Large Scale Topology Optimization Using Preconditioned Krylov Subspace Recycling and Continuous Approximation of Material Distribution

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Abstract. Large-scale topology optimization problems demand the solution of a large number of linear systems arising in the finite element analysis. These systems can be solved efficiently by special iterative solvers. Because the linear systems in the sequence of optimization steps change slowly from one step to the next, we can significantly reduce the number of iterations and the runtime of the linear solver by recycling selected search spaces from previous linear systems, and by using preconditioning and scaling techniques. We also provide a new implementation of the 8-node brick (B8) element for the continuous approximation of material distribution (CAMD) approach to improve designs of functionally graded materials. Specifically, we develop a B8/B8 implementation in which the element shape functions are used for the approximation of both displacements and material density at nodal locations. Finally, we evaluate the effectiveness of several solver and preconditioning strategies, and we investigate large-scale examples, including functionally graded materials, which are solved with a special version of the SIMP (solid isotropic material with penalization) model. The effectiveness of the solver is demonstrated by means of a topology optimization problem in a functionally graded material with 1.6 million unknowns on a fast PC.

Keywords: Topology optimization, material distribution, fast solution schemes, functionally graded materials, finite elements.

INTRODUCTION

The desired result of topology optimization is a domain where each element either is void or contains material. However, it is mathematically difficult to work with integer variables, thus relaxation is usually applied. By allowing intermediate material density between 0 and 1, we can compute the desired sensitivities. To obtain a final solution without intermediate densities, an intermediate density is penalized and made uneconomical in terms of the stiffness as a function of density or volume. At an early stage, the homogenization method [1] was used to derive the stiffness of intermediate densities from certain configurations of microstructures. However, the final solution is not supposed to contain microstructures. Therefore, the derivation of the stiffness for intermediate material density based on the homogenization approach only serves as a

means of penalization. Later the Solid Isotropic Material with Penalization (SIMP) approach [2] was proposed as a simpler way to derive the stiffness for intermediate material density (by interpolation). In the finite element setting, we use the nodal approach with continuous approximation of material distribution (CAMD). The CAMD approach is then extended to model functionally graded materials (FGMs) with the so-called FGM-SIMP model [6].

Problem Statement in the Continuum Setting

The problem formulation for topology optimization using the CAMD approach is given below for the minimization of compliance subject to a volume constraint.

$$\min_{\rho_e \in [0,1]} \mathbf{f}^T \mathbf{u}$$

$$\text{such that} \quad \begin{cases} \mathbf{K}(\mathbf{E}_e)\mathbf{u} = \mathbf{f} \\ \mathbf{E}_e = (\rho_e(\mathbf{x}))^p \mathbf{E}_0 \\ \rho_e(\mathbf{x}) = \sum_{i=1}^{n} N_i \rho_e^{(i)} \\ \sum_{e=1}^{m} \int_{\Omega_e} \rho_e dv_e \leq V_0 \end{cases},$$

where n is the number of nodes in each element, and m is the total number of elements. Moreover, $\mathbf{K}$ denotes the stiffness matrix, which is a function of the density distribution ρ, $\mathbf{f}$ is the load vector, $\mathbf{u}$ is the displacement vector, $\mathbf{E}$ denotes the matrix of elastic properties of the material, V_0 is the total volume in use, and N_i refers to the shape functions of the finite element being used. Further details can be found in [6] (addressing FGMs) and related references in [3, 7].

Functionally Graded Material (FGM) Domain

In case the domain is functionally graded, that is, the properties of the material in the domain vary in space, the elasticity tensor is a variable with respect to location. To handle material gradation the FGM-SIMP model is used [6]:

$$\mathbf{E}^H = \rho^p \mathbf{E}_0(\mathbf{x}).$$

For a simple exponentially graded material in 3D, the FGM-SIMP model becomes

$$\mathbf{E}_0(\mathbf{x}) = \mathbf{E}_0 e^{\alpha x + \beta y + \gamma z}.$$

The CAMD approach is recommended to capture the gradient of FGM properties inside each element.

KRYLOV SUBSPACE RECYCLING FOR SYMMETRIC MATRICES

The finite element analysis in topology optimization requires the solution of a sequence of linear systems, which in most applications are symmetric. In each

optimization step, the algorithm updates the density of each element (the topology), and the changes in the design variables tend to be small from one optimization step to the next. This holds especially towards the end of the optimization process, when the topology is converging. Hence, the optimization leads to small changes from one linear system to the next, and certain properties of the solution of one system, or the search space generated for one system, remain useful for subsequent systems. First, the solution of one system can be used as an initial guess of the next system to reduce the initial residual. Second, an approximate invariant subspace derived from the Krylov space generated for one linear system can be used to improve the convergence rate solving the next linear system. Other subspaces may also be used for 'recycling' [5], and these techniques may greatly improve the convergence rate of Krylov solvers if an appropriate subspace is chosen. This is the basic idea of Krylov subspace recycling [5]. For symmetric systems, we adapt the MINRES algorithm [4] for Krylov subspace recycling. By exploiting the symmetry of the matrix, we make the iteration cheaper and the recycling scheme more effective. Further details can be found in reference [8].

