Fast deflated conjugate gradient method with proper orthogonal decomposition for topology optimization

Kota Watanabe¹*, Kaito Oshima¹

¹ Graduate School of Engineering, Muroran Institute of Technology

*k-wata@muroran-it.ac.jp

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Abstract. A fast linear solver for topology optimization using a deflation technique with Proper Orthogonal Decomposition (POD) is discussed. The topology optimization method based on evolutionary algorithms requires huge computational cost. In this reason, a deflated Preconditioned Conjugate Gradient (PCG) method is introduced so as to reduce the cost of finite element analysis. The deflation technique decomposes the solution into fast and slowly converging components. The slow components can be solved by direct methods with low computational cost due to small dimensions. Therefore, the deflated PCC method can improve the convergence of PCG. However, the deflated PCG requires to find the slow components. In this study, a POD method with snapshots is introduced. In the optimization process, solution vectors corresponding to parents are used for the snapshots. Orthogonal vectors for the deflation are constructed from the snapshots. Numerical results show that the present method can reduce the computational cost.

Keywords: Deflation method, Proper Orthogonal Decomposition, Topology optimization

1. Introduction

Fast linear solvers are an important factor to reduce computational cost of finite element analyses. In the optimization for electromagnetic devices, the finite element analysis occupies almost all computational cost in the optimization process. Therefore, it is important to reduce the cost in solver process by introducing fast linear solvers.

The preconditioned conjugate gradient method has been widely used in finite element (FE) analysis of electromagnetic field problem due to good convergence property, stability, and robustness. In particular, the Incomplete Cholesky (IC) preconditioner is known as one of the best performances in view of convergence property. Therefore, The ICCG method is the best solver for symmetry system matrices obtained by FE analyses.
The deflation technique that replaces small eigenvalues with zeros in the system matrix can improve the convergence of ICCG method [1,2,3,4,5]. Therefore, the deflated ICCG method is a useful solver for FE analyses. The relationship between the deflation technique and other methods such as Implicit Error Correction (IEC) and Explicit Error Correction (EEC) method are discussed in [1]. The deflated technique has been applied to diffusion problem with extreme contrasts in the coefficient matrix [2], and to boundary value problems [3]. Reference [4] shows the effect of the deflated technique in magnetostatic problems with large jumps in the magnetic permeability. The authors applied the deflated technique to finite element analysis with infinite elements which affect convergence of CG method [5]. To use the deflated ICCG method, the deflated ICCG requires finding slowly converging components such as eigenvectors corresponding to basic modes. However, it is high computational cost to obtain them. To solve this difficulty, simple quasi vectors instead of eigenvectors can be used [1]. However, the improvement of convergence is limited. In this study, a Proper Orthogonal Decomposition (POD) method is introduced [6]. In the optimization process by using the evolutionary algorithm such as well-known genetic algorithm, solution vectors corresponding to the past-evaluated individuals (shapes) are used for snapshots. A Singular Value Decomposition (SVD) is applied to them, and then we obtain an orthogonal matrix that can be used for the slowly converging components in the deflation method.

The model order reduction using POD with snapshots is known as a method to reduce computational cost for finite element analysis [7,8]. However, the accuracy of solution depends on the choice of snapshots. On the other hand, in the present method, the selection of snapshots does not affect the accuracy of solution, though the convergence depends on the selection. The present method is applied to a topology optimization of shield model. The efficiency of the present method in linear magnetostatic analyses is investigated.

2. Formulations

2.1. Topology optimization based on immune algorithm

In this study, an immune algorithm based on on/off method is adopted for topology optimization [9]. The immune algorithm that is inspired from the clonal selection principle is one of the evolutionary algorithms. This method has a good valance of local and global search characteristics in order to avoid falling into local optima. This is a merit of this method in comparison with the well-known genetic algorithm that leans to the global search. The on/off method uses a 2D map for representing the material distribution in search space. In this study, finite element mesh is used for the 2D map. Each finite element is associated to a binary value indicating either the presence or absence of material. The procedures of the present method are summarized as follows:
1. Generate an initial population of \( N_p \) candidate antibodies.

