallel environment, we need to ensure that aside from the physical decomposition of the domain, the resulting subproblems are well-posed. It turns out that we can achieve this through a simple reformulation of our minimization problem, which targets the mass constraint (3.3).

4.1. Standard definitions and notation. Consider a subdivision of Ω into N nonoverlapping subdomains Ω_k with boundaries $\partial\Omega_k$ such that

$$\bar{\Omega} = \bigcup_{k=1}^N \bar{\Omega}_k, \quad \Omega_k \cap \Omega_j \equiv \emptyset \quad (k \neq j).$$

We denote the resulting interface by Γ :

$$\Gamma := \bigcup_{k=1}^N \Gamma_k, \quad \Gamma_k := \partial\Omega_k \setminus \partial\Omega.$$

For each k , we define the *nodal index set* ν_k to be the set of nodes strictly contained in Ω_k and the *simplex index set* τ_k to be the set of indices of all simplices contained in Ω_k . We further define $m_k := |\tau_k|$.

4.2. Problem reformulation. One of the obstacles in decomposing the VTS problem (2.5)–(2.8), or equivalently the interior point formulation (3.1)–(3.3), is the global mass constraint (2.7), or (3.3), respectively. A suitable way to “decompose” this constraint is provided by the following equivalent formulation:

$$\mathbf{q}_k^T \boldsymbol{\rho}_k = \mu_k \quad (k = 1, \dots, N), \quad \sum_{k=1}^N \mu_k = \mathbf{q}^T \mathbf{1},$$

where \mathbf{q}_k and $\boldsymbol{\rho}_k$ represent the respective subvectors of \mathbf{q} and $\boldsymbol{\rho}$ corresponding to the index set τ_k . We note here that this approach introduces N additional unknowns $\{\mu_k, k = 1, \dots, N\}$, together with N additional constraints. Note also that given the definition of \mathbf{q} , μ_k represents the mass of subdomain Ω_k .

The modified formulation corresponding to (3.1)–(3.3) is included below:

$$(4.1) \quad \min_{(\mathbf{u}, \boldsymbol{\rho}) \in \mathbb{R}^n \times \mathbb{R}^m} \frac{1}{2} \mathbf{u}^T A(\boldsymbol{\rho}) \mathbf{u} - r \sum_{i=1}^m \log(\rho_i - \underline{\rho}) - s \sum_{i=1}^m \log(\bar{\rho} - \rho_i)$$

$$(4.2) \quad \text{subject to: } A(\boldsymbol{\rho}) \mathbf{u} = \mathbf{f},$$

$$(4.3) \quad \mathbf{q}_k^T \boldsymbol{\rho}_k = \mu_k, \quad k = 1, \dots, N,$$

$$(4.4) \quad \sum_{k=1}^N \mu_k = \mathbf{q}^T \mathbf{1}.$$

The above problem is equivalent to minimization problem (2.5)–(2.8) and hence is well-posed.

Following the same procedure of differentiating the corresponding Lagrangian function, one can derive the first-order optimality conditions and set up Newton's iteration in the form (3.10). The resulting Jacobian matrix, also denoted by J , now has the form

$$(4.5) \quad J = \begin{bmatrix} A & B & & & \\ & Q & & & \\ B^T & Q^T & I_m & -I_m & -I_N \\ & & \Phi & X & \\ & & -\Psi & \tilde{X} & \\ & -I_N & & & \mathbf{1}_N^T \end{bmatrix},$$

where $Q \in \mathbb{R}^{N \times m}$ is described below:

$$Q_{kj} := \begin{cases} q_j & \text{if } j \in \tau_k, \\ 0 & \text{otherwise.} \end{cases}$$

