

**A structural design methodology based on
multiobjective and manufacturing-oriented
topology optimization**

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2019

Acknowledgements

I would like to express my appreciation to my supervisors, Professor Shinji Nishiwaki, Professor Kazuhiro Izui, and Professor Takayuki Yamada, for their continuous support and guidance throughout my undergraduate research and the course of master and doctoral degrees. They provided me with a favorable research environment for conducting creative work. Especially, I am grateful to Prof. Izui for providing me with the opportunity to treat the research topic of this thesis.

I am also deeply grateful to Professor Tetsuo Sawaragi in the Department of Mechanical Engineering and Science at Kyoto University, and Professor Atsushi Matsubara in the Department of Micro Engineering, also at Kyoto University, for their thoughtful advise and for serving on my dissertation committee.

I also would like to express my gratitude to co-researchers for their invaluable advise, stimulating discussions, and giving me the opportunity to expose me to the state-of-the-art studies during collaborative research. I received support on reliability-based topology optimization from Professor Nozomu Kogiso in the Department of Aerospace Engineering at Osaka Prefecture University. I got thoughtful advice on topology optimization problems related to thermofluids from Professor Kentaro Yaji, who was in our laboratory and is in the Department of Mechanical Engineering at Osaka University. I could not have accomplished my doctoral research without their kind help. Also, I am grateful to co-researchers in the Mitsubishi Electric Corporation including Ms. Akiko Hamada and Mr. Shota Kameoka for helpful advice and discussions about the manufacturability of the molded products, and would like to express my gratitude to Professor Hisashi Morishita, Professor Naobumi Michishita, and Ms. Yuka Ishii in the Department of Electrical and Electronic Engineering at National Defense Academy for stimulating discussions about optimization problems related to electromagnetism.

In addition, I really thank my colleagues in the Manufacturing Systems Engineering Laboratory at Kyoto University for their kind support and fruitful discussions. They always

created comfortable surroundings and gave me encouragement. I would also like to express my appreciation to Mr. John E. Goodman for his invaluable help in editing my papers in English and for providing English lectures over the years. Also, I am grateful to Mr. Steve Wever for editing my papers in English.

I also sincerely appreciate the financial support from Grant-in-Aid for JSPS Research Fellow, Grant Number JP17J08185.

Finally, I am most grateful to my parents and my sister for their warmth, kindness and good cheer throughout my life.

Kyoto, 2019

Yuki Sato

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Chapter 1

General introduction

1.1 Introduction

Structural optimization has been successfully used in many industries, such as automotive industries, owing to its potential for accelerating the development processes. Structural optimization can be classified into three primary types: sizing [1, 2], shape [3, 4], and topology optimization [5, 6]. In particular, topology optimization techniques have the most potential for exploring superior optimized structures among these three structural optimization types and are suitable for a tool at the conceptual design stage, because topological changes are allowed in addition to changes in shapes during the optimization processes. After a pioneering study by Bendsøe and Kikuchi [5], topology optimization was applied to a variety of problems, including multiphysics problems, such as coupled thermal-fluid problems [7–9] and coupled acoustic-structural problems [10–12], and multimaterial problems [13–17]. Now, there is a lot of commercial software that can perform topology optimization for industrial use. However, existing topology optimization techniques mainly focus on the improvement of the physical performance in the design target and have several major limitations that hinder the industrial application of topology optimization techniques.

The first limitation is that most existing topology optimization methods only provide a single solution that is optimal under the given optimization problem setting with a single objective although optimization problems are often characterized as multiobjective optimization problems in real-world engineering. Certain pairs of multiple objectives usually have trade-off relationships, which makes no single solution exist that can simultaneously minimize or maximize all objectives. Instead, such optimization problems yield multiple

optimal solutions, called non-dominated solutions or Pareto-optimal solutions. Since existing topology optimization methods do not provide a Pareto-optimal solution set, design engineers need to set an optimization problem so that the particular solution that satisfies their needs can be obtained. This setting of an optimization problem is non-trivial because detailed design requirements do not exactly determined prior to the optimization stage.

The second limitation is related to the manufacturability of the obtained solutions. When topology optimization solutions are applied in practical design scenarios, design engineers often must interpret and modify the results to satisfy manufacturability conditions. For example, in casting, molded products must embody certain geometrical features so that mold parts can be separated, and milling cannot proceed unless the desired shape allows tool cutting faces to reach the workpiece. This modification for ensuring the manufacturability may severely degrade the physical performance that the optimal designs have.

The third limitation is related to the reliability of the optimization results with respect to uncertainties. Geometrical uncertainties caused by manufacturing errors and operational wear can affect the physical performance of optimization results. In microfabrication processes, the effect of geometrical uncertainties can be particularly detrimental, due to the small dimensions at these scales. However, since the physical performance of a device usually depends on the details of its shape in implicit and radically non-linear ways, it is difficult for design engineers to predict the effects of geometrical variations and modify their designs accordingly.

This thesis focuses on the construction of topology optimization methods that can mitigate these limitations. For improving the first limitation, exploring a comprehensive set of Pareto-optimal solutions is useful, because decision makers will have a broader range of potential solutions from which to choose the particular solution that best meets their needs. This thesis therefore proposes a Pareto front exploration technique for multiobjective topology optimization problems based on an adaptive weighting scheme. Furthermore, this thesis also construct a data mining method that can glean useful knowledge from a Pareto-optimal solution set so that a design engineer could comprehend the physical mechanism that operates in the optimized designs. For removing the second limitation, topology optimization methods should incorporate geometrical constraints derived from the manufacturability in the optimization procedure. This thesis implements a manufacturing constraint via fictitious physical models which implicitly describe the manufacturability of a design. The third limitation is reduced by consideration of geometrical uncertainties in the optimization stage.

In this thesis, a reliability-based topology optimization method is constructed by modeling geometrical uncertainties using an advection equation.

The thesis consists of six chapters. In the remainder of this chapter, the basic concept and formulation of topology optimization techniques are briefly described. In the second chapter, a Pareto front exploration technique for multiobjective topology optimization problems is constructed. Pareto fronts obtained by the multiobjective topology optimization methods are analyzed by a data mining technique proposed in the third chapter. The fourth chapter constructs a manufacturing constraint scheme using fictitious physical models. The fifth chapter is related to the construction of a reliability-based topology optimization method under geometrical uncertainties. Finally, the general conclusions of this thesis are provided in the sixth chapter.

1.2 Concept of topology optimization

The basic concept of topology optimization is the replacement of the structural optimization problem with a material distribution problem by introducing an extended design domain, called a fixed design domain, and the characteristic function defined in the fixed design domain. The homogenization design method [5], the first proposed topology optimization method, relaxed the design space by assuming that a fixed design domain was filled with a composite material, introducing microstructures whose parameters such as hole sizes were used as design variables. In density approaches [6], which are now the most popular topology optimization methods, the characteristic function was replaced with a continuous function that was treated as a design variable, and material properties intermediate between those of material and void domains were interpolated using a continuous function. The solid isotropic material with penalization (SIMP) method [18] is the most popular interpolation scheme used in density approaches. On the other hand, level set-based approaches [19–22] have also been widely applied in topology optimization problems, where the level set function is introduced to represent structural boundaries.

1.3 Formulation

Consider a structural optimization problem to determine an optimal configuration of a domain filled with a material. Let the fixed design domain be denoted as $D \subset \mathbb{R}^d$ where d is the

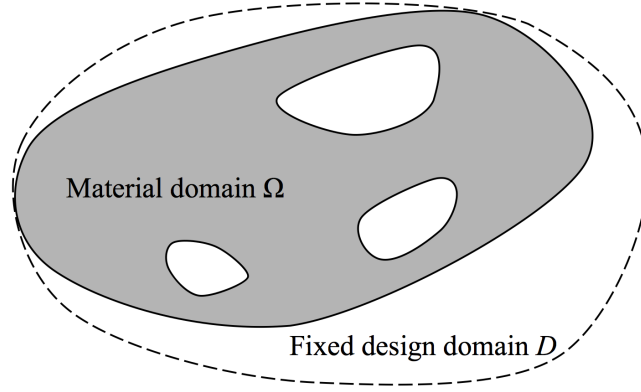


Fig. 1.1 Fixed design domain, D .

number of spatial dimensions. Material domains are then defined as $\Omega \subseteq D$, as shown in Fig. 1.1. Void domains are represented as the complementary domain $D \setminus \Omega$.

The basic idea of topology optimization is the replacement of a structural optimization problem with a material distribution problem by introducing a characteristic function, $\chi_\Omega \in L^\infty(D; \{0, 1\})$, where L^∞ represents a Lebesgue space defined in a fixed design domain D , as

$$\chi_\Omega(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x} \in \Omega \\ 0 & \text{for } \mathbf{x} \in D \setminus \Omega, \end{cases} \quad (1.1)$$

where $\mathbf{x}$ is a position vector. Using the characteristic function $\chi_\Omega(\mathbf{x})$ and a state variable, $u(\mathbf{x})$, given by solving a physical problem, a topology optimization problem is generally formulated as

$$\inf_{\chi_\Omega \in \mathcal{X}_{\text{ad}}} F = \int_D f_d(u, \chi_\Omega) dD + \int_\Gamma f_b(u) d\Gamma, \quad (1.2)$$

where Γ is a specific boundary of D and f_d and f_b are real functions. $\mathcal{X}_{\text{ad}}$ is a subspace of the Lebesgue space $L^\infty(D; \{0, 1\})$ and represents an admissible space defined by certain constraint functionals. Note that a state variable $u(\mathbf{x})$, such as a displacement field in mechanics, implicitly depends on the characteristic function χ_Ω .

It is well-known that the inherited discontinuity of the characteristic function χ_Ω makes the above topology optimization problem ill-posed. Hence, the original topology optimization problem must be replaced by well-posed one.

1.3.1 Density approach

The most popular technique to make the topology optimization problem well-posed is a so-called density method, based on a convexification method (Section 5.2.5 of [23]), in which the design space, $L^\infty(D; \{0,1\})$, is replaced with its convex hull, $L^\infty(D; [0,1])$, introducing a normalized density θ . Then, an intermediate material property tensor $\mathbf{A}$, e.g. the elasticity tensor, between domains Ω and $D \setminus \Omega$ is interpolated using a interpolation function $f(\theta)$ as follows:

$$\mathbf{A}(\theta) = f(\theta)\mathbf{A}_0, \quad (1.3)$$

where $\mathbf{A}_0$ is the material property tensor in Ω . The Solid Isotropic Material with Penalization (SIMP) scheme [18] is an often-used material interpolation scheme in which the interpolation function is defined as

$$f(\theta) = \theta^p, \quad (1.4)$$

where p is a penalty parameter, usually set to 3.

Based on the density approach, a topology optimization problem is formulated as follows:

$$\inf_{\theta \in \Theta_{\text{ad}}} F = \int_D f_d(u, \theta) dD + \int_\Gamma f_b(u) d\Gamma, \quad (1.5)$$

where Θ_{ad} is a subspace of the Lebesgue space $L^\infty(D; [0,1])$ and represents an admissible space defined by certain constraint functionals. This problem can be solved by optimization methods mentioned in Section 1.4.

Heaviside projection method using a PDE-based filter

In density approaches, a filtering scheme is often used to prevent overly complex sub-structures from appearing and numerical instabilities from occurring [24–26]. Here, a Heaviside projection method incorporating a Helmholtz-type of partial differential equation (PDE) filter [27, 28] are discussed. In this method, an auxiliary design variable field, $\hat{\varphi} \in L^\infty(D; [-1,1])$, is introduced and a PDE filter is then applied to the field $\hat{\varphi}$ as follows:

$$-R^2 \nabla^2 \varphi + \varphi = \hat{\varphi}, \quad (1.6)$$

where φ is the filtered variable, and R is a parameter that affects the smoothness of the filtered variable. Note that in Heaviside projection methods, the design variables are conventionally

bounded in $[0, 1]$. But, the raw design variables have no physical meaning and are only used as intermediate mathematical variables [29]. In this thesis, the bound is set to $[-1, 1]$. The filtered variable is projected to 0/1 by zero threshold, using a smoothed Heaviside function defined such as

$$\theta = H_p(\varphi) = \begin{cases} 1 & \text{for } h < \varphi \\ \frac{1}{2} + \frac{15}{16} \left(\frac{\varphi}{h}\right) - \frac{5}{8} \left(\frac{\varphi}{h}\right)^3 + \frac{3}{16} \left(\frac{\varphi}{h}\right)^5 & \text{for } -h \leq \varphi \leq h \\ 0 & \text{for } \varphi < -h, \end{cases} \quad (1.7)$$

or

$$\theta = H_e(\varphi) = \frac{1}{1 + \exp(-\alpha_h \varphi)}, \quad (1.8)$$

where h is the width of the transition from 0 to 1 and α_h is a parameter that controls the curvature of the smoothed Heaviside function. When $\alpha_h \rightarrow \infty$, the smoothed Heaviside function H_e corresponds to the exact Heaviside function. θ is then used as the normalized density. That is, a topology optimization problem now is formulated as follows:

$$\inf_{\hat{\varphi} \in \Phi_{ad}} F = \int_D f_d(u, \theta(\varphi(\hat{\varphi}))) dD + \int_\Gamma f_b(u) d\Gamma, \quad (1.9)$$

where Φ_{ad} is a subspace of the Lebesgue space $L^\infty(D; [-1, 1])$ representing an admissible space.

1.3.2 Level set-based approach

Here, we discuss level set-based structural optimization methods that regularize the design space. In these methods, structural boundaries are clearly expressed by the iso-surface of a scalar function, namely the level set function. Two phases such as material and void domains are discriminated by the sign of the level set function, as follows:

$$\begin{cases} \phi(\mathbf{x}) > 0 & \Leftrightarrow \mathbf{x} \in \Omega \\ \phi(\mathbf{x}) = 0 & \Leftrightarrow \mathbf{x} \in \partial\Omega \\ \phi(\mathbf{x}) < 0 & \Leftrightarrow \mathbf{x} \in D \setminus \bar{\Omega}. \end{cases} \quad (1.10)$$

Note that it is also possible to define the level set function with the opposite sign to the above definition. Using the level set function, a Heaviside function χ_ϕ is defined as

$$\chi_\phi = \begin{cases} 1 & \text{for } \phi \geq 0 \\ 0 & \text{for } \phi < 0. \end{cases} \quad (1.11)$$

Then, an optimization problem is formulated by replacing the characteristic function χ_Ω with the Heaviside function, χ_ϕ , as follows:

$$\inf_{\chi_\phi \in \mathcal{X}_{\text{ad}}} F = \int_D f_d(u, \chi_\phi) dD + \int_\Gamma f_b(u) d\Gamma. \quad (1.12)$$

Note that the definition of the level set function in (1.10) includes arbitrary property, that is the profile of the level set function is not uniquely determined although its sign is fixed. By prescribing the profile of the level set function in the optimization process, the above optimization problem becomes well-posed. Optimization methods to solve the above problem is described in Section 1.4.2.

1.4 Optimization methods

For solving the optimization problems formulated in the previous sections, appropriate optimization methods must be selected. The optimization methods to solve topology optimization problems are classified into two types: gradient-based methods and heuristic methods. Gradient-based methods search the optimal solution based on the gradient information, also called sensitivity, while heuristic methods do not usually require the gradient of the objective functional. Here, several gradient-based optimization methods: mathematical programming, usually used in the density approach, and fictitious time evolution methods, mainly used in the level set-based approach, are discussed. Evolutionary approaches, kinds of heuristic methods, are also briefly mentioned.

1.4.1 Mathematical programming

Mathematical programming is methods to solve linear and non-linear optimization problems. Let $\mathbf{d} = [d_1, \dots, d_n]^T$, $f_0 : \mathbb{R}^n \rightarrow \mathbb{R}$ and $f_i : \mathbb{R}^n \rightarrow \mathbb{R}$ denote the design variable, the objective function and the constraint functions, respectively. We herein consider an optimization

problem formulated as

$$\min_{\mathbf{d} \in \mathcal{D}} f_0(\mathbf{d}) \quad (1.13)$$

$$\text{subject to: } f_i(\mathbf{d}) \leq 0 \quad \forall i \in \{1, 2, \dots, m\}, \quad (1.14)$$

where m is the number of constraint functions and $\mathcal{D}$ is the feasible set defined as

$$\mathcal{D} = \left\{ \mathbf{d} \in \mathbb{R}^n \mid d_i^{\min} \leq d_i \leq d_i^{\max} \quad \forall i \in \{1, 2, \dots, n\} \right\}. \quad (1.15)$$

As in the above formulation, mathematical programming handles optimization problems with the finite dimensional design space. Therefore, the infinite dimensional design space of topology optimization problems must be projected onto the finite dimensional one to apply mathematical programming for topology optimization problems.

Mathematical programming consists of various branches, including linear programming, quadratic programming, convex programming, integer programming, and so on. In the following, sequential linear programming (SLP) and sequential convex programming, which are kinds of non-linear programming, are explained.

Sequential linear programming (SLP)

SLP linearize the objective and constraint functions at a point, $\mathbf{d}^0$, as follows:

$$\min_{\mathbf{d} \in \mathcal{D}_{\text{LP}}} f_0(\mathbf{d}^0) + \left. \frac{\partial f_0}{\partial \mathbf{d}} \right|_{\mathbf{d}=\mathbf{d}^0} (\mathbf{d} - \mathbf{d}^0) \quad (1.16)$$

$$\text{subject to: } f_i(\mathbf{d}^0) + \left. \frac{\partial f_i}{\partial \mathbf{d}} \right|_{\mathbf{d}=\mathbf{d}^0} (\mathbf{d} - \mathbf{d}^0) \leq 0 \quad \forall i \in \{1, 2, \dots, m\}, \quad (1.17)$$

where $\mathcal{D}_{\text{LP}}$ is the feasible set defined as

$$\mathcal{D}_{\text{LP}} = \left\{ \mathbf{d} \in \mathcal{D} \mid -l_i^0 \leq d_i - d_i^0 \leq u_i^0 \quad \forall i \in \{1, 2, \dots, n\} \right\}. \quad (1.18)$$

l_i^0 and u_i^0 are moving limits which are determined so that the accuracy of the linear approximation can be ensured. The above linearized problem can be solved by the simplex algorithm.

In SLP, the solution is iteratively updated by solving the problem linearized at the current solution approximation. That is, a new solution $\mathbf{d}^{k+1}$ is obtained by solving a problem

linearized at the current solution $\mathbf{d}^k$, where k is the iteration number. Since each design variable stops either upper or lower bound of moving limits at every iteration, careful update strategy of moving limits is essential to obtain a converged solution.

Sequential convex programming

Sequential convex programming is based on the convex approximation of the objective function and constraint functions. In the convex linearization method (CONLIN) [30], a kind of convex programming, the objective function and constraint functions are approximated, as follows:

$$f_i(\mathbf{d}) \simeq f_i(\mathbf{d}^0) + \sum_{j=1}^n \left. \frac{\partial f_i}{\partial d_j} \frac{\partial d_j}{\partial p_{ij}} \right|_{\mathbf{d}=\mathbf{d}^0} (p_{ij} - p_{ij}^0) \quad \forall i \in \{0, 1, \dots, m\}, \quad (1.19)$$

where p_{ij} is a variable for convex linearization, and is defined based on the signs of the first partial derivative, as follows:

$$p_{ij} = \begin{cases} d_j & \text{if } \frac{\partial f_i}{\partial d_j} > 0 \\ \frac{1}{d_j} & \text{if } \frac{\partial f_i}{\partial d_j} < 0. \end{cases} \quad (1.20)$$

That is, the objective and constraint functions are linearized with respect to design variables or their reciprocals depending on the signs of the corresponding first derivatives. This approximation is convex and can efficiently be solved via the dual method in which the primal problem is transformed into n single variable minimization problem.