2. Evaluate the objective function for each antibody.

3. Test a stop criterion. If it is satisfied, stop the procedures.

4. Eliminate \( P \% \) low-ranking antibodies.

5. Generate clones for each surviving antibody.

6. Small-modifications called affinity maturation on surface are applied to the clones, which are then evaluated over the objective function. Only the best candidate solution from each subset of (parent antibody + clones) is allowed to survive to the next generation.

7. Add randomly generated antibodies to replace the ones eliminated in Step 4, in order to keep the population size constant.

8. Back to step 2.

2.2. Deflation method with POD

Let us consider a system of linear equations with \( n \) DoF (Degree of Freedom) obtained by a magnetostatic finite element analysis,

\[
Ax = b
\]  

where \( A \) is coefficient matrix, \( x \) and \( b \) are solution and right hand side vector respectively. The solution \( x \) is decomposed into slowly and fast components as,

\[
x = Wy + \hat{x} - Wy
\]  

where \( W = [w_1, w_2, ..., w_k] \in \mathbb{R}^{n \times k}, w_i \in \mathbb{R}^{n \times k} (i = 1, 2, ..., k). A\)-orthogonality is imposed on the vectors \( w_i \) to \( x - Wy \) results in

\[
W^tAWy = W^tAx.
\]  

The slowly converging component \( Wy \) can be expressed as

\[
Wy = W(W^tAW)^{-1} W^tAx
\]  

where \( Q \in \mathbb{R}^{n \times n}. \) Moreover, let us introduce the matrix \( P \) given by,

\[
P = I - Q = I - W(W^tAW)^{-1} W A.
\]  

Consequently, the solution \( x \) can be expressed as,
The fast converging component $Px$ can be obtained by solving $APx = P'Ax = Pb$. The slowly component $Qx$ is obtained from,

$$Qx = W(W'AW)^{-1}W'b.$$  

(7)

The convergence of ICCG method depends on the condition number that is calculated by the ratio of the largest eigenvalue $\lambda_{\text{max}}$ to the smallest non-zero eigenvalue $\lambda_{\text{min}}$ of system matrix. The deflation technique which replaces such the small eigenvalues with zeros in the system matrix can improve the convergence. Here the non-zero eigenvalue of system matrix is sorted in ascending order as $\lambda_{\text{min}} \leq \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{n'}$ is the number of non-zero eigenvalues. If the eigenvectors corresponding to the $\lambda_{i}$ ($i = 1, 2, \ldots, k$) are chosen as $w_i$, the condition number of the deflated system matrix becomes $\lambda_{\text{max}} / \lambda_{k+1}$. In the typical finite element analysis, small number of eigenvalues causes the large condition number. Therefore, even if a small $k (k << n)$ is chosen, the convergence of deflated ICCG can be improved. The inverse matrix $(W'AW)^{-1}$ in (7) can be computed by direct solvers with low computational cost because the dimension of the matrix is $k \times k$.

It is known that the eigenvectors $w_i$ corresponds to the low spatial frequency components of solution vector. Quasi eigenvectors that express simple distribution of solution vector field can be used instead of real $w_i$. In the model order reduction, the solution $x$ is projected into the space spanned by the $w_i$ that is obtained by POD with snapshots. This idea is introduced into the deflated ICCG method in this study. The snapshot matrix is constructed by,

$$X = [x_1^P \ x_2^P \ \cdots \ x_{N_p}^P].$$  

(8)

where $x_i^P, i = 1, 2, \ldots, N_p$ is the solution corresponding to the parent antibody in the step 2 of the procedures of immune algorithm shown in the previous section. The SVD is applied to $X$,

$$X = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_{N_p} u_{N_p} v_{N_p}^T.$$  