Using a node ordering comprising nodes interior to the subdomains Ω_k followed by nodes on the interface Γ , the Jacobian will have the following permuted block form (with subscripts I and Γ indicating this ordering)

$$(4.6) \quad \begin{bmatrix} J_{II} & J_{I\Gamma} \\ J_{\Gamma I} & J_{\Gamma\Gamma} \end{bmatrix} = \begin{bmatrix} A_{II} & B_I & & & A_{I\Gamma} & -I_N \\ & Q & & & & \\ B_I^T & Q^T & I_m & -I_m & B_{\Gamma}^T & \\ & & \Phi_m & X_m & & \\ & & -\Psi_m & \tilde{X}_m & & \\ A_{\Gamma I} & -I_N & \tilde{B}_{\Gamma} & & A_{\Gamma\Gamma} & \mathbf{1}_N^T \end{bmatrix}.$$

Under a further permutation which lists all the unknowns corresponding to subdomains Ω_k , for each $k = 1, \dots, N$, it can be seen that it has the block-diagonal structure $J_{II} := \bigoplus_{k=1}^N J_{II}^k$. Each block J_{II}^k represents the instance of the Jacobian for a minimization problem posed over the subdomain Ω_k with Dirichlet boundary conditions

on $\partial\Omega_k$ and which has the familiar algebraic form (3.11):

$$J_{II}^k := \begin{bmatrix} A_k & B_k & & & \\ & \mathbf{q}_{m_k}^T & & & \\ B_k^T & & I_{m_k} & -I_{m_k} & \\ & \Phi_{m_k} & X_{m_k} & & \\ & -\Psi_{m_k} & & \tilde{X}_{m_k} & \end{bmatrix}.$$

Here, A_k, B_k are the counterparts of A, B assembled on the interior of Ω_k and with Dirichlet boundary conditions applied. By the well-posedness of problems of the form (3.1)–(3.3) for the case $\partial\Omega_N = \emptyset$, we conclude that the associated first-order optimality conditions are well-posed and yield a Jacobian matrix which is nonsingular (cf. Remark 3.1).

The direct-sum structure of J_{II} was achieved through the reformulation of the mass constraint and clearly allows for a parallel implementation of the inverse of J_{II} , which will be a key building block in the solution algorithm described in the next section. It is also an interesting feature in itself to be able to decompose the global Jacobian into local Jacobians associated with similar local minimization problems. One consequence is that the local problems inherit the well-posedness associated with the global problem; the resulting decomposition is hence useful, with the local problems invertible independently of each other.

4.3. A Dirichlet–Dirichlet approach. At each step of the Newton iteration we need to solve linear systems of the form

$$J\mathbf{z} = \mathbf{r},$$

where J is the Jacobian matrix (4.6) corresponding to the first-order conditions for the reformulated problem (4.1)–(4.4). Due to the size and structure of J , we seek to solve such systems using an iterative solver with a suitable preconditioner. A proven candidate is the block upper-triangular matrix below employed as a right preconditioner,

$$(4.7) \quad P = \begin{bmatrix} J_{II} & J_{I\Gamma} \\ & \tilde{S} \end{bmatrix},$$

where \tilde{S} is an approximation to the Schur complement matrix

$$S = J_{\Gamma\Gamma} - J_{\Gamma I} J_{II}^{-1} J_{I\Gamma}.$$

Due to the direct-sum property of J_{II} , this block approach can be classified in domain decomposition terminology as a nonoverlapping Dirichlet–Dirichlet procedure, where each subdomain block represents a Jacobian matrix arising in some topology optimization subproblem posed on Ω_k where the material is clamped on Γ_k . Moreover, at each Newton iteration, the Schur complement S can be seen as the finite element discretization of a generalized Steklov–Poincaré operator corresponding to the interface problem generated by the decomposition. We remark here again that this approach is only available via the reformulation described above.

The preconditioner inverse can be written as the product of three matrices:

$$(4.8) \quad P^{-1} = \begin{bmatrix} J_{II}^{-1} & 0 \\ 0 & I_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} I_{II} & -J_{I\Gamma} \\ 0 & I_{\Gamma\Gamma} \end{bmatrix} \begin{bmatrix} I_{II} & 0 \\ 0 & \tilde{S}^{-1} \end{bmatrix}.$$

The application of P^{-1} would initially involve the action of \tilde{S}^{-1} on the skeleton problem corresponding to the interface Γ . Next, a boundary-to-domain update would be applied through J_{II} , before applying the inversion in parallel of J_{II} on subdomains. With the exception of \tilde{S} , the potential for parallelism in (4.7), or equivalently in (4.8), is evident. Therefore, the task is to seek an appropriate representation of \tilde{S} so that the preconditioner can be assembled, stored, and applied in an efficient manner. This is discussed in detail in the next section.

5. Constraint interface preconditioners. The Schur complement has the following block 3×3 structure

$$(5.1) \quad S = \begin{bmatrix} S_{11} & S_{12} & \mathbf{0} \\ S_{12}^T & S_{22} & \mathbf{1}_N \\ \mathbf{0}^T & \mathbf{1}_N^T & 0 \end{bmatrix},$$

where the matrices $S_{11} \in \mathbb{R}^{n_\Gamma \times n_\Gamma}$, $S_{12} \in \mathbb{R}^{n_\Gamma \times N}$, and $S_{22} \in \mathbb{R}^{N \times N}$. The matrix S_{22} is negative definite and has a nearly diagonal structure with reducing entries as the Newton iteration progresses, while S_{12} can be computed cheaply in parallel. The main focus will therefore be the matrix S_{11} which is associated with the interface displacement nodes. This block dominates the Schur complement for the Jacobian, and so the aim is to design a preconditioning procedure based on the structure of S above and in a manner that provides a suitable approximation \tilde{S}_{11} of S_{11} . We note here that one can view the block structure (5.1) as the discretization of an operator corresponding to S_{11} and constrained by conditions incorporated in the remaining blocks.

Remark 5.1. The Schur complement is symmetric and indefinite, with a negative inertia equal to $i_- = N + 1$, where N is the number of subdomains. Standard optimization approaches, such as the projected conjugate gradient method, cannot be used in this case. Similarly, we expect positive definite preconditioners to be less effective. Consequently, we devised a novel approach which incorporates the indefiniteness (and the constraints) into our preconditioner. The resulting method can be loosely described as being of constrained type (cf. [17]).

Given the structure of S we propose a preconditioner with a similar block form but with S_{11} replaced by a suitable approximation. A direct calculation using the block form (4.6) of the Jacobian matrix yields

$$(5.2) \quad S_{11} = S_{\Gamma\Gamma} + E,$$

where

$$(5.3) \quad S_{\Gamma\Gamma} := A_{\Gamma\Gamma} - A_{\Gamma I} A_{II}^{-1} A_{I\Gamma}$$

is the Schur complement arising in a Dirichlet–Dirichlet nonoverlapping domain decomposition method for the elasticity equations. The above splitting of S_{11} suggests the following candidate for a preconditioner:

$$(5.4) \quad S_0 = \begin{bmatrix} S_{\Gamma\Gamma} & S_{12} & \mathbf{0} \\ S_{12}^T & S_{22} & \mathbf{1}_N \\ \mathbf{0}^T & \mathbf{1}_N^T & 0 \end{bmatrix}.$$

This choice is computationally expensive due to the dense matrix $S_{\Gamma\Gamma}$ and S_0 can only be seen as an ideal preconditioner, very much like the Schur complement itself.

However, the (1-1)-block can afford approximations which make the application of S_0 efficient. In the following, we restrict our attention to $S_{\Gamma\Gamma}$. This matrix is the finite element representation of the Steklov–Poincaré operator corresponding to the interface problem for the elasticity equations, which is known to be continuous and coercive on Λ^2 . The above properties can be shown using the continuity and coercivity of the bilinear form $a_\rho(\cdot, \cdot)$ on V ; for details, see [24]. The restriction to \mathcal{V}_h , in the context of the finite element discretization of our problem, preserves these properties; in turn, $S_{\Gamma\Gamma}$ can be shown to be spectrally equivalent to the matrix representation of a norm on Λ_h^2 . We describe this discrete norm below.

5.1. Discrete fractional Sobolev norms. In order to describe the relevant norms further, we first describe the relevant function spaces defined on the interface Γ . Let ∇_Γ represent the tangential gradient of a scalar function $v(\mathbf{x})$ such that

$$\nabla_\Gamma v(\mathbf{x}) = \nabla v(\mathbf{x}) - \mathbf{n}(\mathbf{n} \cdot \nabla v(\mathbf{x})),$$

corresponding to the projection of the gradient of v onto the plane tangent to Γ at the point $\mathbf{x} \in \Gamma$. We now define

$$H^1(\Gamma) := \left\{ v \in L^2(\Gamma) \mid \int_\Gamma |\nabla_\Gamma v|^2 ds(\Gamma) < \infty \right\}.$$

Let $\gamma := \Gamma \cap \partial\Omega_D$ denote the set of points on the Dirichlet boundary of the domain which are also on the interface Γ ; when this set is nonempty, we define the space

$$H_D^1(\Gamma) := \{v \in H^1(\Gamma) \mid v|_\gamma = 0\}.$$

We recall here that the space Λ introduced above is the fractional Sobolev space of index $1/2$. More generally, we define the scale of spaces Λ_θ as the interpolation spaces of index $\theta \in (0, 1)$ corresponding to the pair of spaces $\{H_0^1(\Gamma), L^2(\Gamma)\}$ in the sense of Lions and Magenes [19]:

$$\Lambda_\theta := [H_\gamma^1(\Gamma), L^2(\Gamma)]_\theta.$$

Using a formulation involving discrete interpolation spaces with application to finite element spaces, one can define a finite-dimensional space $\Lambda_{\theta,h} \subset \Lambda_\theta$, together with the following matrix representation of a discrete interpolation norm [1]:

$$(5.5) \quad H_\theta := [L_\Gamma, M_\Gamma]_\theta := M_\Gamma(M_\Gamma^{-1}L_\Gamma)^{1-\theta},$$

where M_Γ and L_Γ are the mass and Laplacian matrices assembled on Γ using the restriction of the finite element basis for \mathcal{V}_h to the interface. Using this norm representation, the continuity and coercivity properties of the elasticity Schur complement $S_{\Gamma\Gamma}$ translate into the following spectral equivalence [27, p. 129]

$$c_1 \|\mathbf{u}\|_H \leq \|\mathbf{u}\|_{S_{\Gamma\Gamma}} \leq c_2 \|\mathbf{u}\|_H,$$

where $H := H_{1/2} \oplus H_{1/2}$. This equivalence is the basis of our candidate for the approximation of the Schur complement S .

The matrix H_θ is in general full and expensive to compute. However, an implementation of the action of the inverse of H_θ on a given vector can be achieved cheaply using a Krylov subspace approximation constructed via a generalized inverse Lanczos iteration which only requires the application of the inverse of the sparse matrix L_Γ for a small number of steps [1]. In the following section we indicate how to extend this procedure to the case of our proposed preconditioner.

5.2. Constraint preconditioners. Given the constraint form (5.1) of the interface Schur complement, we propose the following choice of preconditioner which preserves the constraining blocks while replacing the (1,1)-block by a spectrally equivalent matrix:

$$(5.6) \quad S_1 := \begin{bmatrix} H & S_{12} & \mathbf{0} \\ S_{12}^T & S_{22} & \mathbf{1}_N \\ \mathbf{0}^T & \mathbf{1}_N^T & 0 \end{bmatrix}.$$

The notion of constraint preconditioning has been extensively analyzed in the context of saddle-point problems [17, 20]. In our case, the matrix structure is of a different nature; however, given the spectral equivalence between S_{11} and H , we hope to achieve a useful similarity between S and \tilde{S} . Our motivation is the following result.

PROPOSITION 5.1. *Consider the generalized eigenvalue problem*

$$\mathcal{K}\mathbf{z} = \lambda\mathcal{G}\mathbf{z},$$

where

$$\mathcal{K} = \begin{bmatrix} K & D & \mathbf{0} \\ D^T & F & \mathbf{1}_N \\ \mathbf{0}^T & \mathbf{1}_N^T & 0 \end{bmatrix}, \quad \mathcal{G} = \begin{bmatrix} G & D & \mathbf{0} \\ D^T & F & \mathbf{1}_N \\ \mathbf{0}^T & \mathbf{1}_N^T & 0 \end{bmatrix},$$

with $K, G \in \mathbb{R}^{n_\Gamma \times n_\Gamma}$, $F \in \mathbb{R}^{N \times N}$ nonsingular. Let Z be a basis for the nullspace of $\mathbf{1}_N$. Then

1. $\lambda = 1$ with multiplicity $N + 1$;
2. the remaining n_Γ eigenvalues satisfy the eigenvalue problem

$$(K - Q)\mathbf{z} = \lambda(G - Q)\mathbf{z},$$

where $Q = DZ(Z^T F Z)^{-1}(DZ)^T$.

Proof. The proof is similar to that given in [17] (see also [27, pp. 180–181]). \square

Remark 5.2. The above result indicates that the increase in size by N due to our problem reformulation (4.1)–(4.4) is automatically taken care of by our constraint interface preconditioner, which maps $N + 1$ eigenvalues to 1. The remaining eigenvalues will depend on the closeness of our preconditioner H to S_{11} . As described above, we tried to incorporate this property by a choice of H that is spectrally equivalent to the dominant part of S_{11} , namely $S_{\Gamma\Gamma}$.

The main issue with the definition of S_1 is the full matrix H arising in the (1,1)-block. This matrix needs to be computed via an expensive matrix square-root calculation; moreover, it needs to be employed in order to implement the action of the inverse of S_1 on a given vector. A practical alternative can be derived from the following constrained Lanczos decomposition of S_1 .

Let

$$V_\Gamma^T L_\Gamma V_\Gamma = T_\Gamma, \quad V_\Gamma^T M_\Gamma V_\Gamma = I_\Gamma$$

denote the generalized Lanczos decomposition of the pencil $[L_\Gamma, M_\Gamma]$ in exact arithmetic, where V_Γ is an orthogonal matrix and T_Γ is a tridiagonal, symmetric, and positive-definite matrix. Define $T = T_\Gamma \oplus T_\Gamma$, $V = V_\Gamma \oplus V_\Gamma$. Then $H = VT^{1/2}V^T$ (see also [1]). Consider the QR-factorization

$$UR = [S_{12} \quad \mathbf{0}] V,$$

where U is orthogonal and define

$$D := U^T \begin{bmatrix} S_{22} & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} U.$$

We obtain the following orthogonal factorization of S_1 ,

$$S_1 = \begin{bmatrix} V & \\ & U \end{bmatrix} \begin{bmatrix} T^{1/2} & R^T \\ R & D \end{bmatrix} \begin{bmatrix} V^T & \\ & U^T \end{bmatrix} =: W\mathcal{T}W^T.$$

We will refer to the above representation of S_1 , seen as a two-by-two block matrix, as the constrained Lanczos factorization of S_1 .

Given our preconditioning task, consider now the product

$$\mathbf{z} = S_1^{-1}\mathbf{v} = W\mathcal{T}^{-1}W^T\mathbf{v}.$$

An approximation to \mathbf{z} can be constructed using a partial factorization:

$$\mathbf{z} \approx \mathbf{z}_k := W_k\mathcal{T}_k^{-1}W_k^T\mathbf{v},$$

where we define

$$W_k := \begin{bmatrix} V_k & \\ & U_k \end{bmatrix}, \quad \mathcal{T}_k := \begin{bmatrix} T_k^{1/2} & R_k^T \\ R_k & D_k \end{bmatrix}, \quad D_k = U_k^T \begin{bmatrix} S_{22} & \mathbf{1} \\ \mathbf{1}^T & 0 \end{bmatrix} U_k.$$

The preconditioning operator implicit in the definition of \mathbf{z}_k will be denoted by S_2 :

$$\mathbf{z} \approx S_2^{-1}\mathbf{v}.$$

Its implementation requires

- i. a partial Lanczos factorization of the (1,1)-block of S_1 ; this yields a matrix V_k of Lanczos vectors and a block tridiagonal matrix T_k ;
- ii. a QR-factorization of the (1,2)-block of S_1 multiplied by V_k ; this yields the factors U_k, R_k arising in W_k and \mathcal{T}_k , respectively.