There also exists an expansion of CONLIN, known as the method of moving asymptotes (MMA) [31]. In this method, the variables for convex linearization are defined as

$$p_{ij} = \begin{cases} \frac{1}{U_j - d_j} & \text{if } \frac{\partial f_i}{\partial d_j} > 0 \\ \frac{1}{d_j - L_j} & \text{if } \frac{\partial f_i}{\partial d_j} < 0, \end{cases} \quad (1.21)$$

where L_j and U_j are moving asymptotes which are updated during the iterations, satisfying the relation $L_j < x_j < U_j$.

It is known that MMA has a good convergence property and is suitable for topology optimization problems. MMA is now one of the most popular solvers for topology optimization,

especially in density approaches. There also exist some works which incorporated MMA with level set-based approaches [32–34].

1.4.2 Fictitious time evolution

In the level set-based structural optimization methods, the shape evolution is usually governed by the fictitious time evolution of the level set function rather than update by mathematical programming because the level set function is used to implicitly represent structural boundaries and is not the design variable. Note that there are methods incorporating the density approaches with the fictitious time evolution for optimization [35].

Here, we consider the following unconstrained optimization problem:

$$\inf_{\Omega} F(\Omega). \quad (1.22)$$

Actually, almost all structural optimization problems are constrained problem because governing equations for physical phenomena must be considered as equality constraints. As for constrained problems, the method of Lagrange multiplier is used to convert them to unconstrained ones. We discuss two fictitious time evolution equations in the following subsections.

Hamilton-Jacobi equation

Wang *et al.* [19] and Allaire *et al.* [20] independently proposed structural optimization methods based on the level set method. In these methods, the shape $\Omega(t)$ is assumed to evolve in fictitious time, t , with a normal velocity, $V_n(\mathbf{x}, t)$, which yields the Hamilton-Jacobi equation, as follows:

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} - V_n |\nabla \phi| = 0. \quad (1.23)$$

Note that the normal vector is represented using the level set function as $\mathbf{n} = -\nabla \phi / |\nabla \phi|$ when the level set function is defined as (1.10). The normal velocity, $V_n(\mathbf{x}, t)$, of the evolution is defined to be a descent direction through the shape sensitivity analysis. The shape sensitivity, also called shape derivative, of $F(\Omega)$ at Ω is defined as the Fréchet derivative of $F((\text{Id} + \mathbf{V})\Omega)$ with respect to $\mathbf{V}$ at 0, and is written in the form as

$$F'(\Omega)(\mathbf{V}) = \int_{\partial \Omega} v \mathbf{V} \cdot \mathbf{n} d\Gamma, \quad (1.24)$$

satisfying the following asymptotic expansion:

$$F((\text{Id} + \mathbf{V})\Omega) = F(\Omega) + F'(\Omega)(\mathbf{V}) + o(\|\mathbf{V}\|), \quad (1.25)$$

where Id is the identity transformation. Therefore, the normal velocity, $V_n = \mathbf{V} \cdot \mathbf{n} = -v$ is a descent direction and can be used in the Hamilton-Jacobi equation for updating the level set function. However, it is known that the level set function becomes too flat or too steep during the evolution by Hamilton-Jacobi equation. In order to regularize the level set function, it is periodically reinitialized so that it would have the property of the signed distance function, as follows:

$$\phi(\mathbf{x}, t) = \begin{cases} \text{dist}(\mathbf{x}, \partial\Omega(t)) & \Leftrightarrow \mathbf{x} \in \Omega(t) \\ 0 & \Leftrightarrow \mathbf{x} \in \partial\Omega(t) \\ -\text{dist}(\mathbf{x}, \partial\Omega(t)) & \Leftrightarrow \mathbf{x} \in D \setminus \bar{\Omega}(t), \end{cases} \quad (1.26)$$

where $\text{dist}(\mathbf{x}, \partial\Omega(t))$ represents the distance from a point $\mathbf{x}$ to the boundary $\partial\Omega(t)$. Finally, the optimal shape can be obtained as

$$\Omega(t_f) = \{\mathbf{x} \in D \mid \phi(\mathbf{x}, t_f) > 0\}, \quad (1.27)$$

where t_f is the final time when a certain convergence criterion is satisfied.

It is well known that this method cannot create new holes during the optimization procedure, although topological changes by merging or cancellation of holes are allowed. As a remedy of this issue, Allaire *et al.* [36] introduced the bubble method [37] using the topological derivative [38, 39]. The topological derivative at a point $\mathbf{x}$ is defined as follows:

$$D_{\text{T}}F(\mathbf{x}) = \lim_{\epsilon \rightarrow 0} \frac{F(\Omega_\epsilon) - F(\Omega)}{b(\epsilon)}, \quad (1.28)$$

where Ω_ϵ is the perturbed domain by subtracting a ball of radius ϵ centered at a point $\mathbf{x}$ from the original domain Ω . $b(\epsilon)$ is a smooth positive function going to zero when $\epsilon \rightarrow 0$ and is chosen so that the topological derivative has a meaning.

Reaction-diffusion equation

Yamada *et al.* [22] proposed a level set-based topology optimization method based on the concept of the phase field method. In this method, the evolution of the level set function is

governed by the reaction-diffusion equation, as follows:

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -F' + \tau \nabla^2 \phi, \quad (1.29)$$

where τ is a diffusion coefficient that affects the smoothness of the level set function, and F' in the reaction term is the design sensitivity. This design sensitivity is determined as the topological derivative of the objective functional, i.e. $F' = -D_T F$.

During the evolution by the reaction-diffusion equation, the level set function has the upper and lower bounds, based on the concept of the phase field method, as follows:

$$\begin{cases} 0 < \phi(\mathbf{x}, t) \leq 1 & \Leftrightarrow \mathbf{x} \in \Omega(t) \\ \phi(\mathbf{x}, t) = 0 & \Leftrightarrow \mathbf{x} \in \partial \Omega(t) \\ -1 \leq \phi(\mathbf{x}, t) < 0 & \Leftrightarrow \mathbf{x} \in D \setminus \bar{\Omega}(t). \end{cases} \quad (1.30)$$

In the same manner as the level set-based method using the Hamilton-Jacobi equation, the optimal configuration can be obtained as

$$\Omega(t_f) = \{\mathbf{x} \in D \mid \phi(\mathbf{x}, t_f) > 0\}. \quad (1.31)$$

This method allows topological changes that create new holes during the optimization procedure, owing to the use of the topological derivative. Furthermore, adjustment of τ allows to qualitatively control the geometrical complexity of the shape. Although the mathematical proofs for optimality of this method has not been provided yet, it has successfully been applied to various design problems.

1.4.3 Evolutionary approach

Here, the existing evolutionary approaches for topology optimization are briefly discussed. Different from the previous gradient-based optimization methods: mathematical programming and fictitious time evolution, evolutionary approaches is based on heuristics. Evolutionary structural optimization (ESO) is a numerical method proposed by Xie and Steven [40] for topology optimization, and was extended as bidirectional ESO (BESO) [41]. These methods are based on the finite element method and can handle the exact 0/1 discrete structural representation.

Evolutionary approaches which used population-based searches have also been applied to topology optimization, including differential evolution [42], ant colony optimization [43], and covariance matrix adaptation evolution strategy (CMA-ES) [44]. Owing to the population-based search strategy, these methods have an advantage of handling multimodality of optimization problems compared to gradient-based methods, although high computational efforts are needed for population-based searches.

1.5 Sensitivity analysis

Gradient-based optimization methods require the gradient, also called sensitivity, of an objective function with respect to design variables to update them to an optimum point. Here, we discuss the three types of sensitivity analysis, i.e. how to evaluate the sensitivity.

We herein consider an optimization problem with an equality constraint formulated as

$$\inf_{\theta} \quad F(u, \nabla u, \theta) = \int_D f_d(u, \nabla u, \theta) dD + \int_{\Gamma} f_b(u, \nabla u) d\Gamma \quad (1.32)$$

$$\text{subject to: } E(u, \theta) = \nabla \cdot (\mathbf{a} \nabla u) - \mathbf{b} \cdot \nabla u - cu + d = 0 \quad \text{in } D \quad (1.33)$$

$$B(u, \theta) = \alpha u + \beta \mathbf{n} \cdot (\mathbf{a} \nabla u) - \gamma = 0 \quad \text{on } \Gamma, \quad (1.34)$$

where $\Gamma = \partial D$ and $\mathbf{n}$ is a unit normal vector pointing outward to the boundary Γ . In the above formulation, the equality constraint E and B respectively represent a state equation and a boundary condition to determine the physical state field $u \in H^1(D)$, which implicitly depends on the design variable θ , i.e. $u(\theta)$. That is, the relationship between the state field and the design variable cannot be expressed in an explicit form, and it is required to solve the state equation for obtaining the state field. Here, it is assumed that $\mathbf{a}$, $\mathbf{b}$, c , and d do not depend on u , but may depend on θ . Furthermore, α , β and γ are assumed to be parameters which can vary depending on the location. Then, the state equation becomes the general linear second-order partial differential equation. Even when the state equation is non-linear, the following discussion about the sensitivity analysis holds. The functional space which θ belongs to depends on the optimization problem, e.g. $L^\infty(D; [0, 1])$ in the density approach of topology optimization. The goal of the sensitivity analysis is to calculate $dF(\theta; \psi)$ which is the Gâteaux derivative of the objective functional with respect to θ in the direction ψ . In the following, $F(u, \nabla u, \theta)$ is simply written as $F(u, \theta)$.

1.5.1 Finite difference method

Finite difference method approximates the derivative by finite differences. Let $\epsilon > 0$ denote the degree of the perturbation of θ . Then the second-order Taylor expansions yield

$$F(u(\theta + \epsilon\psi), \theta + \epsilon\psi) = F(u, \theta) + dF(\theta; \psi)\epsilon + \frac{1}{2}d^2F(\theta; \psi, \psi)\epsilon^2 + O(\epsilon^3) \quad (1.35)$$

$$F(u(\theta - \epsilon\psi), \theta - \epsilon\psi) = F(u, \theta) - dF(\theta; \psi)\epsilon + \frac{1}{2}d^2F(\theta; \psi, \psi)\epsilon^2 + O(\epsilon^3), \quad (1.36)$$

where $d^2F(\theta; \psi_1, \psi_2)$ represents the second-order directional derivative in the directions ψ_1 and ψ_2 . (1.35) gives the forward Euler scheme:

$$dF(\theta; \psi) \approx \frac{F(u(\theta + \epsilon\psi), \theta + \epsilon\psi) - F(u, \theta)}{\epsilon}, \quad (1.37)$$

and (1.36) gives the backward Euler scheme:

$$dF(\theta; \psi) \approx \frac{F(u, \theta) - F(u(\theta - \epsilon\psi), \theta - \epsilon\psi)}{\epsilon}. \quad (1.38)$$

These schemes have the first-order accuracy. On the other hand, subtracting (1.36) from (1.35) yields the centered scheme:

$$dF(\theta; \psi) \approx \frac{F(u(\theta + \epsilon\psi), \theta + \epsilon\psi) - F(u(\theta - \epsilon\psi), \theta - \epsilon\psi)}{2\epsilon}, \quad (1.39)$$

with the second-order accuracy.

The advantage of the finite difference method is its simplicity of implementation. However, the finite difference method has two defects: (1) the difficulty in determining an appropriate ϵ value and (2) the computational cost. As for the first problem, the truncation error becomes large when ϵ is too large, while cancellation of significant digits may cause large numerical errors when ϵ is too small. Consequently, trial-and-error efforts are required to determine the ϵ value. The second problem is the expensive computational cost. For calculating the finite difference approximation, $u(\theta + \epsilon\psi)$ and/or $u(\theta - \epsilon\psi)$ must be calculated for all admissible direction ψ by solving (1.33) with (1.34). The number of equations to be solved corresponds to the number of the dimensions of the design space when the forward or backward Euler schemes are used, and the twice of the dimensions when the centered scheme is used. Consequently, when the dimension of the design space is large, the computational cost becomes so expensive.

1.5.2 Direct difference method

Next, direct difference method is discussed. The derivative of the objective function with respect to θ is directly taken by using the rule of the composite derivative, as follows:

$$dF(\theta; \psi) = \left\langle \frac{\partial F}{\partial \theta}(u, \theta), \psi \right\rangle + \left\langle \frac{\partial F}{\partial u}(u, \theta), u'(\theta; \psi) \right\rangle. \quad (1.40)$$

Here, $u'(\theta; \psi)$, which is the directional derivative of u and is the function of the spatial coordinates, i.e. $u'(\theta; \psi)(\mathbf{x})$, cannot be written in an explicit form. Differentiating the state equation yields the equation to determine $u'(\theta; \psi)$, as follows:

$$\begin{aligned} dE(\theta; \psi) &= \left\langle \frac{\partial E}{\partial \theta}(u, \theta), \psi \right\rangle + \left\langle \frac{\partial E}{\partial u}(u, \theta), u'(\theta; \psi) \right\rangle \\ &= 0, \end{aligned} \quad (1.41)$$

which is reformulated as

$$\nabla \cdot (\mathbf{a} \nabla u') - \mathbf{b} \cdot \nabla u' - cu' = -(\nabla \cdot (\mathbf{a}' \nabla u) - \mathbf{b}' \cdot \nabla u - c'u + d'), \quad (1.42)$$

where $'$ represents the directional derivative with respect to θ in the direction ψ . In the same manner, differentiating the boundary condition leads to the boundary condition of u' , as follows:

$$\alpha u' + \beta \mathbf{n} \cdot (\mathbf{a} \nabla u') = -\beta \mathbf{n} \cdot (\mathbf{a}' \nabla u). \quad (1.43)$$

To calculate the derivative, $dF(\theta; \psi)$, we need to calculate $u'(\theta; \psi)$ for all admissible direction ψ by solving (1.42) with (1.43). Thus, the number of equations to be solved corresponds to the number of the dimensions of the design space. Consequently, when the dimension of the design space is large, which is typically in topology optimization, the computational cost becomes so expensive.

1.5.3 Adjoint variable method

Finally, the adjoint variable method is discussed. This method is based on the method of Lagrange multiplier and is very powerful for sensitivity analysis because it gives rigorous sensitivity with the computationally reasonable cost.

First, the Lagrangian $\mathcal{L}$ is defined, as follows:

$$\mathcal{L}(\theta, v, q, q_b) = F(v, \theta) + \int_D q E(v, \theta) dD + \int_\Gamma q_b B(v, \theta) d\Gamma, \quad (1.44)$$

where q and q_b are the Lagrange multipliers. It is noting that v is a function independent from θ .

We now consider the optimality conditions for the Lagrangian. A stationary condition requiring the partial derivative of $\mathcal{L}$ with respect to q in the direction $\tilde{q}$ to be equal to zero yields

$$\left\langle \frac{\partial \mathcal{L}}{\partial q}, \tilde{q} \right\rangle = \int_D \tilde{q} E(v, \theta) dD = 0. \quad (1.45)$$

Satisfying this optimality condition for all admissible direction $\tilde{q} \in H^1(D)$ gives the state equation. Another stationary condition requiring the partial derivative of $\mathcal{L}$ with respect to q_b in the direction $\tilde{q}_b$ to be equal to zero yields

$$\left\langle \frac{\partial \mathcal{L}}{\partial q_b}, \tilde{q}_b \right\rangle = \int_\Gamma \tilde{q}_b B(v, \theta) d\Gamma = 0. \quad (1.46)$$

Since $\tilde{q}_b$ is arbitrary on Γ , the boundary condition holds. These two optimality conditions mean that $v = u$ is a stationary point. Next, to consider the stationary condition requiring the partial derivative of $\mathcal{L}$ with respect to v in the direction $\tilde{v}$ to be equal to zero, we reformulate the Lagrangian $\mathcal{L}$ using an integration by parts, in the form as

$$\begin{aligned} \mathcal{L}(\theta, v, q, q_b) = & \int_D f_d(v, \theta) dD + \int_\Gamma f_b(v) d\Gamma + \int_\Gamma q \mathbf{n} \cdot (\mathbf{a} \nabla v) d\Gamma - \int_D \nabla q \cdot (\mathbf{a} \nabla v) dD \\ & - \int_D q \mathbf{b} \cdot \nabla v dD - \int_D q (cv - d) dD + \int_\Gamma q_b (\alpha v + \beta \mathbf{n} \cdot (\mathbf{a} \nabla v) - \gamma) d\Gamma. \end{aligned} \quad (1.47)$$

Then the partial derivative of $\mathcal{L}$ with respect to v in the direction $\tilde{v}$ leads to

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial v}, \tilde{v} \right\rangle = & \int_D \tilde{v} \left(\frac{\partial f_d}{\partial v} - \nabla \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla v)} \right) \right) dD + \int_\Gamma \tilde{v} \mathbf{n} \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla v)} \right) d\Gamma + \int_\Gamma \tilde{v} \frac{\partial f_b}{\partial v} d\Gamma \\ & + \int_\Gamma \nabla \tilde{v} \cdot \left(\mathbf{a}^T \frac{\partial f_b}{\partial (\mathbf{a} \nabla v)} \right) d\Gamma + \int_\Gamma q \mathbf{n} \cdot (\mathbf{a} \nabla \tilde{v}) d\Gamma - \int_D \nabla q \cdot (\mathbf{a} \nabla \tilde{v}) dD \\ & - \int_D q \mathbf{b} \cdot \nabla \tilde{v} dD - \int_D \tilde{v} c q dD + \int_\Gamma \tilde{v} \alpha q_b d\Gamma + \int_\Gamma q_b \beta \mathbf{n} \cdot (\mathbf{a} \nabla \tilde{v}) d\Gamma. \end{aligned} \quad (1.48)$$

This partial derivative is rewritten by using an integration by parts, as

$$\begin{aligned}
\left\langle \frac{\partial \mathcal{L}}{\partial v}, \tilde{v} \right\rangle &= \int_D \tilde{v} \left(\frac{\partial f_d}{\partial v} - \nabla \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla v)} \right) \right) dD + \int_\Gamma \tilde{v} \mathbf{n} \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla v)} \right) d\Gamma + \int_\Gamma \tilde{v} \frac{\partial f_b}{\partial v} d\Gamma \\
&\quad + \int_\Gamma \nabla \tilde{v} \cdot \left(\mathbf{a}^T \frac{\partial f_b}{\partial (\mathbf{a} \nabla v)} \right) d\Gamma + \int_\Gamma q \mathbf{n} \cdot (\mathbf{a} \nabla \tilde{v}) d\Gamma - \int_\Gamma \tilde{v} \mathbf{n} \cdot (\mathbf{a}^T \nabla q) d\Gamma \\
&\quad + \int_D \tilde{v} \nabla \cdot (\mathbf{a}^T \nabla q) dD - \int_\Gamma \tilde{v} \mathbf{n} \cdot \mathbf{b} q d\Gamma + \int_D \tilde{v} \nabla \cdot (\mathbf{b} q) dD - \int_D \tilde{v} c q dD \\
&\quad + \int_\Gamma \tilde{v} \alpha q_b d\Gamma + \int_\Gamma q_b \beta \mathbf{n} \cdot (\mathbf{a} \nabla \tilde{v}) d\Gamma \\
&= 0.
\end{aligned} \tag{1.49}$$

Since $\tilde{v}$ is arbitrary in D , the adjoint equation is given as

$$\nabla \cdot (\mathbf{a}^T \nabla p) + \nabla \cdot (\mathbf{b} p) - c p + \frac{\partial f_d}{\partial u} - \nabla \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla u)} \right) = 0 \quad \text{in } D. \tag{1.50}$$

Arbitrariness of $\tilde{v}$ on Γ gives the boundary conditions of the adjoint equation:

$$\frac{\partial f_b}{\partial u} + p_b \alpha + \mathbf{n} \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla u)} - \mathbf{a}^T \nabla p - \mathbf{b} p \right) = 0 \quad \text{on } \Gamma, \tag{1.51}$$

and arbitrariness of $\mathbf{a} \nabla \tilde{v}$ on Γ also gives the boundary conditions of the adjoint equation:

$$\frac{\partial f_b}{\partial (\mathbf{a} \nabla u)} + \mathbf{n} (p + p_b \beta) = 0 \quad \text{on } \Gamma. \tag{1.52}$$

Cancellation of p_b from these two equations gives adjoint boundary condition for p as

$$\alpha p + \beta \mathbf{n} \cdot (\mathbf{a}^T \nabla p + \mathbf{b} p) = -\alpha \mathbf{n} \cdot \frac{\partial f_b}{\partial (\mathbf{a} \nabla u)} + \beta \frac{\partial f_b}{\partial u} + \beta \mathbf{n} \cdot \left(\mathbf{a}^T \frac{\partial f_d}{\partial (\mathbf{a} \nabla u)} \right) \quad \text{on } \Gamma. \tag{1.53}$$

Then, the optimality conditions are given as $q = p$.