(9)

where $u_i$ and $v_i$ are left and right singular vectors and $\sigma_i$ are the singular values in descending order. In the typical case, the $N_p$ is less than several dozens. Therefore, the computational cost of SVD is negligible. The matrix $W$ is assembled as $W = [u_1 \ u_2 \ \cdots \ u_k], k \leq N_p$ and used the deflation method to evaluate clones in the step 6. The clones have almost same structure as the parents. Thus, it is expected that the matrix $W$ obtained by the SVD works well to improve the convergence of deflated ICCG method. The snapshot matrix is updated in each generation. The procedures of the present method based on [10] are summarized in Fig. 1.
3. Numerical results

We applied the present method to a magnet shield model that is a benchmark problem for topology optimization as shown in Fig. 2(a). The objective is to minimize the flux density in the evaluate region. The finite element analysis for magnetostatic field problem was performed to obtain the flux density. As shown in Fig 2(b) (c), two type of finite element meshes were prepared to compare the convergence property of the present method in different degree of freedoms. Because of the limitation of the optimization method, the finite element mesh consists of square elements and very thin rectangular elements. These thin elements result in poor convergence of ICCG method. The optimization is performed by 100th generation with $N_p = k = 4, P = 0.2$.

The computational cost of present method and conventional ICCG method are summarized in Table 1. The present deflated ICCG method can reduce the CPU time in comparison with the conventional ICCG method. The reduction rate of computational cost is almost same.
in both meshes. The cost to perform the SVD is only less than 7 seconds in the large size mesh (type II). Fig.3 shows the average number of iterations in each generation. We can see that the convergence of the present method becomes better as the optimization progresses. It seems that the snapshots work well as the optimization advances, because variety of shapes are lost and the shapes converge into the optimum shape. The average number of iterations for whole period is 393 (type I) and 839 (type II) in the present method. On the other hand, that in the conventional ICCG method is 711 (type I) and 1424 (type II).

We also investigated a relationship between convergence of present method and the number of snapshots $N_p$. In the range of $N_p = 4$ to 10, we can find a small difference in the convergence, and the case of $N_p = 4$ shows the best convergence under the fixed $k = 4$. In the optimization process of this study, the population size is same as $N_p$. Therefore, the variety of shapes in the population increases with $N_p$. The convergence efficiency gets worse in the case of $N_p > k$. If the value of $k$ increases with $N_p$, the convergence would be maintained. However, the computational cost for each iteration increase with $k$ because of calculation cost in the inverse matrix $(W^T W)^{-1}$ in (7). Taking the above trade-off relationship into consideration, we choices $k = 4$. Figure 4 shows the optimized design obtained by the present method. It is note that the design shown in Fig. 4 coincides with that by the ICCG method.

Table 1: Comparison of Computational cost

| Method                     | Total CPU time (sec) | CPU time for SVD (sec) |
|----------------------------|----------------------|------------------------|
| Mesh type I                |                      |                        |
| Conventional ICCG          | 20702                | -                      |
| Deflated ICCG with POD     | 13238 (2.8)          | 2                      |
| Mesh type II               |                      |                        |
| Conventional ICCG          | 376382               | -                      |
| Deflated ICCG with POD     | 24689 (6.7)          | -                      |

CPU: Intel Xeon E5-2670v2, 8 cores used
Intel C++ compiler with MKL and OpenMP are used.
Figure 2: Magnetic shield model for topology optimization

Figure 3: Average number of iterations in present method.
4. Conclusion

The deflated ICCG with POD method for topology optimization so as to reduce computational cost is proposed in this paper. The topology optimization based on the evolutionary algorithm requires huge computation time. Therefore, fast linear solvers are important to reduce the cost. Numerical results show that the present method can significantly reduce the computational cost of topology optimizations. Moreover, the present method does not lose the accuracy of solution. On the other hand, the conventional model order reduction with POD method cannot ensure the accuracy. The present method can be applied to other optimization problems.

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