The number of Lanczos vectors in V_k is expected to be small; correspondingly, the sizes of R_k, D_k will also be small and the resulting matrix \mathcal{T}_k will be easy to invert. The overall complexity for the above procedure is of order $O(kn_\Gamma)$. Thus, the application of the interface preconditioner will not dominate the cost of a subdomain solve provided we work with subdivisions for which $kn_\Gamma = O(n_{I_i}^2)$, where we assumed that the cost of inverting a subdomain Jacobian matrix is the cost that a direct method requires to invert a banded matrix of size n_{I_i} with bandwidth $\sqrt{n_{I_i}}$.

6. Numerical experiments. In order to illustrate the performance of the solution method described in section 6.1, we consider a model test problem based on compliance design. The problem involves a cantilever beam posed on a rectangular design domain as illustrated in Figure 1, with clamping applied along the left edge and a force applied in the middle of the right edge. The density contour plot corresponding to the optimal design is displayed in Figure 2. Symmetry is a feature which may be exploited computationally; however in this paper we chose to retain the original design domain in order to test the performance of our solution method on the full problem.

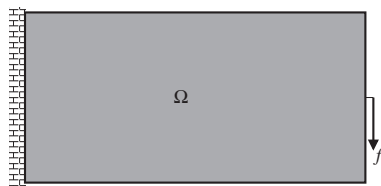


FIG. 1. Illustration of the cantilever beam problem.

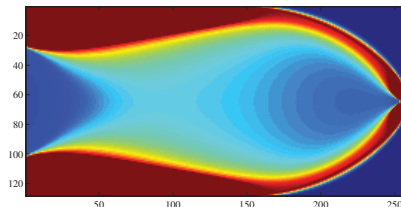


FIG. 2. Contour plots of optimal density distribution for the model problem.

6.1. Implementation details.

6.1.1. Finite element method. We use a subdivision \mathcal{T}_h of Ω into square elements of size h . We seek approximations

$$u_h \in \mathcal{V}_h = \{v \in (H_D^1(\Omega))^2 : v|_T \in \mathcal{P}_2(T)\}, \quad \rho_h \in \mathcal{Q}_h = \{q \in L^\infty(\Omega) : q|_T \in \mathcal{P}_0(T)\}$$

for all $T \in \mathcal{T}_h$, where $\mathcal{P}_k(U)$ denotes the space of degree k polynomials defined on U . We employ uniform refinement, in order to exhibit the behavior of our preconditioning technique with respect to the mesh parameter h . We note here that the space \mathcal{Q}_h^c is not constructed explicitly, and that it was only introduced in order to provide the mathematical description of our problem.

6.1.2. Interior point algorithm. We use a textbook interior point algorithm; the key details are included below; for full details see [23, Chap. 19].

We repeat the following steps until convergence:

1. Solve a sequence of Newton systems (3.10) to get $\Delta \mathbf{y}^k$.
2. Find the step length α (see below).
3. Update the solution

$$\mathbf{y}^k = \mathbf{y}^{k-1} + \alpha \Delta \mathbf{y}^k.$$

4. Update the penalty parameters via

$$r := r/4, \quad s := s/4.$$

We start with $r = s = 1$ and continue until they are brought below a tolerance of 10^{-6} . A more sophisticated version of the code, with an adaptive choice of the penalty parameters r and s can be found in [15]. However, we have never observed any difficulties with this simple update of r and s .

Step length. In the interior point method we cannot take a full Newton step resulting from the solution of (3.10), as this would lead to an infeasible point. We propose a technique that will effectively involve finding α_L such that $\rho_i + \Delta \rho_i \geq \underline{\rho}$

for i such that $\Delta\rho_i < 0$ and α_U such that $\rho_i + \Delta\rho_i \leq \bar{\rho}$ for i such that $\Delta\rho_i > 0$. Therefore, we consider obtaining α_L and α_U as follows:

$$\alpha_L = 0.9 \cdot \min_{i:\Delta\rho_i < 0} \left\{ \frac{\rho - \rho_i}{\Delta\rho_i} \right\},$$

$$\alpha_U = 0.9 \cdot \min_{i:\Delta\rho_i > 0} \left\{ \frac{\bar{\rho} - \rho_i}{\Delta\rho_i} \right\}.$$

The constant 0.9 represents an appropriate shortening of the Newton step to the interior of the feasible region. In the event that both α_L and α_U are greater than 1, the step will be shortened appropriately:

$$\alpha = \min \{ \alpha_L, \alpha_U, 1 \}.$$

This procedure is relatively simple and straightforward to implement. A more sophisticated line search procedure is described in [15] and could potentially be used here. However, it will be illustrated later that the current technique was able to yield desirable results.

Initial approximation. We start the interior point algorithm with a uniform distribution of the design variable $\boldsymbol{\rho}$ chosen with respect to the mass constraint (3.3)

$$\boldsymbol{\rho}_{\text{ini}} = \mathbf{1}.$$

The initial displacements \mathbf{u}_{ini} are then computed from the equilibrium equation

$$A(\boldsymbol{\rho}_{\text{ini}}) \mathbf{u}_{\text{ini}} = \mathbf{f}.$$

6.1.3. Domain decomposition. We used only regular subdivisions into rectangular subdomains. The corresponding sizes of the resulting interfaces are illustrated in Table 1. It is evident (and well known) that in order to balance the complexities of the interface and subdomain problems, the increase in the number of subdomains should be paralleled by a decrease in h . Aside from regular decompositions, one could also decompose the domain in an adaptive fashion based on the changing nature of the design. This could be carried out either at each outer iteration, or alternatively once after a fixed number of outer iterations based on the (previously mentioned) observation that the density will only be subject to minor changes after a relatively small number of iterative steps. In terms of a nonregular subdivision, the graph partitioning tool METIS [16] may be used in order to partition the finite element mesh into nonregular subdomains.

6.1.4. GMRES. We used an inexact Newton-GMRES method preconditioned by either S_0, S_1 ; flexible GMRES was used for the case of S_2 . The GMRES stopping criterion was the reduction of the norm of the initial residual by a factor of 10^6 .

TABLE 1
Mesh information for cantilever beam experiment.

h	n	n_Γ		
		$N = 4$	$N = 16$	$N = 64$
1/64	41,355	384	1,140	2,604
1/128	164,619	768	2,292	5,292
1/256	657,027	1,536	4,584	10,668

TABLE 2
GMRES (Newton) iterations required for solving (3.1) using preconditioners S_0, S_1, S_2 .

		Avg GMRES (Newton)			Total GMRES its.		
No. subdomains:		4	16	64	4	16	64
Preconditioner	$\begin{matrix} h & \theta \end{matrix}$	0.5	0.6	0.7	0.5	0.6	0.7
S_0	1/64	7.29 (14)	10.57 (14)	13.86 (14)	102	148	194
	1/128	5.93 (15)	8.13 (15)	8.93 (15)	89	122	134
	1/256	5.25 (16)	6.81 (16)	7.50 (16)	84	109	120
S_1	1/64	11.36 (14)	25.64 (14)	35.00 (13)	159	359	455
	1/128	10.60 (15)	21.80 (15)	33.12 (16)	159	327	530
	1/256	10.25 (16)	19.94 (16)	29.82 (17)	164	319	507
S_2	1/64	12.21 (14)	31.36 (14)	50.46 (13)	171	439	656
	1/128	12.00 (15)	27.47 (15)	43.47 (15)	180	412	652
	1/256	11.00(16)	26.41 (17)	40.06 (17)	176	449	681

6.1.5. Constrained Lanczos factorization. The implementation of the action of S_2^{-1} requires us first to generate the matrices S_{12} and S_{22} . This is achieved as an additional preprocessing step involving one set of subdomain solves. The number of Lanczos vectors is taken to be $k = O(\sqrt{n_\Gamma})$, so that the overall complexity of using the preconditioner is of order $O(n_\Gamma^{3/2})$.

6.2. Numerical results. Table 2 displays the results for our test case for a range of mesh and subdomain sizes. The results were obtained using a Linux machine with an Intel® Core™ i7 CPU 870 @ 2.93 GHz with 8 cores. The upper and lower limits on the density ρ were set at 1 and 10^{-2} , respectively, with the permissible volume in each test case defined to be $\mathcal{M}_\Omega/2$.

The first observation arising from our numerical experiments is that S_0 has performance independent of mesh size and almost independent of the number of subdomains; moreover, the number of iterations is low (averages between 5–8 iterations on the largest problem), with only a small departure from the optimal count of 2 iterations corresponding to the case where the exact Schur complement is used. This confirms the earlier assumption that the matrix E in (5.2) is negligible and that the preconditioner S_0 is optimal in the same sense as the Schur complement.

With regard to parameter dependence, we note that the number of iterations decreases with h in all experiments. This is somewhat expected, given that S_2 is essentially an approximate implementation of S_1 , which incorporates in the (1-1) block the finite element discretization of the continuous Steklov–Poincaré operator for the elasticity equations. An interesting fact is that the preconditioning technique S_2 appears to occasionally outperform the preconditioner S_1 ; however, different preconditioners lead to different Newton convergence histories given the adaptive stopping criterion employed, which may result in overall complexities more favorable for the constrained preconditioning approach.

The table also indicates what appears to be a logarithmic dependence on the number of subdomains. We found this difficult to analyze, but this behavior is not unlike that exhibited by similar substructuring preconditioning techniques in [1]. This

suggests that the preconditioner S_2 has the ability to match the properties of the discrete fractional Sobolev norm in a constrained setting. This represents a novel approach which could be useful in other constrained optimization settings and for other PDE models.

The values of θ listed in Table 2 were chosen by experimentation based on similar observations for the linear elasticity problem reported in [28], where it is noted that different values of θ may be able to provide a closer approximation to the decay of the associated Steklov–Poincaré operator. Similar findings were found numerically in this work also, with the best values of θ used in order to produce the results reported in the table.

Despite the fact that a logarithmic dependence is noted for an increasing number of subdomains, the computational benefits gained as a result of distributing calculations amongst an increasing number of processors can lead to a significant speedup when compared to solving the original problem on the global domain Ω . Exact calculations displaying this behavior are not included here, however, the interested reader is referred to [28], where notable speedup was observed under the preconditioner described in (5.5) for the optimality criteria method for topology optimization, which, unlike the interior point approach in this paper, requires the solution of a linear elasticity problem at each step.

7. Conclusions. We described a novel domain decomposition approach coupled with an interior point method for compliance minimization problems arising in the field of topology optimization. The problem was reformulated in order to allow for well-posed subdomain problems which could be viewed as local Jacobian solves. This was an important step which allowed for the domain decomposition method to be well-defined. The resulting interface Schur complement problem yielded an indefinite matrix which included a global volume constraint; consequently, an indefinite preconditioner was devised in order to incorporate the properties and the structure of the interface Schur complement matrix. This resulted in a technique requiring the inversion of a so-called constrained discrete fractional Sobolev norm, the application of which was performed via a certain constrained Lanczos procedure. We tested the resulting method on a standard test problem of topology optimization, with experiments indicating independence from the mesh parameter, although a dependence on the number of subdomains was noticed.

Some of our current investigations include nonregular decompositions, as well as adaptive decompositions based on current iterates. The constrained Lanczos factorization, which allowed the sparse implementation of our interface preconditioner, will be the subject of further study. The precise role played by the parameter θ also requires more analysis and experimentation in order to quantify the most appropriate value of θ for a decomposition into any given number of subdomains. Finally, the reformulation of the problem resulting in Jacobian subproblems on subdomains is also worthy of further investigation as it points to nonlinear domain decomposition approaches, such as that described in [29].

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