Finally, the Gâteaux derivative of the objective functional with respect to θ in the direction ψ is calculated as the partial derivative of $\mathcal{L}$ with respect to θ in the direction ψ at the optimal point (u, p) , as follows:

$$dF(\theta; \psi) = \left\langle \frac{\partial \mathcal{L}}{\partial \theta}, \psi \right\rangle = \int_D \left(\frac{\partial f_d}{\partial \theta} - \nabla p \cdot \left(\frac{\partial \mathbf{a}}{\partial \theta} \nabla u \right) - p \frac{\partial \mathbf{b}}{\partial \theta} \cdot \nabla u - p \frac{\partial c}{\partial \theta} u \right) \psi dD. \tag{1.54}$$

When using the adjoint variable method, the number of adjoint equations to be solved for calculating the sensitivity corresponds to the number of the state equation. (If the optimization problem has the self-adjoint property, solving the adjoint equation can be omitted). In topology optimization, the number of the state equations is much smaller than the number of the dimensions of the design space which is theoretically infinite. Therefore, the adjoint variable method is suitable to evaluate the sensitivity.

1.6 Summary

This chapter clarified the objective of this thesis and summarized existing topology optimization methodologies. First, challenges of existing topology optimization methodologies are discussed, and the objective of this thesis are clarified. Then, existing topology optimization methodologies are summarized. First, a topology optimization problem was formulated in a general form. Then several topology optimization approaches, the density and the level set-based approaches, which convert the ill-posed topology optimization problem to the well-posed one, were discussed. In the density approaches, the design space of the original topology optimization problem is convexified, introducing a normalized density of material. In the level set-based approaches, the design space of the original topology optimization problem is regularized by introducing the level set function which implicitly represent structural boundaries and restricting the evolution of the level set function. Optimization methods, which are loosely classified into gradient-based methods and heuristic methods, for solving the topology optimization problems were introduced in the next section. Mathematical programming is a kind of gradient-based optimization methods and is often used as a solver of the density approach. Fictitious time evolution is also a kind of gradient-based methods, more precisely the steepest descent method, and is often used in the level set-based approaches. Two time evolution equations, the Hamilton-Jacobi equation and a reaction-diffusion equation, are discussed. Evolutionary approaches, which have an advantage of handling multimodality of optimization problems, are also briefly discussed. Finally, the sensitivity analysis to calculate the gradient of an objective functional were provided.

Chapter 2

Multiobjective topology optimization

2.1 Introduction

In real-world engineering, structural optimization problems, including topology optimization problems, are often characterized by the presence of the multiple objective functions, for example, when the goal is to obtain maximum stiffness and minimum mass of a target structure. When a conflicting relationship exists among multiple objective functions, the design problem does not have a single solution. Instead, a set of optimal solutions called a non-dominated solution set or a Pareto-optimal solution set is obtained. To facilitate the handling of multiobjective optimization problems, a scalarization technique such as the weighted-sum method [45, 46] or the ε -constraint method [47] is often used, so that a multiobjective optimization problem can be converted to a single-objective optimization problem.

A converted single-objective optimization problem obtains one particular solution on the Pareto front, and each different single-objective optimization problem converted according to a certain scalarization parameter obtains a different optimal solution. Therefore, time-consuming adjustment of the scalarization parameters is required to obtain a desired solution that represents a particular compromise to the conflicting relationship between the objective functions.

Obtaining an entire set of Pareto-optimal solutions is another approach to handle multi-objective optimization problems. This approach does not require predetermined preference parameter settings, and has an advantage because design engineers can easily choose a particular solution that best meets their needs. The concept of Pareto-optimal solutions have

been extended to the concept of s-Pareto fronts for concept selection [48]. Furthermore, Pareto-optimal solution information can aid the analysis of trade-off conditions among the objective functions [49, 50], by applying data mining techniques such as cluster analysis or a self-organizing map.

The most popular and powerful approaches to obtain a Pareto-optimal solution set are metaheuristic-based approaches such as multiobjective evolutionary algorithms (MOEAs) [51–54], including genetic algorithms (MOGAs) [55, 56], and multiobjective particle swarm optimization methods [57–59]. Most metaheuristic methods use a population-based search strategy in which many points in the design space are simultaneously evaluated and new points are generated from the population so that they migrate toward non-dominated points. Population-based search strategies are advantageous for global searches and can provide a Pareto front approximation in a single optimization calculation. Furthermore, since many metaheuristic methods do not require gradient information from the objectives, they can easily be applied in a variety of engineering problems.

Metaheuristic-based techniques have also been applied to multiobjective topology optimization problems [60–63]. One of the merits of using metaheuristic-based techniques for topology optimization is that these techniques do not require design sensitivities, which make implementation simpler. However, metaheuristic-based techniques are inefficient when searching for fine-tuned solutions near optimal solutions, since these algorithms do not include the use of design sensitivities. Metaheuristic-based techniques are also inefficient when applied to large-scale problems that have many thousands of design variables. Metaheuristic-based approaches that can handle multiobjective topology optimization problems in which the number of design variables is roughly 10^3 at most are described in the literature [64]. However, topology optimization problems are often characterized by large-scale problems in which the number of design variables is on the order of 10^3 – 10^6 , since a design variable is typically assigned to each finite element, or node, of the discretized design domain [65]. As a result, additional techniques to forcibly reduce the number of design variables are required when using metaheuristic-based approaches applied to topology optimization problems [66–68], and these become increasingly problematic as the multiobjective topology optimization problem becomes more complex.

On the other hand, several gradient-based multiobjective optimization methods that use design sensitivities in the optimization procedure have been proposed. For non-constrained problems, the multiobjective steepest descent method [69] and multiobjective optimization

based on Newton's method [70] have been proposed. For constrained problems, the normal boundary intersection method [71] and the normal constraint method [72] have been proposed. Furthermore, multiobjective optimization methods using an adaptive weighted-sum method [73] and an aggregative gradient-based multiobjective optimization (AGMO) method [74] have also been proposed. The use of design sensitivities in the optimization procedure is advantageous since this enables optimal solutions to be obtained efficiently. In many structural optimization problems that include continuous design variables, design sensitivities can be obtained by conducting sensitivity analysis prior to the optimization procedure. In particular, the adjoint variable method is an effective technique, in which adjoint equations are used to calculate the design sensitivities.

Gradient-based multiobjective optimization methods have also been applied to multiobjective topology optimization problems. Suresh [75] constructed code for Pareto-optimal tracing in a multiobjective topology optimization problem and the AGMO method cited above has also been applied to the same. However, this code can only be applied to topology optimization problems that have two objective functions, and in AGMO, points located some distance from a Pareto front are updated along with points near a Pareto front, which is computationally inefficient. Furthermore, AGMO requires that some scheme be used to ensure the diversity of the obtained Pareto-optimal solutions [76].

As described above, multiobjective optimization methods that are especially suitable for multiobjective topology optimization problems have not yet been fully developed. This chapter presents a new multiobjective optimization algorithm that adroitly handles multiobjective topology optimization problems that include tens of thousands of design variables, before data mining techniques are applied to the structural data of the topology optimization result, which is mentioned in the next chapter.

2.2 Multiobjective optimization

Here, we discuss the basic concept of multiobjective optimization problems. Let $\mathbf{d}$ denote a design variable vector, and $\mathbf{f}$ represent a objective function vector. A multiobjective optimization problem which has m -objectives is then generally formulated, as follows:

$$\min_{\mathbf{d} \in \mathcal{D}_{\text{ad}}} \mathbf{f} = [f_1, f_2, \dots, f_m], \quad (2.1)$$

where $\mathcal{D}_{\text{ad}}$ represents an admissible space of the design variable vector. When an objective function is to be maximized, it can be converted to a minimization function simply by prefixing it with a minus sign. In multiobjective optimization, no single solution exists that simultaneously yields minimal values for all objectives. Instead, a set of multiple solutions is obtained, called non-dominated solutions, or Pareto-optimal solutions. A feasible solution, $\mathbf{d}_1$, is said to dominate another feasible solution, $\mathbf{d}_2$, if and only if the following conditions hold:

1. $f_i(\mathbf{d}_1) \leq f_i(\mathbf{d}_2)$ for all indices $i \in 1, \dots, m$,
2. $f_j(\mathbf{d}_1) < f_j(\mathbf{d}_2)$ for at least one index $j \in 1, \dots, m$.

A feasible solution is called a non-dominated solution or a Pareto-optimal solution if no other solution dominates it. The mapping of Pareto-optimal solutions in the design space into the objective space is called a Pareto front. The result of solving a multiobjective optimization problem usually provides a set of design variable vectors that are Pareto-optimal, and a corresponding Pareto front approximation.

Now, we formulate a multiobjective topology optimization problem. Let $\mathbf{F}$ denote a objective functional vector whose components are to be minimized. A multiobjective topology optimization problem is then formulated as follows:

$$\inf_{\chi_{\Omega} \in \mathcal{X}} \mathbf{F} = [F_1, \dots, F_m], \quad (2.2)$$

with

$$F_i = \int_D f_{\text{di}}(u_i, \chi_{\Omega}) dD + \int_{\Gamma} f_{\text{bi}}(u_i) d\Gamma, \quad (2.3)$$

for all indice $i \in \{1, 2, \dots, m\}$ where f_{di} and f_{bi} are integrands of each objective functional, and u_i is a state variable governed by a state equation describing certain physical phenomenon.

2.3 Stiffness maximization problems for multiple loads

2.3.1 Formulation of an optimization problem

We first consider the minimum mean compliance problem, which is well-known as a benchmark problem of topology optimization methods. In multiple loading cases, mean compliances for each loading case are the objective functionals to be minimized.

Let $\mathbf{t}^i, \forall i \in \{1, \dots, m\}$, respectively denote a traction applied on the boundary Γ_i , a part of the boundaries of the fixed design domain, ∂D . We consider a structural optimization problem to determine an optimal configuration of the material domain $\Omega \subseteq D$ which minimizes mean compliances against m loads. Here, the level set-based approach [22] mentioned in Section 1.3.2 is used. Then, a multiobjective topology optimization problem for minimum mean compliances is formulated as

$$\inf_{\chi_\phi} \quad \mathbf{F} = [F_1, F_2, \dots, F_m], \quad (2.4)$$

$$\text{subject to:} \quad (2.5)$$

$$G = \int_D \chi_\phi dD - V_{\max} \leq 0, \quad (2.6)$$

with

$$F_i = \int_{\Gamma_i} \mathbf{t}^i \cdot \mathbf{u}^i d\Gamma, \quad \forall i \in \{1, \dots, m\}. \quad (2.7)$$

$\mathbf{u}^i \in \mathcal{U}$ is a displacement field and satisfies the following variational formulation for $\forall \mathbf{v} \in \mathcal{U}$:

$$E_i = \int_{\Gamma_i} \mathbf{t}^i \cdot \mathbf{v} d\Gamma - \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{v}) : \mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}^i) d\Omega = 0, \quad \forall i \in \{1, \dots, m\}, \quad (2.8)$$

where $\mathbf{C}$ is the elastic tensor, $\boldsymbol{\varepsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ is the strain tensor, and $\mathcal{U}$ is a functional space defined as

$$\mathcal{U} = \{\mathbf{v} \in H^1(D)^d \mid \mathbf{v} = \mathbf{0} \text{ on } \Gamma_u\}, \quad (2.9)$$

with H^1 being a Sobolev space and d the number of dimensions.

2.3.2 Optimization method

Concept of a population-based approach

In the proposed method, a population-based approach is used to explore the Pareto front based on a modified version of the study by [74]. Figure 2.1 shows the conceptual scheme of a population-based approach for a case with two objective functions. Many points exist in the objective space and each point corresponds to a single solution candidate. Arrows emanating

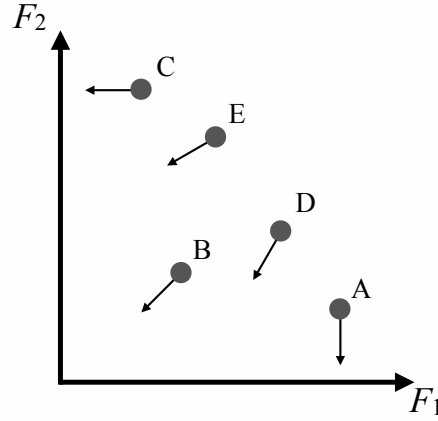


Fig. 2.1 Conceptual scheme of a population-based approach.

from each point indicate the direction in which each point should proceed to search the Pareto front efficiently. To determine these directions, adaptive weighting coefficients are calculated considering the relative position of the points in the objective space.

Adaptive weighting coefficients

In the proposed method, multiobjective topology optimization problems are converted into conventional single-objective topology optimization problems based on the idea of the weighted-sum method. Although the weighted-sum approach has limitations when applied in problems that have a non-convex Pareto front, it is reasonable to assume that the Pareto fronts in most engineering design problems are convex. Therefore, the weighted-sum approach remains a useful approach for many practical multiobjective optimization problems, and is discussed in numerous studies [77, 78].

Let a weighting coefficient vector assigned to the p th point be denoted as

$$\mathbf{w}^p = [w_1^p, w_2^p, \dots, w_m^p]. \quad (2.10)$$

In (1.29), the sensitivity is replaced with the weighted-sum of the sensitivities derived from each objective functional, as follows:

$$F'_{\text{total}} = \sum_{i=1}^m w_i \frac{F'_i \int_D dD}{\int_D |F'_i| dD}, \quad (2.11)$$

where $\int_D dD / \int_D |F'_i| dD$ is a scaling factor.

A method for determining the weighting coefficients adaptively, considering the distribution of the Pareto front, is now explained. Suppose that the value for the p th point of F_i^p , which represents the i th objective functional, is the l th largest among the values of the i th objective functional for the existing points. The value of weighting coefficient w_i^p is then determined using

$$w_i^p = l - 1. \quad (2.12)$$

The weighing coefficients for each point are then normalized so that the sum of the weighting coefficients for each point becomes 1, as follows:

$$\bar{w}_i^p = \frac{w_i^p}{\sum_{j=1}^m w_j^p}, \quad (2.13)$$

where $\bar{w}_i^p$ represents a normalized weighting coefficient. Consequently, the smaller the value of an objective functional, the larger the value of the weighting coefficient assigned for that objective functional. For example, point A in Fig. 2.1 has the largest value of the F_1 functional among all points, and its F_2 functional value is the smallest among all points. Weighting coefficient $\bar{w}^A = [\bar{w}_1^A, \bar{w}_2^A]$ is then determined as $[0, 1]$. As a result, point A will proceed in the direction indicated by the arrow. The application of adaptive weighting coefficients thereby enables efficient exploration of the Pareto front.

Point selection

As mentioned above, a population-based approach is used in the present study. That is, many points corresponding to solution candidates are updated during each iteration of the optimization procedure, and the non-dominated points are output as Pareto-optimal solutions when the terminal condition is satisfied. Since the number of the non-dominated points increases overall as the optimization progresses, the computational cost would increase dramatically if all non-dominated points were updated at every iteration. Therefore, we introduce a point selection scheme to reduce the number of points requiring calculations. The point selection scheme selects points along a portion of the Pareto front where Pareto-optimal solutions are sparsely obtained in the current iteration. It is expected that these selected points will explore unexplored regions after the gradient-based update of the design variables, owing to the use of the adaptive weighting scheme, and that the distribution of the

Pareto-optimal solutions will be improved. To detect portions of the Pareto front where Pareto-optimal solutions are relatively sparse, we employ the concept of the “crowded comparison” approach, which is usually applied in NSGA-II [55]. It is worth noting, however, that the ε -dominance approach replaced the “crowded comparison” approach about a decade ago in MOEA literature [79, 80]. It is well known that the ε -dominance approach can select points uniformly, whereas the “crowded comparison” approach tends to favor the selection of points in areas where points are sparsely distributed. Thus, we use the “crowded comparison” in the point selection scheme so that regions along Pareto front where Pareto-optimal solutions are relatively sparse would be preferentially selected. In this chapter, we use an indicator, the “crowding distance” (CD), based on the idea of the “crowded comparison”. The CD value of the p th non-dominated point is calculated as

$$CD^p = \sum_{i=1}^m \frac{F_i^{p+1} - F_i^{p-1}}{F_i^{\max} - F_i^{\min}}, \quad (2.14)$$

where $F_i^{\max}$ and $F_i^{\min}$ represent the maximum and minimum values of the i th objective functional among all non-dominated points. F_i^{p+1} and F_i^{p-1} represent the values of the i th objective functionals of points to either side of the p th non-dominated point when all non-dominated points are sorted in order of their value for the i th objective functional. Figure 2.2 shows the relationship between the functional values for F_i^p , F_i^{p+1} and F_i^{p-1} in a two-dimensional objective space. Note that if F_i^p is the largest or smallest among the values of the i th objective functional for all non-dominated points, F_i^{p+1} , or F_i^{p-1} , will not exist. In such cases, the numerator $F_i^{p+1} - F_i^{p-1}$ in (2.14) is replaced with $2(F_i^p - F_i^{p-1})$ or $2(F_i^{p+1} - F_i^p)$, respectively. The larger the value of the CD, the fewer the number of points in the area. Therefore, it is advantageous to explore the regions near points that have large CD values.

