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Reaction-diffusion equation based topology optimization combined with the modified conjugate gradient method

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ABSTRACT

The reaction-diffusion equation (RDE) based design method is a type of topology optimization methods generally employing the finite element method for physical field analysis. It uses the RDE as the design variable update scheme and its diffusion term contributes to regularize the density field. The drawback of the method is that the diffuse interfacial layer which affects the complexity of the optimization result contains the gray scale area. Moreover, the update scheme of the RDE based optimization method has employed the steepest descent method so far, although its convergence rate becomes slow near the optimum. To overcome such drawbacks, this study proposes a modified conjugate gradient method for the RDE based design method to stabilize the convergence with some numerical restrictions. It also contributes for effective elimination of intermediate materials by supplying the implicit mechanism to change the influence between the reaction and the diffusion term in the RDE. Electromagnetic as well as structural design results are given to confirm the validity of the proposed approach.

1. Introduction

Since the first proposal by Bendsøe and Kikuchi [1], topology optimization has been regarded as an effective tool for structural optimization in various physics systems such as statics [1–3], dynamics [4–6], magneto-statics and electromagnetics [7–11], heat [12,13] and so forth. Different from traditional design approaches such as size or shape optimization, topology optimization enables the generation of holes in a structure, so that it may produce an unprecedented design result with a small amount of material. Representative approaches of topology optimization are classified into the homogenization design method [1–5,8], the solid isotropic material with penalization (SIMP) method [7,9,10,12, 14,15], the level set method [16–19], and the phase field method [20, 21]. In topology optimization results, the existence and the void of a material is indicated as the value of 0 and 1, respectively, and the intermediate material is assigned to a value between 0 and 1 in the design result. Among them, the SIMP method has been widely used because it has intuitively simple conception and is easy to use with filtering schemes or perimeter constraints to relax the numerical instability and gray portion [22–24].

The original level set method for structural design derives the optimal shape by finding the appropriate shape boundary based on the level set function using Hamilton-Jacobi equation [16,17]. However, it cannot create new holes because the method allows the shape change tracing the existing boundary only. As a result, the topological derivative [18,19] is added to realize topological structure design. The level set method also requires the re-initialization process to update the displacement characteristics and it may cause expensive computation cost. To avoid such defects, Yamada et al. [25] proposed the new approach to construct a reaction-diffusion equation (RDE) by using the fictitious energy term. The method updates the level set function by the RDE based on the topological derivative and it enables topological design because the reaction terms work as the topological derivative. It has been applied to structural design in various physical fields [13,26,27].

The phase field method has been widely applied to simulate interfacial dynamics for phase transition phenomena [28] and it is also used for crack simulation [29]. The phase field method is also used to perform structural optimization using the fourth order Cahn-Hilliard equation [20,30] or the second order Allen-Cahn equation [31]. The article by Blank et al. [32] compares the Cahn-Hilliard and Allen-Cahn equations for evolving the phase field parameter and it indicates that the Allen-Cahn equation is better than the Cahn-Hilliard equation in the

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viewpoint of efficiency and computational cost. The shape optimization study performed by Takezawa et al. [31] proposed the Allen-Cahn equation based phase field method where the objective function is combined with double well potential (DWP) functions in Van der Waals free energy. Choi et al. [33] introduced the RDE based design method using the RDE without the DWP function and it has been modified and applied to structural design in the elastic [6,34] and the electromagnetic field [11,35,36].

This study employs the RDE based design method for topological design based on the works by Takezawa et al. [31] and Choi et al. [33] and the finite element method is employed for structural and electromagnetic field analysis. Except the combination with DWP functions, both approaches use the material interpolation scheme similar to the SIMP method [14] with the phase field parameter, which works as the design variable during the design process. The former method may not generate new holes because DWP functions restrict the shape variation only along structural boundaries [31,35]. This is classified as the phase field design method and it may control the thickness of the diffuse interfacial layer by adjusting diffusion coefficient κ as designated in Fig. 1(a). The complexity of an optimal structure is inversely proportional to the interfacial layer thickness. The diffusion coefficient must have large enough value to enclose boundary elements to avoid zig-zag boundary shapes as shown in Fig. 1(b). Although the large interfacial layer contributes to the simple final shape, it may cause gray scale representation along the structure boundary [33,35,37]. The study by Petersson and Sigmund [22] also reports the relevance between the perimeter constraint and intermediate materials in case of using the SIMP method.

The design process by the RDE based design method with the time evolutionary partial differential equation (PDE) is similar to updating the design variable through steepest descent method (SDM) with the perimeter constraint in the SIMP method. However, the implicit perimeter constraint is defined as the update solution in case of the RDE based design method while the ordinary perimeter constraint is defined in general filtering schemes. The formulation of the time differential equation facilitates the use of the SDM and the diffusion term in the PDE corresponds to the perimeter constraint. It is noteworthy that previous studies report that SDM is slow and inefficient [38,39]. Although its convergence rate is fast in the early design stage, it gradually becomes slow, especially near the optimum. In addition, the time step of the evolutionary PDE is restricted by the Courant–Friedrichs–Lewy (CFL) condition because the size of the time step affects the convergence stability [31]. The RDE used as the update scheme in the RDE based design method has the formulation which combines the optimizer and the perimeter constraints into a PDE. Therefore, an appropriate solution scheme of the optimization problem may improve the convergence rate. It enables the method to generate fast and reliable results.