PRECONDITIONING AND SCALING

For Krylov subspace methods applied to symmetric or Hermitian systems the ratio between the absolute largest and smallest eigenvalues, which is the condition number of the matrix, governs an upper bound on the convergence rate. The linear systems arising from large-scale finite element simulations in physics and engineering are generally ill-conditioned. In topology optimization, the ill-conditioning is significantly exacerbated by the wide range of element densities. To remedy this ill-conditioning, we rescale the stiffness matrices such that the diagonal coefficients are all the same, which is the case for a problem with homogeneous density. We propose to rescale the stiffness matrices $\mathbf{K}$ by multiplying with a diagonal matrix on both sides,

$$\widetilde{\mathbf{K}} = \mathbf{D}^{-1/2} \mathbf{K} \mathbf{D}^{-1/2},$$

where $\mathbf{D}$ is the diagonal of $\mathbf{K}$. The importance of such scaling and why it helps is explained for an idealized 1D problem in [8]. To further improve the conditioning and reduce iterations, we apply an incomplete Cholesky preconditioner with zero fill-in to the *explicitly* rescaled system,

$$\widetilde{\mathbf{K}} = \mathbf{D}^{-1/2} \mathbf{K} \mathbf{D}^{-1/2} \approx \widetilde{\mathbf{L}} \widetilde{\mathbf{L}}^{T}.$$

Figure 1 compares the condition numbers of four matrices, the original stiffness matrix $\mathbf{K}$, the diagonally scaled stiffness matrix $\widetilde{\mathbf{K}}$, and both matrices multiplied with their respective incomplete Cholesky preconditioners. The rescaling significantly reduces the condition number, and also improves the effectiveness of the incomplete Cholesky preconditioning. Note that applying the Cholesky preconditioner to the stiffness matrix without first scaling leads to a condition number that is worse than that of the diagonally scaled system (without a Cholesky preconditioner).
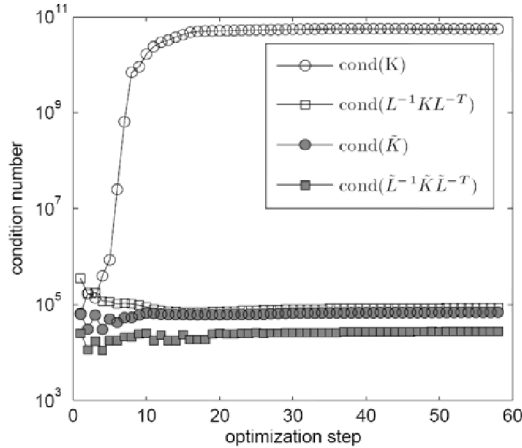
FIGURE 1. Condition numbers for (1) the original stiffness matrices, $\mathbf{K}$, (2) their incomplete Cholesky preconditioned forms, $\mathbf{L}^{-1}\mathbf{K}\mathbf{L}^{-T}$, (3) the diagonally scaled stiffness matrices, $\widetilde{\mathbf{K}}$, and (4) their incomplete Cholesky preconditioned forms, $\widetilde{\mathbf{L}}^{-1}\widetilde{\mathbf{K}}\widetilde{\mathbf{L}}^{-T}$.

NUMERICAL RESULTS

In this section, we give numerical results to illustrate the effectiveness of our recycling MINRES method and preconditioning as well as two large-scale design examples with the CAMD scheme.

Krylov Subspace Recycling

To test the effectiveness of our recycling MINRES solver, we solve a cantilever beam that is subject to a point load at the center of the free surface. The domain is discretized using 84×28×28 brick elements and continuous distribution of material density inside each element (B8/B8). Figure 2 shows a comparison of iteration counts and run times for the standard and recycling MINRES (RMINRES) solvers for several parameters choices (see [8]). Without recycling, the time to solve each linear system in the optimization problem is roughly constant. After an initial phase, this time is about 80% higher than the time to solve linear systems using the RMINRES solver with the best parameter choice. Our recycling method exploits the slow variation of the linear systems, and thus reduces the number of iterations significantly.

Large-Scale Design with CAMD Approach

To demonstrate the effectiveness of the iterative solver and the CAMD approach, we solve a design problem of approximately 1.6 million unknowns on a single processor PC. The smooth approximation of material density using the CAMD approach for large problems leads to a higher fidelity solution with smoother boundary surfaces. Figure 3 shows the final design in a homogeneous material.
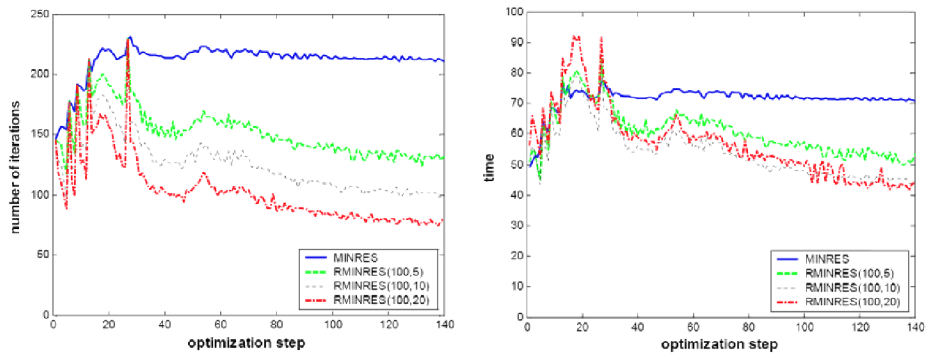
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FIGURE 2. Comparison of iteration counts and runtimes between the standard MINRES solver and the recycling MINRES (RMINRES) solver for several parameters choices.
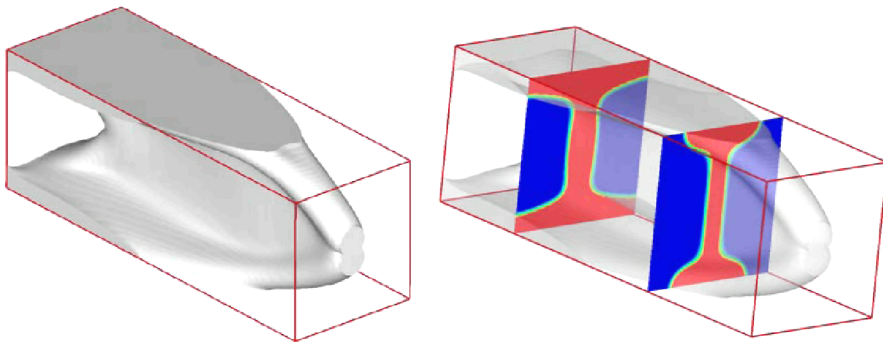

FIGURE 3. A cantilever beam design solved using the preconditioned, recycling MINRES solver and the CAMD approach; mesh size: $210 \times 70 \times 70$ B8/B8 elements; total number of unknowns: approximately 1.6 million. Left: final design of an homogeneous material. Right: Two cross-sections from the final design.

Large-Scale Design in a Functionally Graded Domain

We also implemented the cantilever beam design for a simple exponentially graded material in 3D using the FGM-SIMP model, described earlier. In this example, the material is only graded along the height of the beam with non-homogeneity coefficient $\beta = 2/h$ ($a = g = 0$), where h is the height of the beam. The configuration of the problem is the same as in the previous example. The results shown in Figure 4 refer to a non-symmetric structural configuration, which illustrates the effect of the material gradation in the design domain.
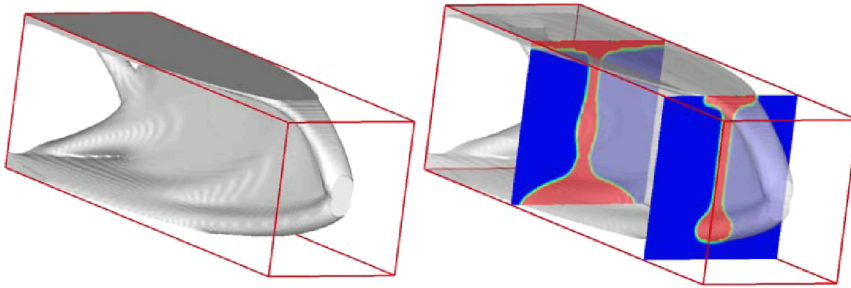
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FIGURE 4. A cantilever beam solved in the FGM domain using the preconditioned, recycling MINRES solver and the CAMD approach; mesh size: 210×70×70 B8/B8 elements; total number of unknowns: approximately 1.6 million. Left: final design of FGM beam. Right: two cross-sections from the final design.

CONCLUSIONS

As suggested by the examples in this paper, the use of topology optimization is moving from conceptual designs towards final designs that can be used for fabrication. This evolution of the technology can be achieved by combining more accurate modeling (CAMD) with efficient solution schemes for large-scale problem (Krylov subspace recycling and preconditioning).

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