We set the number of points that will be updated at each iteration, N , and these points are selected in the order of their CD value, starting with the point whose CD value is the largest. The weighting coefficients for the N points are assigned using (2.12) and the N points are updated until each one converges. As a result, the proposed method can efficiently explore areas in the objective space in which points are sparse. Note that in NSGA-II, if the value of F_i for a point is the largest or smallest among the values of the i th objective function in a population, the CD value for this point assumes a very large value, ideally infinity, so that points at the extreme ends of the Pareto front are always selected. Since, in the proposed

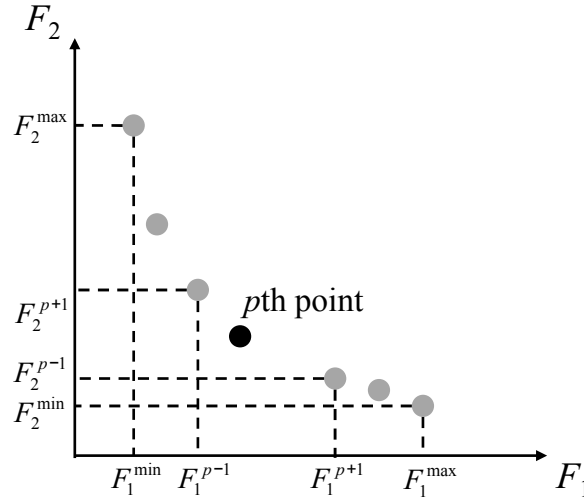


Fig. 2.2 Relationship between F_i^p , F_i^{p+1} and F_i^{p-1} in the two-dimensional objective space.

method, the limits of the Pareto front are easily obtained, points at the extreme ends are treated in the same manner as other points.

Optimization algorithm

Figure 2.3 shows the flowchart of the optimization algorithm. The proposed method is now described in detail.

– Step 1: Perform initial optimization

$m + 1$ optimization problems, composed of m single-objective optimization problems decomposed from the original multiobjective optimization problem, and one problem in which the weighting coefficients for all objective functionals are set to $1/m$, are solved. Non-dominated points are updated at every iteration in this procedure.

– Step 2: Select points to be updated

N points are selected from the set of non-dominated points according to their CD values, using (2.14). Set $k = 1$.

– Step 3: Calculate weighting coefficients

Calculate the weighting coefficients for the k th point, using (2.12).

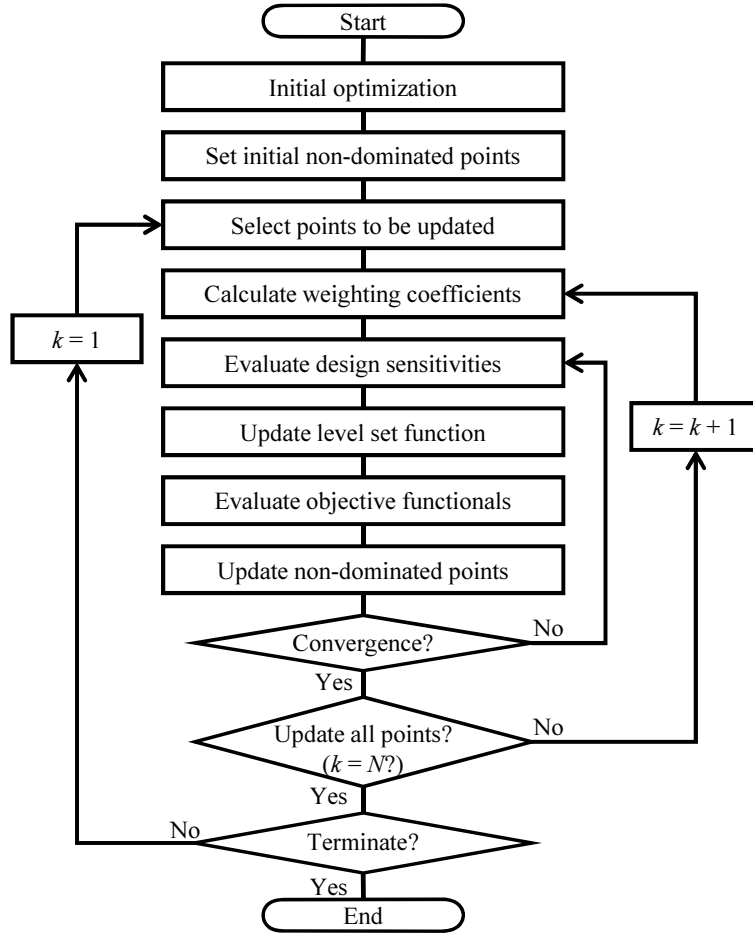


Fig. 2.3 Flowchart of the proposed algorithm.

– **Step 4: Evaluate design sensitivities**

Evaluate the design sensitivities for all objective functionals, using the adjoint variable method.

– **Step 5: Update the level set function**

The level set function of the k th point is updated, using (1.29).

– **Step 6: Evaluate objective functionals and check non-domination condition**

The objective functionals are evaluated for the updated level set function of the k th point and the updated point is checked to determine whether or not it is a non-dominated point. If the updated point is a non-dominated point, it is added to the set of non-dominated points.

– **Step 7: Check convergence**

If the objective functionals are converged, set $k = k + 1$, otherwise return to Step 4. If the new value of k is less than or equal to N , return to Step 3, otherwise proceed to Step 8.

– **Step 8: Check termination condition**

If the termination condition is satisfied, the optimization process is halted, otherwise set $k = 1$ and return to Step 2. The termination condition is set at the beginning as the maximum number of calls for Step 8, i.e., the maximum number of cycles from Step 2 to Step 8. The set of non-dominated points at the time when the optimization process is halted is output as a Pareto-optimal solution set.

Here, we use two terms, “inner iteration” and “outer iteration,” to distinguish the two subroutines in the optimization process. The former means iterations in which a point is updated until it converges, based on Steps 4–6. The latter means iterations in which N points are selected and then updated through the operation of the “inner iteration.” The “outer iteration” corresponds to Steps 2–8, i.e., the termination condition is set to the maximum number of “outer iterations” in this chapter.

The key techniques in the proposed method are the use of adaptive weighting coefficients and the point selection scheme, which is based on the “crowded comparison” concept. Since the weighting coefficients are adaptively assigned to each point considering the relative position of the non-dominated points, setting weighting coefficients to predetermined values is not required, even though the proposed method uses the weighted-sum approach. Furthermore, the point selection scheme enables efficient Pareto front exploration because points in areas where points are sparse are preferentially selected and updated, so that the vicinities of these points are explored based on their weighting coefficients.

2.3.3 Numerical example

Here, we consider two loading cases. Figure 2.4 shows the non-dimensional fixed design domain, in which tractions t^1 and t^2 are applied at the center of the bottom and top edges of the fixed design domain D , respectively. Since the boundary conditions are symmetric at the symmetric boundary indicated in Fig. 2.4 by the vertical dash-dotted line, we deal with only the right half of the fixed design domain, which is discretized using 80×120 quadrilateral first-order finite elements. The upper limit of the volume, $V_{\max}$, is set to 40% of the right half

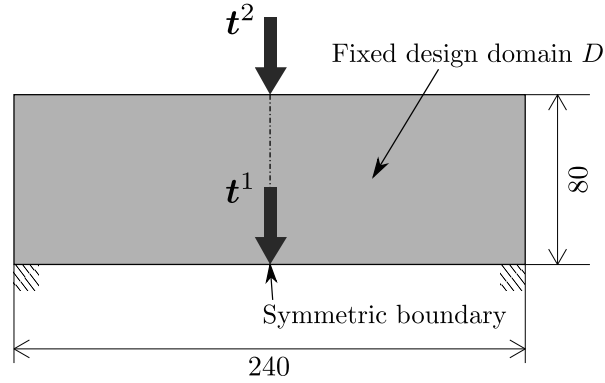


Fig. 2.4 Fixed design domain and boundary conditions.

Table 2.1 Parameter settings in the two-objective topology optimization.

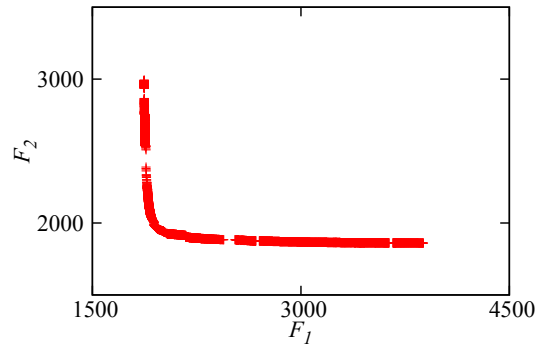
	N	$O_{\max}$
Case 1	10	20
Case 2	20	20
Case 3	10	40

of the fixed design domain. The Young's modulus and Poisson's ratio was set to 1 and 0.3, respectively.

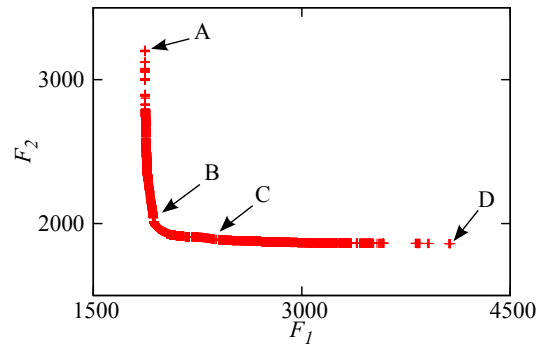
Effects of setting the number of points and number of outer iterations

First, we examine the effects of setting the number of points treated and the number of outer iterations conducted during the optimization procedure. Let $O_{\max}$ denote the maximum number of times the outer iteration is run. In this problem, optimization was conducted for three cases: Case 1, with N , the number of points updated during each outer iteration = 10 and $O_{\max} = 20$; Case 2, with $N = 20$ and $O_{\max} = 20$; and Case 3, with $N = 10$ and $O_{\max} = 40$, as listed in Table 2.1.

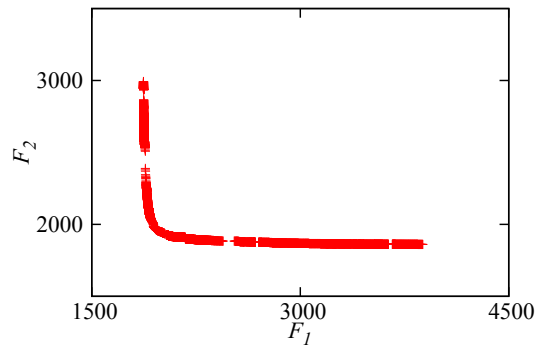
Figure 2.5 shows the Pareto-optimal solution sets for the three cases and Fig. 2.6 shows the optimal configurations at points A, B, C and D in Fig. 2.5(b). As Fig. 2.5 reveals, the Pareto-optimal solutions obtained in Case 2 are more diverse than those in Cases 1 and 3, and the Pareto-optimal solutions in Cases 1 and 3 are almost identical. This implies that, to obtain well-distributed Pareto-optimal solutions, the number of points N updated during every



(a)



(b)



(c)

Fig. 2.5 Pareto optimal solutions in (a) Case 1; (b) Case 2; (c) Case 3.

outer iteration has a greater effect than the maximum number of times the outer iteration is performed. Therefore, parameter N should be given priority when adjusting parameters to improve the distribution of the Pareto-optimal solutions.

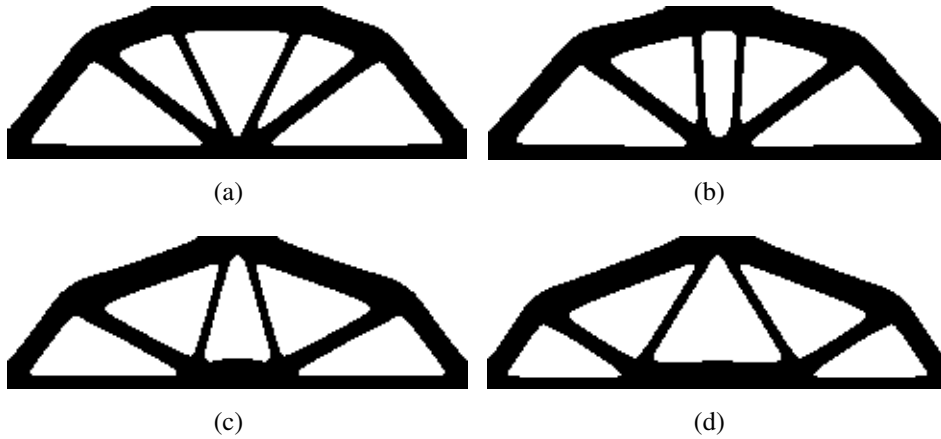
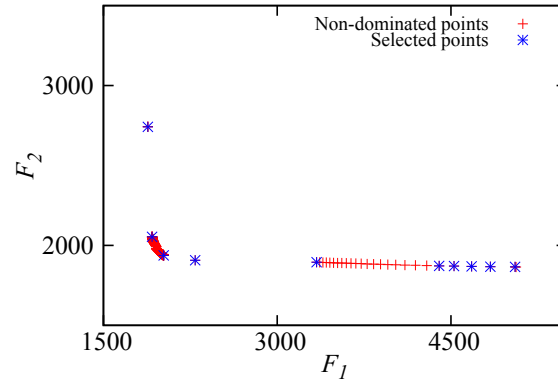


Fig. 2.6 Optimal configurations for Pareto-optimal solutions in Case 2: (a) Point A; (b) Point B; (c) Point C; (d) Point D.

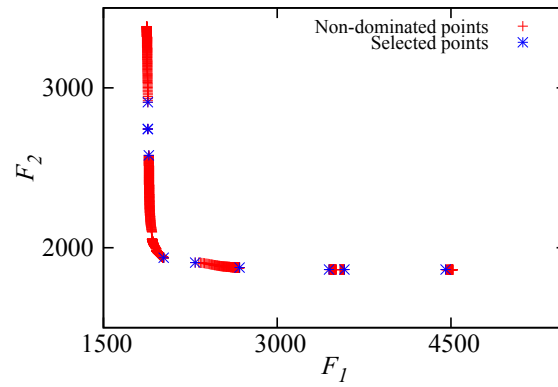
Next, we consider the relationship between the optimal configurations and the values of the objective functionals. As can be seen in Fig. 2.6, the optimal configurations for each of the chosen Pareto-optimal solution have the same geometric topology, the five apertures included in each structure. However, the orientation of the central pair of beam structures is radically different, depending on the location of the solution chosen along the Pareto front. Specifically, in the structure shown in Fig. 2.6(a), obtained with traction t^1 greatly outweighing the influence of traction t^2 , the two central beam structures intersect at the bottom and are widely spaced at the top. A markedly different geometry is obtained when the influence of the upper and lower tractions is reversed, as shown in Fig. 2.6(d), where the central pair of beam structures now intersect at the top. The dramatic differences between the structures shown in Fig. 2.6(a)–(d) illustrate how Pareto-optimal solution information enables an understanding of the trade-off relationships between objective functionals and how they affect the optimal structures. Data mining techniques to analyze multiobjective topology optimization results are provided in the next chapter.

Effectiveness of the point selection and adaptive weighting schemes

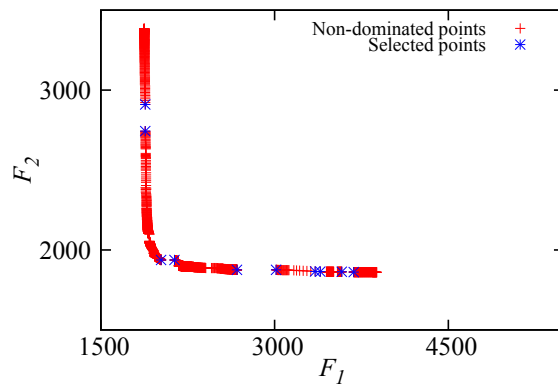
Next, we verify the effectiveness of the proposed adaptive weighting and point selection schemes. Here, N was set to 10. Figure 2.7(a)–(c) shows the selected points and non-dominated points after one, two, and three outer iterations, respectively. At each successive iteration, points located in areas with sparse distributions of points were appropriately selected



(a)

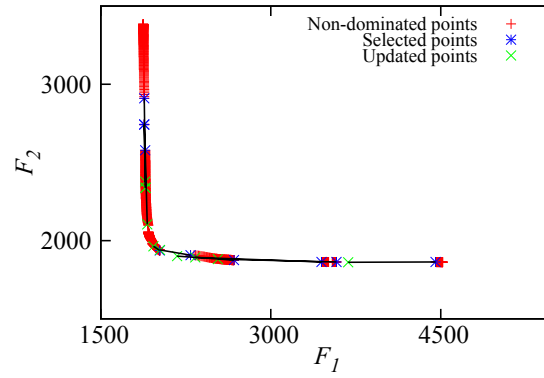


(b)

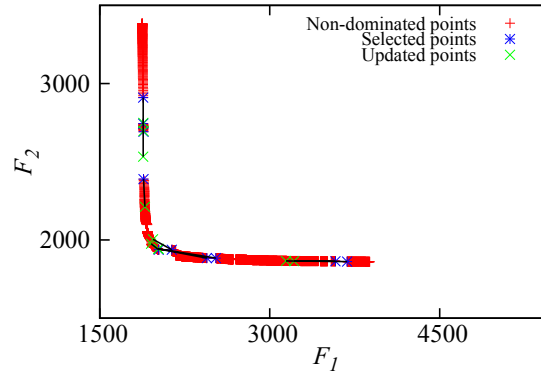


(c)

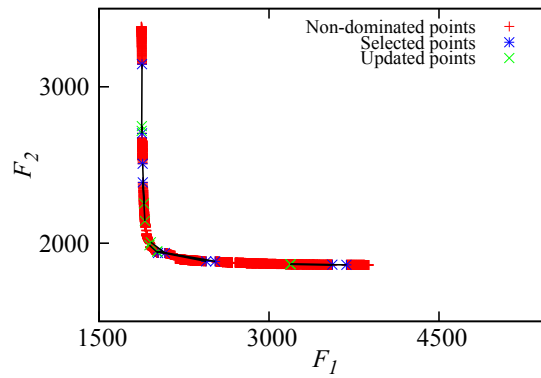
Fig. 2.7 Selected points and non-dominated points at the time the outer iteration was conducted: (a) after one iteration; (b) after two iterations; (c) after three iterations.



(a)



(b)



(c)

Fig. 2.8 Selected points prior to outer iteration (“*” in blue), points corresponding to selected points after outer iteration (“x” in green), and non-dominated points after outer iteration (“+” in red): (a) after two iterations; (b) four iterations; (c) six iterations.

and the population of Pareto solutions along the Pareto front was further increased. We therefore confirm that the point selection scheme works effectively in the proposed method.

Figure 2.8 illustrates how the adaptive weighting scheme functions. The ten selected points (“*” in blue) are updated during each outer iteration of the optimization procedure and moved to new locations along the Pareto front (“×” in green). Non-dominated points (“+” in red) created during the inner iteration during the optimization procedure are placed along the black lines connecting blue and green points, where non-dominated points are sparse or do not exist. At each successive iteration, areas with few or no non-dominated points were correctly identified and subsequently populated with non-dominated solutions. We therefore confirm that the adaptive weighting scheme functions appropriately in the proposed method.

2.4 An optimum design problem of a no-moving-part valve

2.4.1 Background

No-moving-part (NMP) valves such as Tesla valves are fluid channels whose flow resistance depends on flow direction. Having no moving parts, they rely on fluidic inertial forces so that the fluid flows preferentially in one direction. NMP valves are widely used in the field of microfluidics as components of pumps [81–83]. Although NMP valves do not eliminate reverse flow completely, they have significant advantages over active valves that rely on moving parts actuated by external forces, because NMP valves are more reliable and easier to fabricate. Furthermore, NMP valves can handle particle-laden, multiphase and oscillating flows [84].

A number of previous studies have explored improvements in NMP valve design. Truong and Nguyen [85] conducted a parametric optimization of an NMP valve design and analyzed relationships between the geometric parameters of an NMP valve and its performance as measured by its diodicity. Gamboa *et al.* [86] conducted shape optimization for an NMP valve design. Topology optimization methods have also been proposed for the optimum design of an NMP valve [87, 84].