This study employs the conjugate gradient method (CGM) [40] to solve the optimization problem. The CGM modifies present sensitivity according to previous sensitivity value and it may be a powerful alternative of the SDM to improve the convergence rate. Moreover, the RDE based topology optimization with the CGM contributes to the decrease of the interfacial layer thickness even in the case of a large diffusion coefficient value. The CGM combined with the RDE offers an implicit mechanism to change the influence between the reaction and the diffusion term in the RDE and enables the generation of a simple shape having little intermediate materials. It is different from previous study results [33,36,37] which show optimal structures having large gray portion in spite of simple shapes due to the large diffusion coefficient. However, the direct application of the CGM to RDE may cause ill convergence problem. This study reports instability factors for the CGM and suggests necessary complements in the CGM formulation to stabilize the convergence history. Derived results for benchmark problems in previous studies are investigated with respect to intermediate material portions and the convergence rate.

The outline of this manuscript is as follows. The RDE based design method and the modified CGM are described in detail in Section 2. In Section 3, optimization problems for three numerical examples are formulated; The first one is MBB beam design to minimize compliance and second example is magnetic force maximization problem in magnetic actuator design. Last one is to derive the dielectric collimator lens structure for maximizing the electric field intensity at a target area [41]. Section 4 explains numerical experiment results to verify the effect of the proposed method. Concluding remarks are given in Section 5.

2. Design method combined with the CGM

The optimization problem to minimize the design objective taking the inequality volume constraint into account is expressed as

$$\begin{aligned} &\underset{\phi}{\textbf{minimize}} \quad F(\phi,\ \mathbf{u}(\phi)) \\ &\textbf{subject to} \quad G(\phi) = \int_{\Omega_D} \phi \, dx - V_{req} \le 0, \quad \text{where } 0 < \phi_{\min} \le \phi \le 1 \end{aligned} \tag{1}$$

where $F(\phi,\ \mathbf{u}(\phi))$ is the design objective function. ϕ is the design variable that is the phase field parameter in the RDE based design method. $\mathbf{u}(\phi)$ is a state variable and it is determined according to the related physical field. $G(\phi)$ stands for the volume constraint having the pre-determined allowed total volume of V_{req} over the design domain Ω_D. $\phi_{\min}$ represents the lower bound of ϕ to avoid possible singularity problems. Ω_D is classified into the void or the solid region according to the variance of ϕ which varies in the interval from 0 to 1 during the design process. The area of $\phi = 1$ corresponds with solid while regions of $\phi = 0$ and $0 < \phi < 1$ stands for the void and the intermediate material, respectively.

2.1. RDE based design method

The RDE based design method employs the RDE for updating ϕ for structural optimization [33]:

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = \kappa \nabla^2 \phi(\mathbf{x},t) - \left\{ \eta \frac{\partial F(\phi, \mathbf{u}(\phi))}{\partial \phi} + \frac{\partial \widehat{G}(\phi)}{\partial \phi} \left[\lambda + \xi \widehat{G}(\phi) \right] \right\}$$
$$\text{where } \Omega \ \& \ \Omega_D \subset \mathbf{R}^n (n = 2 \text{ for 2D cases},\ n = 3 \text{ for 3D cases}) \tag{2}$$

where Ω and Ω_D are domains enclosed by the boundary domain $\partial\Omega$. Ω and Ω_D are the sensitivity calculation domain and the design domain, respectively. $\mathbf{x}$ represents the position vector. The boundary domain has the property of $\partial\phi(\mathbf{x},t)/\partial\hat{\mathbf{n}} = 0$ where $\hat{\mathbf{n}}$ is the outer unit vector normal to the boundary. The diffusion coefficient κ in the diffusion term of Eq. (2) is defined by $\kappa_0 \int_\Omega dx$. It determines the thickness of the diffuse interfacial layer and the complexity of the optimal structure as shown in Fig. 1(b) so that the amount of the intermediate materials increases as κ increases [25,31,33]. In the reaction term expressed in the bracket, η is for the normalized design sensitivity and it is defined by dividing the design domain area by the design sensitivity L^2–norm as $\eta = \int_{\Omega_D} d\mathbf{x} / \|\partial F/\partial\phi\|_{L^2(\Omega)}$. Because of the augmented Lagrangian formulation, the reaction term also includes the volume constraint $\widehat{G}(\phi)$ where $\widehat{G}(\phi) = \max(0, G(\phi))$. λ and ξ represent the Lagrange multiplier and the penalty parameter, respectively.

2.2. Modified CGM for the RDE based design method

To determine the updated design variable, the CGM combines the sensitivity of the design objective at the current iteration with that of previous iteration. Therefore, the design variable increment even in the late stage of the design process may keep a large value as displayed in Fig. 2 [40]. The CGM combined with the design sensitivity is formulated as follows: