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Topology optimization using a reaction–diffusion equation

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ABSTRACT

This paper presents a structural topology optimization method based on a reaction–diffusion equation. In our approach, the design sensitivity for the topology optimization is directly employed as the reaction term of the reaction–diffusion equation. The distribution of material properties in the design domain is interpolated as the density field which is the solution of the reaction–diffusion equation, so free generation of new holes is allowed without the use of the topological gradient method. Our proposed method is intuitive and its implementation is simple compared with optimization methods using the level set method or phase field model. The evolution of the density field is based on the implicit finite element method. As numerical examples, compliance minimization problems of cantilever beams and force maximization problems of magnetic actuators are presented to demonstrate the method's effectiveness and utility.

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1. Introduction

Reaction–diffusion systems are mathematical models that use partial differential equations to model two processes: one is a 'reaction,' referring to how two substances react locally, and the other is a 'diffusion' that tends, over time, to equalize the concentration of substances occupying a space. The reaction–diffusion equation can model many complicated natural phenomena that occur due to the propagation of interfaces between substances. For example, in population dynamics [1,2], combustion [3], chemical reactions [4,5] and biological morphogenesis [1,6], the phases of interacting substances create unique patterns as their fronts propagate.

The simplest reaction–diffusion system is a one-dimensional model describing the propagation of a gene population, introduced by Fisher [7]. In Fisher's equation, a non-linear quadratic form is used as the reaction term. Fisher showed that there exists a minimal velocity of the propagating interfaces. While Fisher's equation is a reaction–diffusion system with only one component, it is possible to expand the expression to an N-component vector field. Generally, two- or three-component systems have much broader application compared with one-component systems. In this study, one- and two-component reaction–diffusion systems are applied in methods to solve several structural topology optimization problems.

Since a seminal paper by Bendsøe and Kikuchi [8], structural topology optimization has become an established and effective design tool in various physical systems for stiffness maximization problems [8,9], compliant mechanism design problems [10,11] and microstructure designs [12–14]. In contrast with traditional methods like sizing or shape optimization, topology optimization permits radical design evolution beyond initially proposed models. A widely used topology optimization method is based on the SIMP (Solid Isotropic Material with Penalization) method [15], an approach that allows density values from 0 to 1 while suppressing intermediate densities in the optimal design by penalization [16]. However, the utility of SIMP method optimal results is often degraded by the generation of intermediate densities, checkerboard patterns and mesh dependency [16,17]. To avoid these numerical instabilities, filtering techniques [18] and the perimeter control method [19] have often been employed.

Another well known structural optimization approach is level set-based methods. A structural design using this method was first performed by Sethian and Wiegmann [20], in which evolution of the level set function was based on the stress distribution of the current design. This method implicitly represents structural boundaries by the iso-contour of the level set function, which is generally updated based on the Hamilton–Jacobi formulation [21], allowing level set-based optimization methods to avoid the numerical problems of the SIMP method described above. However, since the level set method originally tracks free boundaries, using shape derivatives, it does not allow for the nucleation of new inner holes (at least in two-dimensional problems). In order to resolve this problem, the bubble method (or the topological

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gradient method) [22,23] is typically coupled with a conventional level set-based method.

In the level set-based optimization method using the Hamilton–Jacobi equation, during the evolution of the level set function, the level set function does not maintain the signed distance function characteristic, and reinitialization is therefore required. The need for reinitialization is one of the main drawbacks of the level set method, since it is computationally troublesome and expensive. Recently, other reinitialization-free level set approaches, different from traditional level set methods based on the Hamilton–Jacobi equation, have been proposed by some researchers. Wei and Wang [24] introduced a structural optimization method using a piecewise constant level set method first proposed for segmentation of digital images by Lie et al. [25]. In this method, the interfaces are represented by discontinuities of constant level set functions and as a result, the level set function has sharp interfaces. Another approach for avoiding reinitialization is the method proposed by Yamada et al. [26], where an objective functional including a fictitious interface energy is used.

Currently, phase field methods are accepted as structural optimization methods. Although phase field methods are not yet widely employed for structural optimization, unlike level set-based methods, they are useful for simulating interfacial dynamics for phase transition phenomena such as solidification [27], dendritic growth [28] and fluid interface modeling [29]. In common with the level set-based method, this approach implicitly tracks the interface between phases, but does not need a reinitialization process, and this approach has recently been used for topology optimization by some researchers. Bourdin and Chambolle [30] applied a phase field method to dam design. Wang and Zhou [31,32] explored structural optimization using the Cahn–Hilliard equation [33]. Most recently, Takezawa et al. [34] proposed a structural optimization method based on the Allen–Cahn equation [35], a kind of reaction–diffusion equation with low computational cost compared to the fourth order Cahn–Hilliard equation. In phase field models, a Lyapunov energy functional includes a smooth double-well potential that takes a globally minimum value at each phase level.

In this work, we introduce a new topology optimization method based on a reaction–diffusion equation. In addition to our approach, two structural optimization methods using a reaction–diffusion equation have recently been reported. One is a phase field-based optimization method using the Allen–Cahn equation proposed by Takezawa et al. [34] and the other is the level set-based method proposed by Yamada et al. [26]. The former is similar to our approach except that it includes the double-well potential in the reaction term, so that intermediate densities can be avoided. However, free changes in structural topology are as problematic as with conventional level set-based methods, since the design sensitivity is available only in phase transition regions. The latter is a level set-based topology optimization method using topological derivatives [22,23], which supports the generation of new void holes. The structural boundaries are determined by using a relaxed Heaviside function and thus it is regarded as a level set-based method. Unlike conventional level set methods, the level set function is updated based on a reaction–diffusion equation, and optimized results using this approach show clear and smooth configurations. However, no explanation on how to derive the design sensitivity using topological derivatives was provided, nor was a mathematically rigorous proof regarding this issue given.

Our proposed optimization method does not include the double-well potential, so it supports flexible changes in structural topology according to the design sensitivity. The employed design sensitivity is the derivative of the objective function with respect to the design variables and it is directly used as the reaction term in the reaction–diffusion equation. Our optimization method thus has an advantage due to its simple and intuitive implementation. Furthermore, it converges quickly and supports the free nucleation of new holes, in contrast with level set-based optimization methods, since the sensitivity is loaded over the whole design domain. Our approach is applied in several examples of structural designs subject to elastic fields and magnetic fields. The state variables of these systems and the reaction–diffusion equation are solved using the finite element method.

The plan of this paper is as follows. In Section 2, we propose the optimization method and develop an algorithm based on the

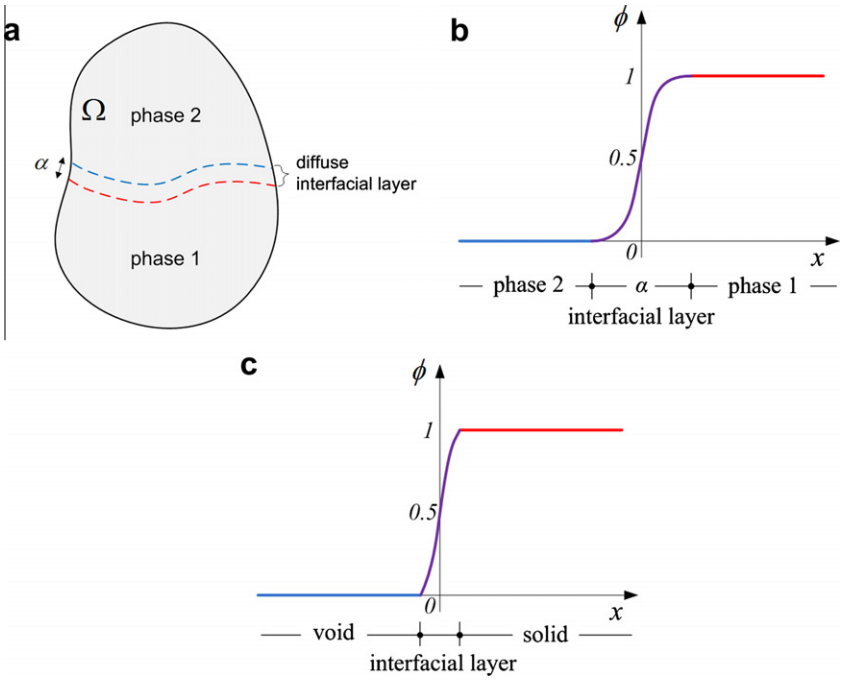

Fig. 1. Partition of material phases by a diffuse interface: (a) material separation by an interfacial layer; (b) phase transition of the phase-field function; and (c) phase transition of the density field proposed in our approach.

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