For fluid mechanics problems, Borrvall and Petersson [88] first developed a topology optimization method in which the fixed design domain is composed of both fluid and solid domains, with the former governed by the Stokes equation and the latter assumed to have a property of porous media, based on Darcy’s law [89]. That is, a fictitious force applied only in the solid domain was introduced and flow in the solid domain was slowed depending on the

magnitude of this fictitious force that depends on the characteristic function. Consequently, the fixed design domain was governed by an expanded governing equation that includes a fictitious force term, and optimal fluid channel configurations can then be obtained using this expanded governing equation. Several previous studies have extended this approach to the Navier-Stokes equation and it to fluid channel design problems, including minimization of fluid dissipation energy [90, 91], fluid-structure interaction problems [92], and others [93–95].

In almost all previous studies for the design of NMP valves, performance is measured using diodicity, defined as the ratio of the pressure drop in reverse flow to that of the forward flow at the same flow rate. However, higher diodicity does not necessarily indicate better NMP valve performance. Although higher diodicity values indicate a higher ratio of pressure drop between reverse and forward flows, the pressure drop in the forward flow may be higher than desired, leading to increased pumping power requirements and inefficient fluid flow. Therefore, for the optimum design of an NMP valve, the pressure drop in the forward and reverse flows should be considered independently, using a multiobjective formulation, rather than treating the diodicity alone.

In this section, the proposed multiobjective optimization method is applied to an optimum design problem for an NMP valve formulated as a bi-objective optimization problem. One objective function is to minimize the dissipation energy in the forward flow, and the other is to maximize the dissipation energy in the reverse flow. Pareto-optimal solutions that can be obtained by treating the forward and reverse flows independently can provide design engineers with practical information, such as multiple design candidates that then allow choices adapted to particular requirements, and insights concerning the physical mechanisms responsible for desired performances, by comparing each Pareto-optimal solution.

2.4.2 Governing equations

Consider an internal flow channel problem in which an iso-thermal incompressible steady-state fluid flow is assumed. The formulation of the governing equations therefore must include the conservation of mass and momentum. Let the gradient operator, fluid velocity and pressure be denoted $\bar{\nabla}$, $\bar{\mathbf{u}}$ and $\bar{p}$, respectively. The Reynolds number Re , non-dimensional gradient operator ∇ , and non-dimensional variables $\mathbf{u}$ and p are then defined as follows:

$$Re = \frac{\rho UL}{\mu}, \quad \nabla = L\bar{\nabla}, \quad \mathbf{u} = \frac{\bar{\mathbf{u}}}{U}, \quad \text{and} \quad p = \frac{\bar{p}}{\rho U^2}, \quad (2.15)$$

where U and L represent a characteristic fluid velocity and a characteristic length, respectively. In this research, U and L represent the average fluid velocity at the inlet and the width of the inlet, respectively. The non-dimensional continuity and Navier-Stokes equations that govern the flow are then given as follows:

$$\text{Continuity equation:} \quad -\nabla \cdot \mathbf{u} = 0, \quad (2.16)$$

$$\text{Navier-Stokes equation:} \quad (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T). \quad (2.17)$$

As the general boundary condition for $\mathbf{u}$, we define a Dirichlet boundary condition on Γ_D , as follows:

$$\mathbf{u} = \mathbf{u}_D \text{ on } \Gamma_D, \quad (2.18)$$

where $\mathbf{u}_D$ represents the fluid velocity on Γ_D . A Neumann boundary condition is defined as

$$\mathbf{n} \left(-p \mathbf{I} + \frac{1}{\text{Re}} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right) = 0 \text{ on } \Gamma_N, \quad (2.19)$$

where $\mathbf{I}$ is the identity matrix and $\mathbf{n}$ is the outward unit normal vector on Γ_N .

To formulate the governing equations for the fixed design domain, no-slip boundary conditions are approximated by introducing a fictitious force applied only in the solid domain [88]. That is, the solid domain is treated as a permeable material which has the inverse permeability of a porous medium $\alpha_{\max}$, and a fictitious force $-\alpha \mathbf{u}$ is added to the governing Navier-Stokes equation. Based on the density approach described in Chapter 1, the extended Navier-Stokes equation is written as follows:

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \alpha(\theta) \mathbf{u} \quad \text{in } D, \quad (2.20)$$

where α is defined such that

$$\alpha(\theta) = \frac{q(1-\theta)}{q+\theta} \alpha_{\max}, \quad (2.21)$$

and q is a parameter that controls the convexity of $\alpha(\theta)$. If $\alpha_{\max}$ is set infinitely large, then the solid domain represents an impermeable material. In practice, $\alpha_{\max}$ is set to a very large value. Consequently, since $-\alpha \mathbf{u}$ in (2.20) forces the flow velocity in the solid domain to approach zero, the fluid and solid domain can both be governed by (2.20), which can then be defined in the fixed design domain D .

2.4.3 Optimization problem

Let $\mathbf{u}_f$ and p_f respectively denote the fluid velocity and pressure in the forward flow, and similarly, let $\mathbf{u}_r$ and p_r respectively denote the fluid velocity and pressure in the reverse flow. The total dissipation energy is then represented as the sum of the viscous dissipation and the potential energy of the body force, based on Darcy's law, as follows:

$$D_f = \frac{1}{2\text{Re}} \int_D (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) : (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) dD + \int_D \alpha(\theta) \mathbf{u}_f \cdot \mathbf{u}_f dD, \quad (2.22)$$

$$D_r = \frac{1}{2\text{Re}} \int_D (\nabla \mathbf{u}_r + \nabla \mathbf{u}_r^T) : (\nabla \mathbf{u}_r + \nabla \mathbf{u}_r^T) dD + \int_D \alpha(\theta) \mathbf{u}_r \cdot \mathbf{u}_r dD, \quad (2.23)$$

where D_f and D_r represent the dissipation energy of the forward flow and the reverse flow, respectively.

In most previous studies of NMP valve designs, the performance of the NMP valve is assessed by its diodicity, Di , defined as

$$\text{Di} = \frac{\Delta p_r}{\Delta p_f} = \frac{\int_{\Gamma_{\text{in},r} \cup \Gamma_{\text{out},r}} p_r (-\mathbf{u}_r \cdot \mathbf{n}) d\Gamma}{\int_{\Gamma_{\text{in},f} \cup \Gamma_{\text{out},f}} p_f (-\mathbf{u}_f \cdot \mathbf{n}) d\Gamma}, \quad (2.24)$$

where $\mathbf{n}$ is a unit vector normal to the boundaries and the diodicity is almost equal to the ratio of the dissipation energies, Di' , as follows:

$$\text{Di}' = \frac{D_r}{D_f} \simeq \frac{\Delta p_r}{\Delta p_f} = \text{Di}, \quad (2.25)$$

as shown in a previous study [84]. Larger diodicity values indicate increasingly large differences between the reverse and forward flow pressure drops, hence better performance of an NMP valve.

However, higher diodicity does not guarantee better performance of NMP valves because the ratio does not indicate the degree of forward flow dissipation, D_f , and high dissipation in the forward flow implies that more pumping power is required, which spoils fluid flow efficiency. Therefore, we handle the forward and reverse dissipations independently, and formulate a bi-objective optimization problem that aims to obtain optimal channel configurations for a no-moving part valve. One objective function minimizes the total dissipation energy of the forward flow D_f , and the other maximizes the total dissipation energy of the

reverse flow D_r . The boundary conditions for $\mathbf{u}_f$, p_f , $\mathbf{u}_r$ and p_r are formulated as follows:

$$\left\{ \begin{array}{ll} \mathbf{u}_f = \mathbf{u}_{\text{in},f} & \text{on } \Gamma_{\text{in},f} \\ \mathbf{u}_f = 0 & \text{on } \Gamma_{\text{wall}} \\ p_f = 0 & \text{on } \Gamma_{\text{out},f} \\ \mathbf{u}_r = \mathbf{u}_{\text{in},r} & \text{on } \Gamma_{\text{in},r} \\ \mathbf{u}_r = 0 & \text{on } \Gamma_{\text{wall}} \\ p_r = 0 & \text{on } \Gamma_{\text{out},r}, \end{array} \right. \quad (2.26)$$

where $\Gamma_{\text{in},f}$ and $\Gamma_{\text{out},f}$ represent the inlet and the outlet for the forward flow, and $\Gamma_{\text{in},r}$ and $\Gamma_{\text{out},r}$ represent the inlet and the outlet for the reverse flow, respectively. That is, $\Gamma_{\text{in},r}$ corresponds to $\Gamma_{\text{out},f}$ and $\Gamma_{\text{out},r}$ corresponds to $\Gamma_{\text{in},f}$. Γ_{wall} represents wall boundaries. $\mathbf{u}_{\text{in},f}$ and $\mathbf{u}_{\text{in},r}$ are the prescribed flow velocities at $\Gamma_{\text{in},f}$ in the forward flow and at $\Gamma_{\text{in},r}$ in the reverse flow, respectively. Based on the Heaviside projection method described in Section 1.3.1, a bi-objective optimization problem is then formulated as follows:

$$\inf_{\hat{\phi}} \mathbf{F} = [F_1, F_2] = \left[D_f, \frac{1}{D_r} \right], \quad (2.27)$$

where state variables $(\mathbf{u}_f, p_f) \in \mathcal{U}_f \times \mathcal{P}_f$ and $(\mathbf{u}_r, p_r) \in \mathcal{U}_r \times \mathcal{P}_r$ satisfy the following variational formulations:

$$E_1 = - \int_D \nabla \cdot \mathbf{u}_f \tilde{p}_f dD = 0 \quad (2.28)$$

$$E_2 = \int_D (\mathbf{u}_f \cdot \nabla) \mathbf{u}_f \cdot \tilde{\mathbf{u}}_f dD - \int_D p_f \nabla \cdot \tilde{\mathbf{u}}_f dD \quad (2.29)$$

$$+ \int_D \frac{1}{\text{Re}} (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) : \nabla \tilde{\mathbf{u}}_f dD + \int_D \alpha(\theta) \mathbf{u}_f \cdot \tilde{\mathbf{u}}_f dD = 0 \quad (2.30)$$

$$E_3 = - \int_D \nabla \cdot \mathbf{u}_r \tilde{p}_r dD = 0 \quad (2.31)$$

$$E_4 = \int_D (\mathbf{u}_r \cdot \nabla) \mathbf{u}_r \cdot \tilde{\mathbf{u}}_r dD - \int_D p_r \nabla \cdot \tilde{\mathbf{u}}_r dD \quad (2.32)$$

$$+ \int_D \frac{1}{\text{Re}} (\nabla \mathbf{u}_r + \nabla \mathbf{u}_r^T) : \nabla \tilde{\mathbf{u}}_r dD + \int_D \alpha(\theta) \mathbf{u}_r \cdot \tilde{\mathbf{u}}_r dD = 0. \quad (2.33)$$

for all variables $(\tilde{\mathbf{u}}_f, \tilde{p}_f) \in \mathcal{U}_f^0 \times \mathcal{P}_f^0$ and $(\tilde{\mathbf{u}}_r, \tilde{p}_r) \in \mathcal{U}_r^0 \times \mathcal{P}_r^0$ where

$$\mathcal{U}_f = \{\mathbf{u}_f \in H^1(D)^d \mid \mathbf{u}_f = \mathbf{u}_{\text{in},f} \text{ on } \Gamma_{\text{in},f} \text{ and } \mathbf{u}_f = 0 \text{ on } \Gamma_{\text{wall}}\} \quad (2.34)$$

$$\mathcal{U}_r = \{\mathbf{u}_r \in H^1(D)^d \mid \mathbf{u}_r = \mathbf{u}_{\text{in},r} \text{ on } \Gamma_{\text{in},r} \text{ and } \mathbf{u}_r = 0 \text{ on } \Gamma_{\text{wall}}\} \quad (2.35)$$

$$\mathcal{U}_f^0 = \{\tilde{\mathbf{u}}_f \in H^1(D)^d \mid \tilde{\mathbf{u}}_f = 0 \text{ on } \Gamma_{\text{in},f} \cup \Gamma_{\text{wall}}\} \quad (2.36)$$

$$\mathcal{U}_r^0 = \{\tilde{\mathbf{u}}_r \in H^1(D)^d \mid \tilde{\mathbf{u}}_r = 0 \text{ on } \Gamma_{\text{in},r} \cup \Gamma_{\text{wall}}\} \quad (2.37)$$

$$\mathcal{P}_f = \{p_f \in L^2(D) \mid p_f = 0 \text{ on } \Gamma_{\text{out},f}\} \quad (2.38)$$

$$\mathcal{P}_r = \{p_r \in L^2(D) \mid p_r = 0 \text{ on } \Gamma_{\text{out},r}\} \quad (2.39)$$

$$\mathcal{P}_f^0 = \{\tilde{p}_f \in L^2(D) \mid \tilde{p}_f = 0 \text{ on } \Gamma_{\text{out},f}\} \quad (2.40)$$

$$\mathcal{P}_r^0 = \{\tilde{p}_r \in L^2(D) \mid \tilde{p}_r = 0 \text{ on } \Gamma_{\text{out},r}\}. \quad (2.41)$$

$E_i (i = 1, 2, 3, 4)$ represents the functionals of equality constraints in weak forms, derived from the equilibrium equations, and $\tilde{\mathbf{u}}_f$, $\tilde{\mathbf{u}}_r$, $\tilde{p}_f$ and $\tilde{p}_r$ are the test functions. L^2 is a Lebesgue space. Note that the second objective functional is formulated as the inverse of D_r , so that the maximization problem is replaced with a minimization problem.

2.4.4 Optimization method

Here, we use the optimization method described in Section 2.3.2. The two objective functionals for the k th point defined in (2.27) are scalarized using the weighting coefficient as follows:

$$F_{\text{total}}^k = \bar{w}_1^k \frac{F_1^k}{\hat{F}_1} + \bar{w}_2^k \frac{F_2^k}{\hat{F}_2}, \quad (2.42)$$

where the superscript “ k ” indicates the values for the k th point and $\bar{w}_i^k$ represents a normalized weighting coefficient. $\hat{F}_1$ and $\hat{F}_2$ represent the initial values of F_1 and F_2 in the current outer iteration, respectively.

2.4.5 Numerical example

In this section, the proposed method is applied to an optimum design problem for an NMP valve. Figure 2.9 shows the fixed design domain D and boundary conditions for (a) the forward flow, and (b) the reverse flow. We assume an incompressible steady state flow with a Reynolds number Re of 100. Inverse permeability α_{max} was set to 1.0×10^3 based on numerical experiments prior to the optimization, so that the velocities in the

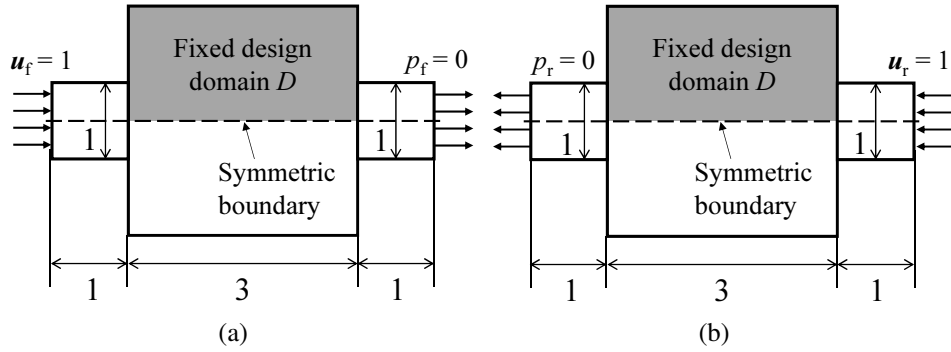


Fig. 2.9 Design domain and boundary condition: (a) forward flow; (b) reverse flow.

solid domain would approach zero. Parameter q was set to 0.05. The design domain was discretized using quadrilateral elements whose size, Δx , is 0.02. In this example, we used the Heaviside projection method by a PDE filter for topology optimization, which was described in Section 1.3.1. The width of the smoothed Heaviside function h in (1.7) was set to 1.0, and parameter R in (1.6) was set to $0.03 (= 1.5\Delta x)$. The number of points, N , that are updated at every outer iteration was set to 10, and the number of outer iteration cycles was set to 10. The convergence criterion parameter ε was set to 10^{-5} and the maximum number of inner iteration was set to 150. Note that we do not need to set any parameters for the importance of the two objective functionals prior to the optimization procedure.

Figure 2.10 shows the obtained Pareto front, and Fig. 2.11 shows a plot of D_r vs. D_f for the obtained Pareto-optimal solutions. The blue dotted line in this figure represents the line: $D_r = D_f$. Pareto-optimal solutions located above this line have greater values of the total dissipation energy D_r in the reverse flow than those of the forward flow D_f , which indicates solutions that can operate as NMP valves.

Figure 2.12 shows the Pareto-optimal configurations for points A, B, C, D and E along the Pareto front shown in Fig. 2.10. As shown in Fig. 2.12(a)–(e), optimal configurations that have different features are obtained as Pareto-optimal solutions. The optimal configuration shown in Fig. 2.12(a) has no solid material in the center of the channel, which minimizes the dissipation of the forward flow, whereas the optimal configuration shown in Fig. 2.12(e) is filled with solid material, which maximizes the dissipation of the reverse flow. Note that since we assume that the solid domain is composed of a porous medium which has a high inverse permeability, the fluid does flow in the configuration shown in Fig. 2.12(e), although

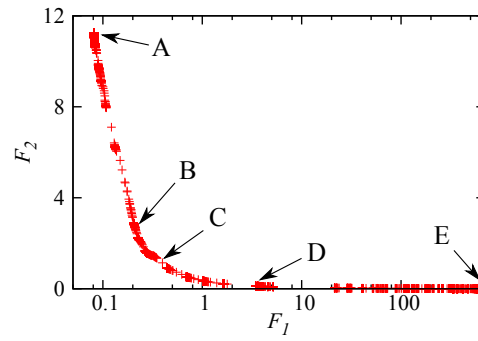


Fig. 2.10 Pareto front obtained by the proposed method.

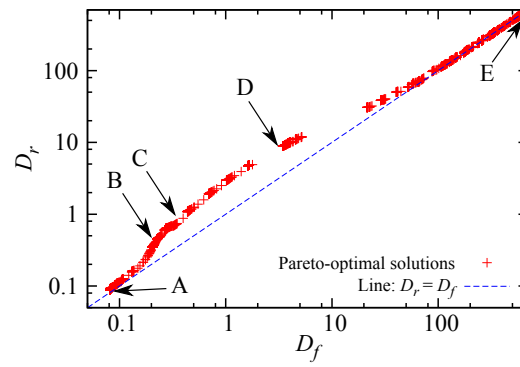


Fig. 2.11 Plot of D_r vs. D_f for obtained Pareto-optimal solutions.

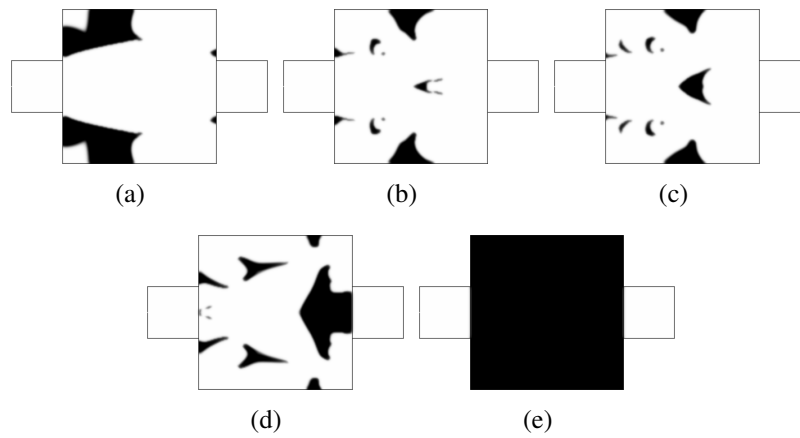


Fig. 2.12 Pareto-optimal configurations (black solid; white fluid) for selected points along the Pareto front in Fig. 2.10: (a) A; (b) B; (c) C; (d) D and (e) E.

extremely slowly. These illustrations are extreme solutions for this bi-objective optimization problem.

On the other hand, the optimal configurations shown in Fig. 2.12(b)–(d) utilize common features. These optimal designs have fang-shaped features, similar to those appearing in the original Tesla valve. The solid material in the center of channel has forward ends shaped so that forward flow is unimpeded and minimal energy is dissipated, whereas the wall-like reverse ends inhibit reverse flow and maximize energy dissipation. These features are similar to those found in the literature [84]. Furthermore, Fig. 2.12(b)–(d) indicates that larger solid material shapes in the center of the optimal configurations are associated with larger values of F_1 and smaller values of F_2 along the Pareto front. In other words, the presence of larger solid material shapes in the center of a channel inhibits reverse flow more successfully than do smaller shapes, but simultaneously increases the dissipation of energy in the forward flow. The Pareto front clearly illustrates this trade-off relationship, and design engineers can choose a particular solution according to their needs at the conceptual design stage. However, the optimal configurations clearly include grayscale areas. To compare the relative errors between pressure drops for the forward and reverse flows of an optimal configuration with the pressure drops calculated by solving the fluid problems with a no-slip boundary condition imposed on the boundaries of the fluid and the solid domains, we evaluated Pareto-optimal solutions using a continuous system version of the “measure of non-discreteness” [29], defined as

$$M_{nd} = \frac{\int_D 4\theta(1 - \theta)dD}{\int_D dD} \times 100\%, \quad (2.43)$$

which returns a value of 0% if no grayscales are present and 100% if the configuration is totally filled with grayscales. Note that we only focused on Pareto-optimal solutions whose D_f value was less than 10, since solutions with very large D_f for the forward flow are unsuitable design candidates for a no-moving-part valve, due to the excessive pumping power requirements. As a result, the maximum measure of non-discreteness was 8.4%. By extracting the fluid-solid interfaces as iso-surfaces with $\varphi = 0$ for the Pareto-optimal solution that has the largest measure of non-discreteness, and imposing a no-slip boundary condition on the extracted fluid-solid interfaces, we obtained pressure drop errors of -17.5% in the forward flow and -12.4% in the reverse flow. That is, for the forward flow, the presence of grayscales improved the value of objective functional D_f , whereas for the reverse flow, the pressure drop was underestimated, which led to the degradation in the value of the objective functional $1/D_r$, due to the treatment of the solid domains as porous media. Therefore,

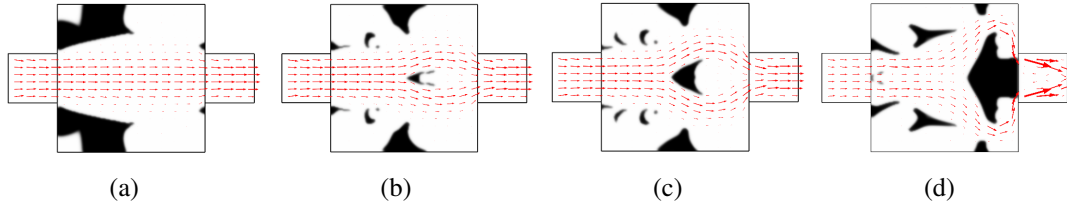


Fig. 2.13 Streamlines for the forward flow of the Pareto-optimal configurations shown in Fig. 2.12.

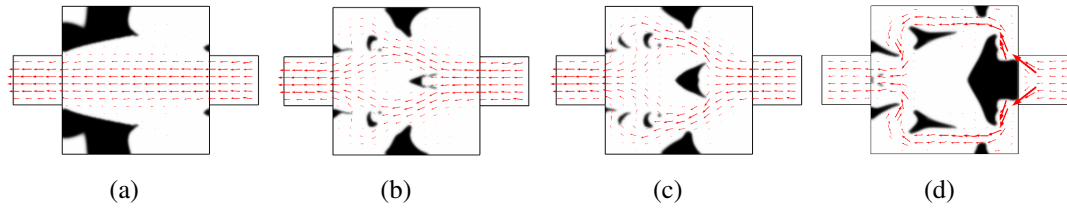


Fig. 2.14 Streamlines for the reverse flow of the Pareto-optimal configurations shown in Fig. 2.12.

at a detailed design stage, after a particular solution is selected from the obtained Pareto-optimal solution set, further tuning using a more accurate analysis free from the influences of grayscales and the permeability of solid domains would be required.

Next, we provide velocity vector plots to aid visualization of the forward and reverse flows in the main channel. The velocity vector plots for the forward and reverse flow of the optimal designs in Fig. 2.12(a)–(d) are given in Figs. 2.13 and 2.14, respectively. As shown in Fig. 2.13, the fluid takes a winding path in the forward direction. On the other hand, the reverse flow is steered into the fang-like channel by inertial forces, and this leads to high dissipation in the reverse flow, and flow inhibition. This mechanism is common in the optimal designs in Fig. 2.12(b)–(d), and appears to be essential for NMP valves. Therefore, it can be expected that similar optimal configurations would be obtained for different Reynolds numbers as long as they are relatively high. Correspondingly, if the Reynolds number were small enough to allow the inertial term to be neglected, the Navier-Stokes equation could then be replaced with the Stokes equation and the mechanism that depends on inertial forces would stop working, which would make designing an NMP valve problematic. The amounts by which the forward and reverse flows are diverted from a straight path are reflected in

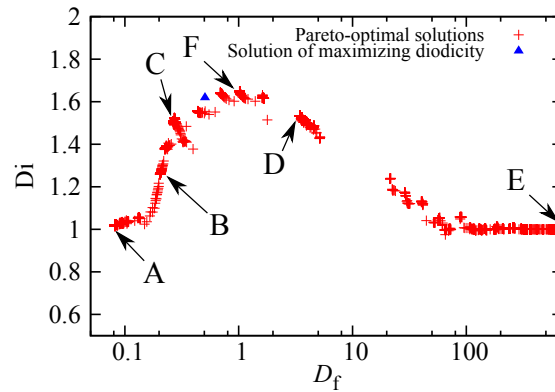


Fig. 2.15 Diodicity of the Pareto-optimal solutions. Points A–E correspond to those in Fig. 2.10 and point F indicates the solution that has the highest diodicity.

the different positions of the solutions along the Pareto front. Again, design engineers can choose a particular solution from the set of Pareto-optimal solutions according to their needs.

To discuss the optimization results in terms of diodicity values that are commonly used to measure the performance of NMP valves, Fig. 2.15 provides a plot of the dissipation in the forward flow (that is the value of F_1) of the Pareto-optimal solutions vs. the corresponding diodicity. Points A–E correspond to those in Fig. 2.10 and point F indicates a solution that has the highest diodicity among the Pareto-optimal solutions. This figure also shows the solution obtained when the objective functional was formulated to maximize the diodicity. Figure 2.16 shows the optimal configuration of the solution F and its streamlines for the forward and reverse flow. Figure 2.17 shows the optimal configuration of the solution obtained by maximizing diodicity and its streamlines for the forward and reverse flow. Solution F and the solution obtained by maximizing diodicity have similar features to those of solutions B–D. It is worth noting that the diodicity value of the solution obtained by maximizing diodicity is not the largest among those of the Pareto-optimal solutions. It is conjectured that this obtained solution may represent a local optimum. On the other hand, the solution obtained when maximizing diodicity has a larger pressure drop in the reverse flow than that of the Pareto front for the same pressure drop in the forward flow. This reinforces the idea that the proposed method does not find global Pareto-optimal solutions, which is always the case when using a gradient-based approach in topology optimization. We hope to develop an optimization algorithm that can avoid local optima more effectively than the current version in future research.

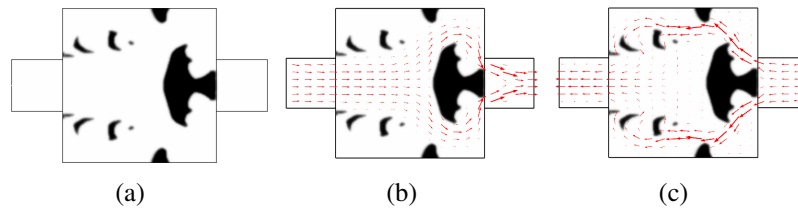


Fig. 2.16 Solution F which has the highest diodicity among the Pareto-optimal solutions: (a) optimal configurations; (b) streamline for the forward flow; (c) streamline for the reverse flow.

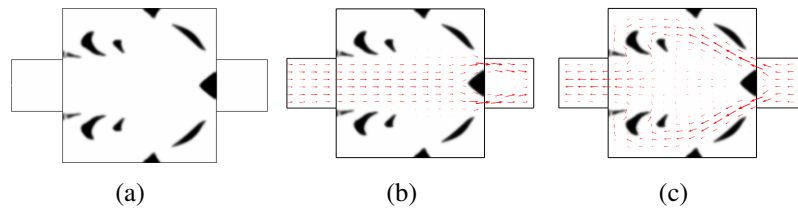


Fig. 2.17 Solution that was obtained using maximizing diodicity as the objective functional: (a) optimal configurations; (b) streamline for the forward flow; (c) streamline for the reverse flow.

Figure 2.15 indicates that solutions C and D have almost the same diodicity values, implying that the suitability of these two solutions cannot be distinguished using diodicity. However, the suitability of solutions C and D depends on the particular design problem. For example, if a design engineer requires an NMP valve design that has a particularly low pressure drop for the forward flow, solution C in this example is superior to solution D, but if a higher pressure drop for the reverse flow is desired, solution D is better. Furthermore, although conventional design methods for NMP valve design problems that focus on diodicity will favor solution F over the other solutions, solution F is not necessarily the best design for an NMP valve, since solution C has a lower pressure drop for the forward flow and solution D has a higher pressure drop for the reverse flow. This illustrates how design engineers can adjust their choice of the most suitable solution, using the set of Pareto-optimal solutions, to meet the needs of a particular design problem. This highlights the significant advantage of the Pareto front exploration approach for the design of NMP valves.

2.5 An optimum design problem of a thermal-fluid device

2.5.1 Background

Thermal-fluid devices such as a heat sink are widely used for cooling mechanical and electronic devices and applied in various products, such as automotive engines, brake disks and semiconductor cooling devices. In particular, based on advances in the fabrication of micro-electromechanical systems (MEMS) and very large-scale integration (VLSI) technologies, micro-channel heat sinks have increasingly attracted attention for their ability to remove a large amount of heat energy [96, 97]. A micro-channel heat sink is a miniature heat exchanger in which fluid draws heat from a heated mechanical or electric device via thermal and fluid interactions. To maximize heat sink performance, an appropriate geometrical configuration of flow channels is required, so that the heat exchange between the fluid and heated solid will be maximized. Many researchers have explored heat sink design methods experimentally [98, 99], numerically [100–102], and by using structural optimization approaches [103–105]. In particular, a structural optimization approach allows an optimal configuration to be obtained based on mathematical and physical principles and can be effective for the development of heat sink designs, since the governing physical phenomena can be described as a thermal-fluid multiphysics problem despite their complexity.

Topology optimization methods for coupled thermal-fluid problems that consider the conservation of energy in addition to that of mass and momentum have been proposed. Matsumori *et al.* [7] developed a topology optimization method in which heat sink performance was evaluated in terms of the heat exchange between a fluid flowing in a channel and a heated structure, which was later extended in a level set-based topology optimization method [8]. Some researchers obtained optimal heat sink designs through topology optimization and confirmed their validity by experiment [106, 107]. Topology optimization methods for the design of a heat sink in which natural convection is considered have also been proposed [108, 9]. In addition, topology optimization methods for coupled thermal-fluid incorporating the Lattice Boltzmann Method (LBM) [109, 110] are recent additions to the literature. In most of these investigations, topology optimization problems were formulated as single-objective problems [7–9, 108–110]. In practical design scenarios, however, device performance must often satisfy multiple demands, such as minimization of pressure drop or required pumping power while maximizing heat exchange. Consequently, an optimum design problem for a heat sink is fundamentally a multiobjective optimization problem.

In this section, the proposed multiobjective optimization method is applied to a two-dimensional micro-channel heat sink design problem under a laminar flow assumption. An optimal heat sink design problem is formulated as bi-objective optimization problem in which maximal heat exchange and minimal pressure drop are objectives, and multiple optimal configurations are obtained as Pareto-optimal solutions. A comparison of individual Pareto-optimal solutions can provide design engineers with practical information, such as multiple design candidates that can be selected to meet particular requirements, and insights concerning the physical mechanisms responsible for certain desired performances.

2.5.2 Governing equations

Consider an internal flow channel problem in which an incompressible steady-state fluid flow is assumed. For heat sink designs, the formulation of the governing equation must include the conservation of energy in addition to that of mass and momentum. Let $\bar{T}$, C_p and k respectively denote the temperature, specific heat capacity at constant pressure and thermal conductivity. The Prandtl number Pr , and non-dimensional temperature T are then defined as follows:

$$Pr = \frac{\mu C_p}{k}, \quad T = \frac{\bar{T} - T_r}{T_s - T_r}, \quad (2.44)$$

where T_s and T_r represent the characteristic temperature and a reference temperature that determines the baseline of the non-dimensional temperature, respectively. The heat transfer equation that govern the behavior of flow in addition to the continuity and Navier-Stokes equations in (2.16) and (2.17) are then given as follows:

$$-\nabla^2 T + RePr(\mathbf{u} \cdot \nabla)T = 0. \quad (2.45)$$

Let T_{in} denote the prescribed temperature. In this study, the boundary conditions for temperature T are considered as follows:

$$\begin{cases} T = T_{in} & \text{on } \Gamma_{in} \\ \mathbf{n} \cdot \nabla T = 0 & \text{on } \Gamma_{out} \cup \Gamma_{wall}. \end{cases} \quad (2.46)$$

We now discuss the formulation of the governing equations for the entire fixed design domain that includes both fluid and solid domains. No-slip boundary conditions are

approximated based on the level set-based approach described in Chapter 1.3.2, as follows:

$$(\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \alpha(\chi_\phi) \mathbf{u} \quad \text{in } D, \quad (2.47)$$

where α is defined as

$$\alpha(\chi_\phi) = (1 - \chi_\phi) \alpha_{\max}, \quad (2.48)$$

Based on previous research dealing with heat exchange maximization problems [7, 8], we next expand the heat transfer equation to the entire fixed design domain by assuming that the internal heat generation Q_s only occurs in the solid domain, as follows:

$$Q_s = \beta_{\max}(1 - T) \quad \text{in } D \setminus \Omega, \quad (2.49)$$

where $\beta_{\max}$ is a non-dimensional coefficient that controls the heat generation according to the temperature difference between that in the solid domain and the characteristic temperature. That is, the heat conduction equations in the fluid and solid domains are respectively given as

$$\begin{cases} -\nabla^2 T + \text{RePr}(\mathbf{u} \cdot \nabla) T = 0 & \text{in } \Omega \\ -\nabla^2 T = \beta_{\max}(1 - T) & \text{in } D \setminus \Omega. \end{cases} \quad (2.50)$$

These equations can be expressed as a single equation using the Heaviside function χ_ϕ :

$$-\nabla^2 T + \text{RePr}(\mathbf{u} \cdot \nabla) T = \beta(\chi_\phi)(1 - T) \quad \text{in } D, \quad (2.51)$$

where β is defined as

$$\beta(\chi_\phi) = (1 - \chi_\phi) \beta_{\max}. \quad (2.52)$$

Note that the second term in (2.51) vanishes in solid domains, since the velocity approaches zero in such domains due to the force term in (2.47). Consequently, the governing equations defined in the fixed design domain for the thermal-fluid problem are summarized as follows:

$$\begin{cases} -\nabla \cdot \mathbf{u} = 0 \\ (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \alpha(\chi_\phi) \mathbf{u} \\ -\nabla^2 T + \text{RePr}(\mathbf{u} \cdot \nabla) T = \beta(\chi_\phi)(1 - T). \end{cases} \quad (2.53)$$

2.5.3 Optimization problem

We now formulate the optimum design problem for a cooling device such as a heat sink. Cooling performance can be evaluated as the heat exchange occurring between the flow channel and the heated structure. However, numerically evaluating this heat transfer is problematic since fluid-solid boundaries must be extracted at every iteration during the optimization procedure. Thus, for simplicity and based on previous research [7, 8], we assume that the heat exchange can be evaluated according to the internal heat generation in the fixed design domain. Therefore, we evaluate cooling performance using the following index, Q , that represents the amount of internal heat generation in the fixed design domain:

$$Q = \int_D \beta(1 - T) dD. \quad (2.54)$$

The topology optimization problem to maximize cooling performance can now be formulated as a problem to maximize internal heat generation Q .

On the other hand, an important performance index that should generally be considered in the design of a fluid device is a total pressure drop, representing the energy loss in the flow channel, formulated as

$$\Delta E = \int_{\Gamma_{in} \cup \Gamma_{out}} (p + \frac{1}{2} |\mathbf{u}|^2) (-\mathbf{u} \cdot \mathbf{n}) d\Gamma. \quad (2.55)$$

However, an objective functional defined as a volume integral is generally useful in numerical optimization [84]. Therefore, the total potential energy represented as

$$\Phi = \int_D \left(\frac{1}{2\text{Re}} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \alpha(\chi_\phi) |\mathbf{u}|^2 \right) dD, \quad (2.56)$$

is used as the performance index in the present study. The total potential energy is equal to the total pressure drop under the condition that the flow is fully developed at the inlet and outlet.

To show the relationship between the total potential energy and the total pressure drop, we first multiply the extended incompressible steady-state Navier-Stokes equation, (2.47), by

$\mathbf{u}$ and integrate it over the entire domain D , as follows:

$$\begin{aligned} & \int_D (\mathbf{u} \cdot \nabla) \mathbf{u} \cdot \mathbf{u} dD + \int_D \nabla p \cdot \mathbf{u} dD \\ & - \int_D \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \mathbf{u} dD + \int_D \alpha(\chi_\phi) \mathbf{u} \cdot \mathbf{u} dD = 0. \end{aligned} \quad (2.57)$$

Then we apply the integration by parts formula to the result, using the conservation of mass, $\nabla \cdot \mathbf{u} = 0$, as follows:

$$\begin{aligned} & \int_{\partial D} \frac{1}{2} (\mathbf{u} \cdot \mathbf{u}) \mathbf{u} \cdot \mathbf{n} d\Gamma + \int_{\partial D} p \mathbf{u} \cdot \mathbf{n} d\Gamma - \int_{\partial D} \frac{1}{\text{Re}} \mathbf{n} \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \mathbf{u} d\Gamma \\ & + \int_D \frac{1}{\text{Re}} \nabla \mathbf{u} : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) dD + \int_D \alpha(\chi_\phi) \mathbf{u} \cdot \mathbf{u} dD = 0, \end{aligned} \quad (2.58)$$

where $\partial D = \Gamma_{\text{in}} \cup \Gamma_{\text{out}} \cup \Gamma_{\text{wall}}$. The no-slip boundary condition on the wall, $\mathbf{u} = 0$ on Γ_{wall} , leads to

$$\begin{aligned} & \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \left(p + \frac{1}{2} |\mathbf{u}|^2 \right) (\mathbf{u} \cdot \mathbf{n}) d\Gamma - \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \frac{1}{\text{Re}} \mathbf{n} \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \mathbf{u} d\Gamma \\ & + \int_D \frac{1}{\text{Re}} \nabla \mathbf{u} : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) dD + \int_D \alpha(\chi_\phi) \mathbf{u} \cdot \mathbf{u} dD = 0. \end{aligned} \quad (2.59)$$

By assuming that the curvature of the inlet and outlet boundaries equals to zero, the fully developed flows can be represented as $\mathbf{u} = U\mathbf{n}$ and $\mathbf{n} \cdot \nabla U = 0$. Consequently, the second term in (2.59) becomes zero when the flow on $\Gamma_{\text{in}} \cup \Gamma_{\text{out}}$ fully developed, as follows:

$$\begin{aligned} \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \frac{1}{\text{Re}} \mathbf{n} \cdot (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \mathbf{u} d\Gamma &= \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \frac{1}{\text{Re}} U \mathbf{n} \otimes \mathbf{n} : (\mathbf{n} \otimes \nabla U + \nabla U \otimes \mathbf{n}) d\Gamma \\ &= 0. \end{aligned} \quad (2.60)$$

Note that this term can be assumed to be zero even when the Reynolds number is large because the boundary integral which includes $1/\text{Re}$ can be ignored compared to the other terms.

On the other hand, the third term in (2.59) can be rewritten as

$$\int_D \frac{1}{\text{Re}} \nabla \mathbf{u} : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) dD = \int_D \frac{1}{2\text{Re}} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) dD. \quad (2.61)$$

Therefore, we obtain the following equation:

$$\begin{aligned} & \int_D \left(\frac{1}{2\text{Re}} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \alpha(\chi_\phi) \mathbf{u} \cdot \mathbf{u} \right) d\Omega \\ &= \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{out}}} \left(p + \frac{1}{2} |\mathbf{u}|^2 \right) (-\mathbf{u} \cdot \mathbf{n}) d\Gamma, \end{aligned} \quad (2.62)$$

with the left-hand side representing the total potential energy and the right-hand side the total pressure drop.

The optimum design problem for the cooling device is now formulated by considering two primary objective functionals, one to maximize Q and the other to minimize Φ , as the following bi-objective optimization problem:

$$\inf_{\chi_\phi \in L^\infty(D, [0,1])} [-Q, \Phi] \quad (2.63)$$

subject to:

$$G_1 = \int_D \chi_\phi dD - V_{\max} \leq 0, \quad (2.64)$$

$$G_2 = \Phi - \eta \Phi_0 \leq 0, \quad (2.65)$$

where G_1 is a volume constraint and $V_{\max}$ is the upper limit of the allowable volume. It is worth noting that this volume constraint is introduced to stabilize the optimization computation and reduce the time required for convergence, regularizing the design space; similar use is reported in previous research [84]. G_2 is a constraint applied as the upper limit of the total potential energy, where Φ_0 represents the initial value of the total potential energy Φ and η is a parameter. State variables $(\mathbf{u}, p, T) \in (\mathcal{U} \times \mathcal{P} \times \mathcal{T})$ satisfy the following variational formulation:

$$E_1 = - \int_D \nabla \cdot \mathbf{u} \tilde{p} dD = 0, \quad (2.66)$$

$$E_2 = \int_D (\mathbf{u} \cdot \nabla) \mathbf{u} \cdot \tilde{\mathbf{u}} dD - \int_D p \nabla \cdot \tilde{\mathbf{u}} dD + \frac{1}{\text{Re}} \int_D \nabla \tilde{\mathbf{u}} : (\nabla \mathbf{u} + \nabla \mathbf{u}^T) dD + \int_D \alpha(\chi_\phi) \tilde{\mathbf{u}} \cdot \mathbf{u} dD = 0, \quad (2.67)$$

$$E_3 = \int_D \nabla T \cdot \nabla \tilde{T} dD + \int_D \text{RePr}(\mathbf{u} \cdot \nabla) T \tilde{T} dD - \int_D \beta(\chi_\phi) (1 - T) \tilde{T} dD = 0, \quad (2.68)$$

for all variables $(\tilde{\mathbf{u}}, \tilde{p}, \tilde{T}) \in (\mathcal{U}^0 \times \mathcal{P} \times \mathcal{T}^0)$. E_1 , E_2 and E_3 are weak forms of the governing equations in (2.53), where test functions are denoted as $\tilde{\mathbf{u}}$, $\tilde{p}$ and $\tilde{T}$. The notations $\mathcal{U}$, $\mathcal{P}$, $\mathcal{T}$,

$\mathcal{U}^0$ and $\mathcal{T}^0$ represent the spaces of admissible variables, defined as

$$\mathcal{U} = \{v \in H^1(D)^d \mid v = u_{\text{in}} \text{ on } \Gamma_{\text{in}}, v = 0 \text{ on } \Gamma_{\text{wall}}\}, \quad (2.69)$$

$$\mathcal{U}^0 = \{v \in H^1(D)^d \mid v = 0 \text{ on } \Gamma_{\text{in}} \cup \Gamma_{\text{wall}}\}, \quad (2.70)$$

$$\mathcal{P} = \{q \in L^2(D) \mid q = 0 \text{ on } \Gamma_{\text{out}}\}, \quad (2.71)$$

$$\mathcal{T} = \{S \in H^1(D) \mid S = T_{\text{in}} \text{ on } \Gamma_{\text{in}}\}, \quad (2.72)$$

$$\mathcal{T}^0 = \{S \in H^1(D) \mid S = 0 \text{ on } \Gamma_{\text{in}}\}, \quad (2.73)$$

where d is the number of spatial dimensions. The design sensitivity of this problem can be obtained using the adjoint variable method (see Appendix A.2 for details of the derivation).

2.5.4 Optimization method

Overview of the proposed method

Here, we used the weighted-sum method to convert the bi-objective optimization problem into a single objective optimization problem. When applied in problems that have a non-convex Pareto front, the weighted-sum approach has well-known limitations that prevent solutions in such cases [111, 51]. However, it remains a useful approach for many practical multiobjective optimization problems [77, 112, 74], including heat sink design problems [106, 107] where the front is convex. The scalarized objective function is defined as

$$\inf_{\chi_\phi} -\bar{w}_1 Q + \bar{w}_2 \Phi, \quad (2.74)$$

where $\bar{w}_1$ and $\bar{w}_2$ are weighting coefficients that satisfy the following equations:

$$\bar{w}_1 + \bar{w}_2 = 1, \bar{w}_1 \geq 0, \bar{w}_2 \geq 0. \quad (2.75)$$

Since all possible settings of the weighting coefficients result in a local Pareto front if it is convex, a finite number of local Pareto-optimal solutions can be obtained using a finite number of weighting coefficient combinations. However, since the relationship between the weights and the position of a corresponding Pareto-optimal solution on the Pareto front is unknown at the outset, it is difficult to determine an appropriate set of weighting coefficients to obtain an appropriate Pareto front approximation. Furthermore, topology optimization problems usually encounter multiple local optima that yield low-quality locally optimal configurations.

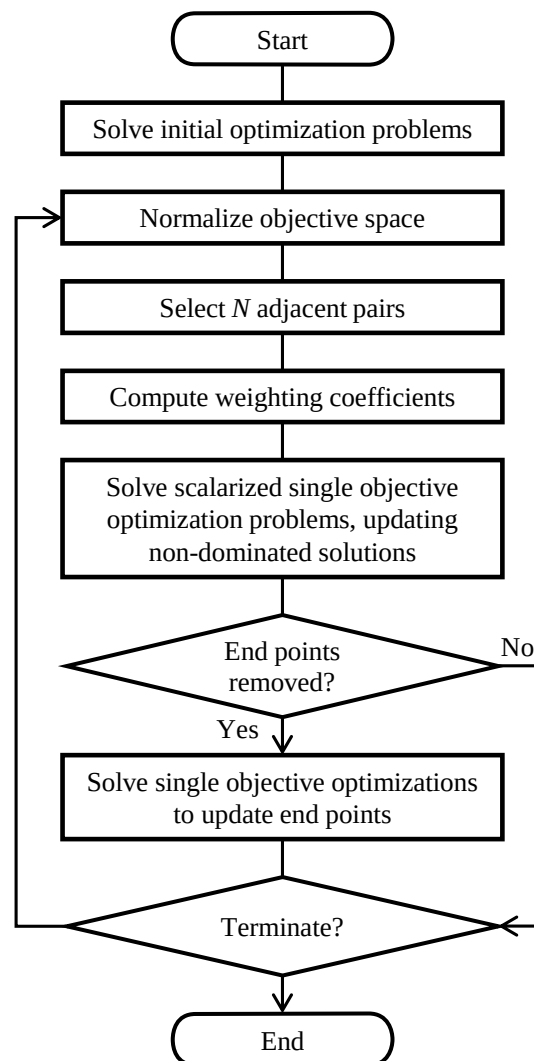


Fig. 2.18 Flowchart of the proposed method, the main algorithm

Therefore, this study propose a Pareto front exploration scheme that iteratively updates a Pareto front approximation using adaptively determined weighting coefficients that are based on the non-dominated solutions obtained in the previous iteration, which avoids low-quality local optima as far as possible. Figure 2.18 illustrates the flowchart of the proposed Pareto front exploration algorithm, the details of which are described in the following subsection.

2.5.5 Optimization algorithm

We now describe two optimization algorithms, one of which is nested within the main algorithm. That is, the main algorithm is used to obtain a Pareto front approximation, and a second algorithm is executed within it to solve a single objective topology optimization problem. The details of the main algorithm (Fig. 2.18) are as follows:

– **Step 1: Perform initial optimization**

Three optimization problems are initially solved. In the first two optimization problems, objective functionals $-Q$ and Φ are individually minimized as single objective optimization problems, and in the third optimization, the two weighting coefficients, one for each objection functional, are set so that $w_1 = w_2 = 1/2$. The obtained solutions are saved as initial non-dominated solutions.

– **Step 2: Normalize the objective space**

Each objective functional is then normalized, as follows:

$$F_1 = \frac{-Q + Q_{\max}}{Q_{\max} - Q_{\min}}, \quad (2.76)$$

$$F_2 = \frac{\Phi - \Phi_{\min}}{\Phi_{\max} - \Phi_{\min}}, \quad (2.77)$$

where subscripts max and min mean the maximum or minimum value among the current non-dominated solutions, respectively.

– **Step 3: Select non-dominated solutions**

N adjacent pairs (F_A^k, F_B^k) for $k = 1, \dots, N$ of the non-dominated solutions are selected in descending order of their Euclidean separation distance in the normalized objective space, and the corresponding N desired points, F_D^k for $k = 1, \dots, N$, that improve the distribution of non-dominated solutions are defined as

$$F_D^k = \frac{F_A^k + F_B^k}{2}. \quad (2.78)$$

Figure 2.19(a) shows an example when $k = 1$, i.e. for the adjacent pair that has the greatest separation distance in the normalized objective space. When the number of adjacent pairs is less than N , all adjacent pairs have been selected.

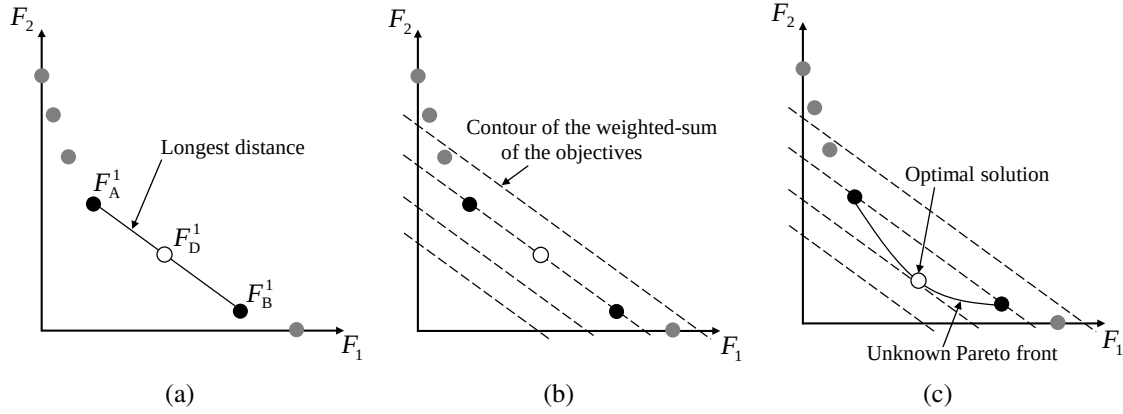


Fig. 2.19 Adaptive weighted sum method: (a) setting a desired point; (b) determining weighting coefficients; (c) update non-dominated solutions

– **Step 4: Calculate weighting coefficients**

Two new optimization problems for every desired point are defined. First, weighting coefficients $w^k = [w_1^k, w_2^k]$ are determined for each desired point so that each weighted sum of the objective functionals at each corresponding desired point is minimized, by solving the following linear programming problem:

$$\min_{w^k} w^k \cdot F_D^k \quad (2.79)$$

subject to

$$w^k \cdot F \geq 1 \quad \text{for all non-dominated solutions,} \quad (2.80)$$

$$w^k \geq 0, \quad (2.81)$$

where $F = [F_1, F_2]$. Using the calculated weighting coefficients, for example, the weighted sum of the objective functionals for $k = 1$ has the contours shown in Fig. 2.19(b).

– **Step 5: Solve single objective optimization problems**

Scalarized objective functional $w^k \cdot F$ is now minimized in a pair of optimizations nested within the main algorithm, starting from two initial configurations, the two non-dominated solutions for the adjacent pair selected in Step 3. By solving these two new optimization problems based on different initial configurations but using the same

weighting coefficients, new non-dominated solutions located between the two initial configurations are obtained. That is, the initial configurations are determined based on non-dominated solutions previously obtained for certain weights, and newly determined weights are applied so that these initial configurations will search unexplored regions of the Pareto front. Figure 2.19(c) shows the situation when $k = 1$. Since N desired points are obtained in Step 3, $2N$ single objective optimization problems must be solved in this step. During each optimization procedure, non-dominated solutions are successively updated.

– **Step 6: Update extreme solutions**

If a non-dominated solution located at an end point of the Pareto front approximation is dominated by a newly obtained non-dominated solution and removed from the set of non-dominated solutions in Step 5, a new optimization problem is solved, in which the objective functional is either F_1 or F_2 , depending on which end point was removed. The initial configuration is set to a solution located at the new end point after Step 5.

– **Step 7: Check convergence**

If the termination condition is satisfied, the optimization procedure ends, otherwise it returns to Step 2.

In Step 3, N desired points rather than a single point are determined, which lets the optimization procedure continue to search the Pareto front even if no non-dominated solutions dominating a desired point are obtained in certain optimization problems due to getting stuck at a low-quality local optimum.

In the present study, the termination condition in Step 7 is the convergence of a hypervolume indicator I_H [113, 114], which represents a volume enclosed by a Pareto front approximation and a reference point in the objective space. The optimization procedure is stopped when the following convergence criterion is satisfied:

$$\left| \frac{I_H^l - I_H^{l-1}}{I_H^{l-1}} \right| < \epsilon_H, \quad (2.82)$$

where l is an iteration number. The criterion value was set to $\epsilon_H = 10^{-5}$, and the reference point when calculating the hypervolume was set to $(0, \eta\Phi_0)$.

Next, the details of the nested algorithm used in Steps 1, 5 and 6 of the main algorithm are described.

– **Step 1: Initialize the level set function**

The initial level set function is set.

– **Step 2: Solve governing equations**

The governing equations are solved using the finite element method (FEM).

– **Step 3: Update non-dominated solutions**

The two objective functionals are computed. If the corresponding point in the objective space, whose position is determined according to the computed objective functionals, dominates a certain point of a non-dominated solution, the new point is added to the set of non-dominated solutions and the originally dominated point is deleted from the set of non-dominated solutions.

– **Step 4: Check convergence**

If the weighted sum of the objective functionals is converged, this algorithm is stopped, otherwise the adjoint equations are solved using the FEM.

– **Step 5: Evaluate design sensitivities**

The design sensitivities are computed.

– **Step 6: Update the level set function**

The level set function is updated using the reaction-diffusion equation. The optimization algorithm then returns to Step 2.

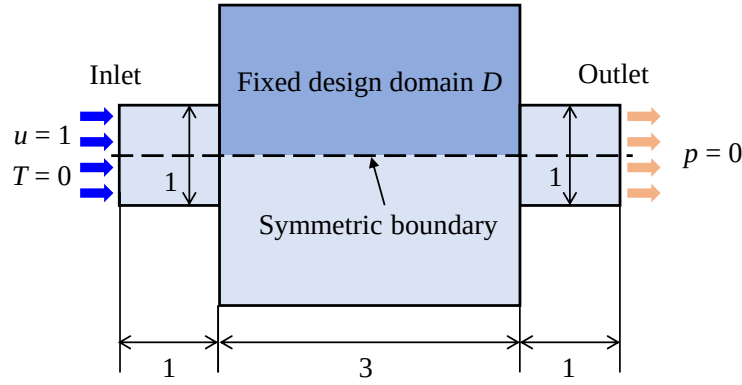
In Step 4, the algorithm is stopped when the following criterion is satisfied:

$$\left| \frac{F_{\text{total}}^t - F_{\text{total}}^{t-\Delta t}}{F_{\text{total}}^{t-\Delta t}} \right| < \epsilon_{\text{top}}, \quad (2.83)$$

where F_{total} is a weighted sum of the normalized objective functionals. In the present study, the criterion value was set to $\epsilon_{\text{opt}} = 10^{-4}$.

2.5.6 Numerical example

In this section, the proposed method is applied to a heat sink design problem to confirm its validity and applicability. Figure 2.20 shows the design model including the fixed design domain D and boundary conditions. Since the design model is vertically symmetric, the fixed design domain is defined as the upper half of the design domain, as shown in Fig. 2.20.

Fig. 2.20 Design model and fixed design domain D

A Reynolds number of 20 was used for the fluid flow, and the fluid had a Prandtl number of 6.7, typical for water. Parameter $\beta_{\max}$ for heat generation was set to 20. The dependencies of optimal configurations on the Reynolds number and the value of parameter $\beta_{\max}$ were investigated in previous research [7, 8], which revealed that the complexity of the optimal configurations increases as the Reynolds number and the value of parameter $\beta_{\max}$ is increased. The upper limit of the allowable fluid volume was set to 70% of the volume of the fixed design domain, and parameter η for the upper limit of the total potential energy was set to 50. The regularization parameter τ used in the reaction-diffusion equation in (1.29) was set to 1×10^{-4} .

Dependency of Pareto front approximation on parameter N

First, we investigated the dependency of the obtained Pareto front approximation on the value of parameter N . Figure 2.21 shows the obtained Pareto front approximation for different parameter settings: $N = 1, 2, 3$. As clearly shown, the Pareto front approximation for $N = 1$ includes large sparse areas and is inferior to those for $N = 2$ and $N = 3$. When $N = 1$, only one desired point in the objective space is explored at Step 5 in the main algorithm. As a result, if new non-dominated solutions that dominate a desired point cannot be obtained at Step 5 of the main algorithm due to adhesion at a low-quality local optimum, the optimization procedure then stops. On the other hand, when $N > 1$, the optimization procedure can continue to search the Pareto front even if no non-dominated solutions are obtained in certain optimization problems due to a low-quality local optimum adhesion. The fact that the Pareto front approximations obtained when $N = 2$ and $N = 3$ are similar led us to conclude that parameter N should be set larger than 1.

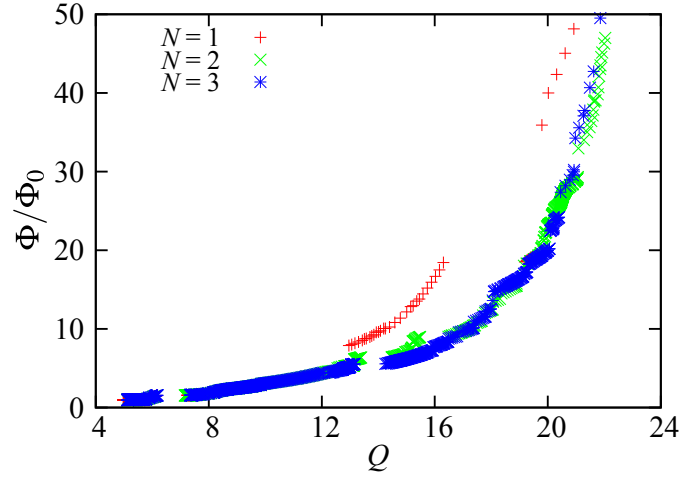


Fig. 2.21 Obtained Pareto front approximation for various settings of parameter N

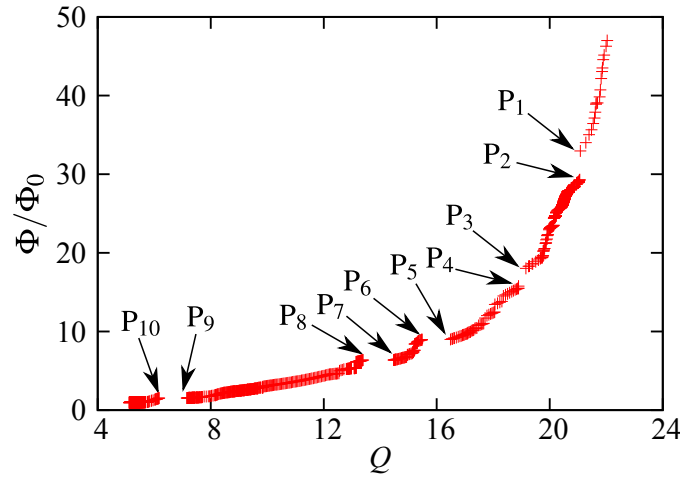


Fig. 2.22 Obtained Pareto front approximation for $N = 2$

Detailed results and discussion

Next, we detail and analyze obtained non-dominated solutions and their corresponding optimal configurations, using the Pareto front exploration obtained when $N = 2$.

Figure 2.22 shows the obtained Pareto front approximation, and Fig. 2.23 illustrates a histogram of the fluid volume fraction in the obtained Pareto-optimal solutions. As shown in Fig. 2.23, the volume constraint is not always active in the set of Pareto-optimal solutions. When considering a heat sink design problem, some solid domains must be included in an optimal configuration to remove heat. Thus, when setting $V_{\max}$ to a relatively large value,

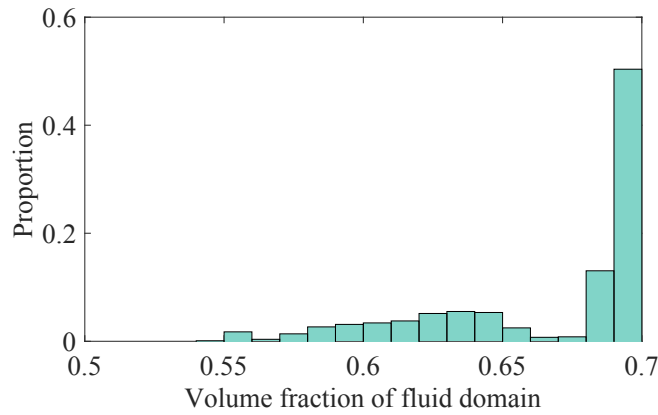


Fig. 2.23 Histogram of fluid volume fraction in obtained Pareto-optimal solutions

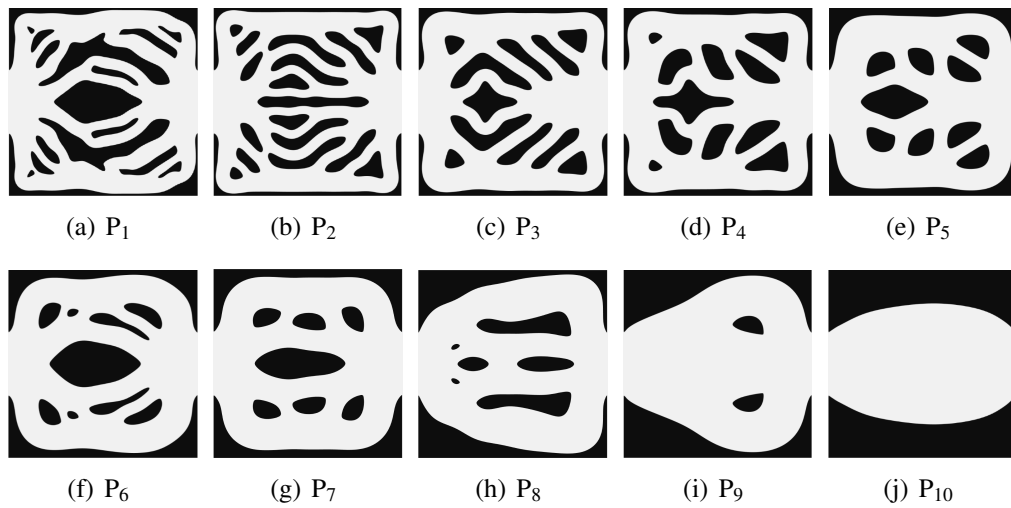


Fig. 2.24 Optimal configurations on the Pareto front approximation

the obtained solutions have little dependence on the volume constraint value, which leads to certain volume constraints being inactive.

Figure 2.24 shows the Pareto-optimal solutions corresponding to points P_i for $i = 1, 2, \dots, 10$ in Fig. 2.22. These obtained configurations as Pareto-optimal solutions embody a variety of complex channels owing to the use of topology optimization, and they therefore may provide higher performance compared to some existing micro-channel heat sink such as a straight micro-channel heat sink or a manifold micro-channel heat sink, in which a channel is designed based on a combination of simple geometries.

Profound differences between the optimal configurations included in the obtained Pareto front approximation are easily observed, and the geometrical complexity greatly depends on the position on the Pareto front approximation. That is, the number of branched flow channels increases as the amount of heat exchange increases, which increases the total surface area of a channel. Unfortunately, the total potential energy also increases as the number of branched flow channels increases, whereas the total potential energy minimization, which represents pressure drop minimization, prefers geometrically simple channels. The obtained Pareto front approximation clearly illustrates this trade-off relationship and allows design engineers to choose a particular solution among radically different Pareto-optimal solutions, one that best meets their immediate requirements. The geometrical complexity of the obtained Pareto-optimal solutions also depends on the set value of the regularization parameter τ . The physical performance of a heat sink and the degree of geometrical simplicity of the design have a trade-off relationship [8]. That is, the Pareto front obtained for larger values of the regularization parameter will be located toward the upper left portion of the Pareto front shown in Fig. 2.22. Therefore, the regularization parameter should be adjusted to produce the desired degree of geometrical complexity in the obtained solutions, while considering the trade-off relationship between heat exchange performance and manufacturability.

On the other hand, the obtained Pareto front approximation includes some discontinuous regions, e.g. between points P_1 and P_2 . In these regions, the shape and topology of optimal configurations undergo dramatic changes, as the value of one of the two objective functionals varies considerably. These changes, in shape and/or topology, are responsible for the discontinuities.

Next, we compared the results obtained with the proposed method with those using a conventional weighted sum method in which the weighting coefficients are given prior to the optimization procedure, and with results obtained using our previous method described in Section 2.3.2. In the conventional weighted sum method, weighting coefficients in (2.74) were given as

$$\bar{w}_1 = 0.9 \times \frac{i_w}{n_{\text{div}} - 1}, \quad (2.84)$$

$$\bar{w}_2 = 1 - \bar{w}_1, \quad (2.85)$$

for $i_w = 0, 1, \dots, n_{\text{div}} - 1$ where $n_{\text{div}} = 40$ in this chapter. That is, 40 single objective optimization problems were independently solved using the second algorithm described in

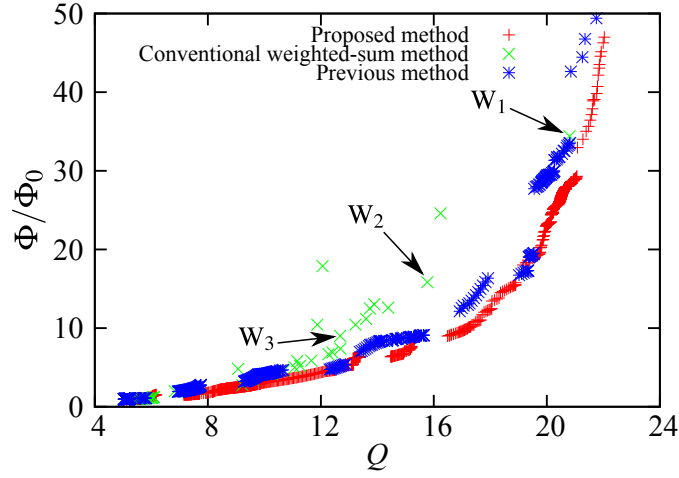


Fig. 2.25 Comparison of the proposed method to a conventional weighted sum method and our previous method

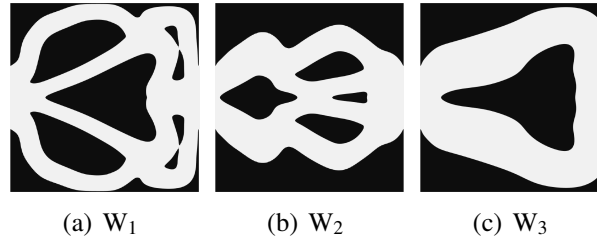


Fig. 2.26 Optimal configurations obtained by the conventional weighted sum method: (a) $\bar{w} = (0.900, 0.100)$; (b) $\bar{w} = (0.831, 0.169)$; (c) $\bar{w} = (0.646, 0.354)$.

Section 2.5.5. On the other hand, in our previous method described in Section 2.3.2, the weighting coefficients are determined adaptively during the optimization procedure. Suppose that the initial solution has the j th largest value of the objective functional F_i ($i = 1$ or 2) among the current non-dominated solution set, then the weighting coefficient are simply given as

$$w_i = j - 1, \quad (2.86)$$

where w_i is the weighting coefficient for F_i . In addition, the initial solutions were selected from the current non-dominated solutions according the “crowded comparison” indicator [55]. Although weighting coefficients are adaptively given according to the distribution of the current non-dominated solutions in our previous method, improvement in the distribution of non-dominated solutions using newly given weighting coefficients is not guaranteed.

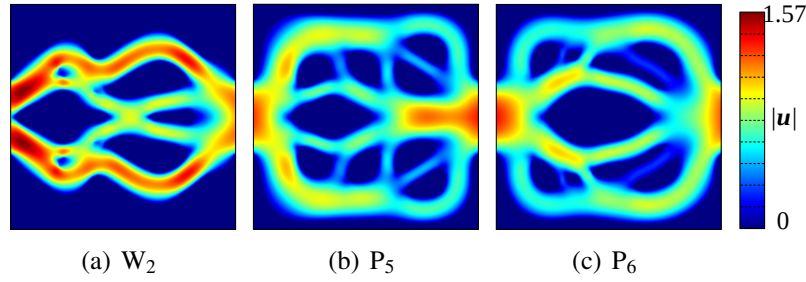


Fig. 2.27 Velocity magnitudes

Figure 2.25 shows the optimal solutions in the objective space obtained by the conventional weighted sum method and our previous method, together with the Pareto front approximation obtained by the proposed method. This figure clearly illustrates that the optimal solutions obtained by both the conventional weighted sum method and our previous method more often reflect lower-quality local optima than those obtained by the proposed method; the proposed method can obtain higher-quality Pareto front approximations by avoiding certain low-quality local optima. This is because the newly proposed method provides appropriate weights for each initial solution according to the current distribution of non-dominated solutions, by solving a linear programming problem as discussed in Section 2.5.5. In the conventional weighted-sum method, weights and initial configurations are fixed to those given at the first step of the optimization procedure, and in the previously presented method described in Section 2.3.2, the adaptive weighting scheme was heuristic, which led to deterioration of the distribution of the obtained Pareto front.

On the other hand, in the currently proposed method, even if a particular design has converged at a local optimum with respect to certain weights, this design can be used to further explore the Pareto front by being selected as an initial design for the next iteration and having different weights assigned. That is, weights and initial solutions are adaptively adjusted according to the distribution of the current Pareto front approximation, and the distribution and quality of the Pareto front are iteratively improved during the optimization procedure. As a result, the proposed method is more capable of avoiding lower-quality local optima and can obtain a more diverse Pareto front approximation.

Figure 2.26 shows the optimal configurations denoted as W_1 , W_2 and W_3 in Fig. 2.25. These configurations are geometrically simple compared to the configurations in the Pareto front approximation. To investigate these solutions in more detail, we first focus on solution W_2 , whose internal heat generation Q is close to that of solutions P_5 and P_6 obtained by the

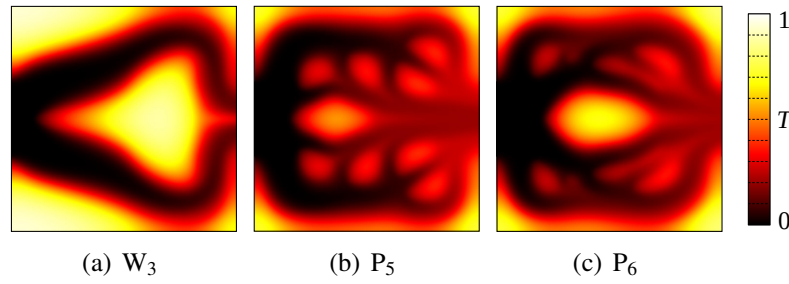


Fig. 2.28 Temperature distributions

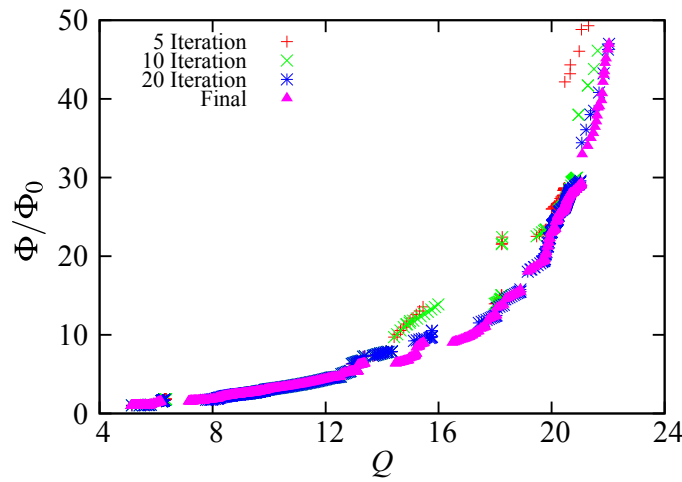


Fig. 2.29 Intermediate and obtained Pareto front approximations

proposed method. Solution W_2 also has a greater total potential energy Φ than solutions P_5 and P_6 , as illustrated in Fig. 2.25. Figure 2.27 shows the magnitude of the flow velocities for solutions W_2 , P_5 and P_6 . In solution W_2 , the fluid flows along a winding path and the velocity gradient is relatively high in the main channel. Consequently, solution W_2 has a higher total potential energy than solutions P_5 or P_6 , although all of these solutions provide quantitatively similar heat exchange.

We next focus on solution W_3 whose value of Φ is close to that of solutions P_5 and P_6 , whereas solution W_3 has lower value of Q than solutions P_5 or P_6 , as illustrated in Fig. 2.25. Figure 2.28 shows the temperature distributions for solutions W_3 , P_5 and P_6 . Solution W_3 is geometrically simple, with only one large solid island, and the solid domain has a relatively high temperature due to reduced surface area in contact with fluid, which degrades internal heat generation Q . Consequently, solution W_3 provides less heat exchange than solutions P_5

or P_6 , although the total potential energy of these solutions is, again, quantitatively similar. Although the channel in solution W_3 would have improved heat exchange if the solid domains were further subdivided, such geometrical changes would increase the total potential energy, which would negatively affect the weighted sum of the objective functionals. As a result, solution W_3 indicates an adhesion at a lower-quality local optimum, unlike solutions P_5 and P_6 . Therefore, the proposed method does a good job of avoiding local optima as far as possible, owing to the adaptive adjustment of the weighting coefficients. Figure 2.29 illustrates the intermediate and final Pareto front approximations obtained by the proposed method. This figure clearly illustrates that the Pareto front approximation was improved, by avoiding certain local Pareto fronts.

2.6 Summary

This chapter presented multiobjective topology optimization techniques incorporating Pareto front exploration. We achieved the following:

1. We briefly discussed the concept of multiobjective optimization and formulated a multiobjective topology optimization problem in the general form.
2. A multiobjective topology optimization method for stiffness maximization problems under multiple loading cases was proposed in which an algorithm incorporating adaptive weighting and point selection schemes was constructed. The proposed method provides Pareto-optimal solution sets for bi-objective topology optimization problems that can be productively exploited to obtain highly appropriate designs that reflect a detailed understanding of the physical bases for the obtained optimal configurations. Optimal configurations can be chosen based on information that is clearly expressed in the range of solutions along the Pareto front for the particular design problem.
3. An optimum design method of a no-moving part valve was constructed. The optimum design problem was formulated as a bi-objective optimization problem, with one objective functional to minimize the total potential energy in the forward flow, and the other to maximize the total potential energy in the reverse flow. In the numerical example, Pareto-optimal solutions were provided. Although the Pareto-optimal solutions reveal the trade-off relationship between the objective functions, certain solutions had nearly identical features that appear to be essential for NMP valves. The obtained

Pareto-optimal solutions were discussed in terms of their diodicity values, commonly used for comparing the performance of NMP valves. Different Pareto-optimal solutions had almost the same diodicity values, but the proposed Pareto front exploration method enables design engineers to choose a particularly suitable solution from the Pareto-optimal solution set, depending on the requirements of the design problem under consideration.

4. An optimum design method of a micro-channel heat sink was constructed. An optimum design problem for a two-dimensional micro-channel heat sink under a laminar flow assumption was formulated as a bi-objective optimization problem in which maximal heat exchange and minimal pressure drop were the desired objectives. An algorithm for Pareto front exploration was constructed in which weighting coefficients are adaptively determined by solving a linear programming problem, with no prior weighting coefficient settings by design engineers required. In numerical examples, Pareto-optimal solutions were obtained and clearly illustrated the trade-off relationships between heat exchange and pressure drop. That is, increases in the total surface area of the solid domains were coupled with increases in both the amount of heat exchange and the pressure drop. Finally, a comparison of results obtained by the proposed method with those from a conventional weighted sum method and our previous method allow us to confirm that the new scheme for adaptively setting weighting coefficients effectively avoids undesirable trapping in low-quality local Pareto fronts.

Chapter 3

Data mining for knowledge discovery in multiobjective topology optimization

3.1 Introduction

Engineering optimization problems are often characterized as multiobjective optimization problems, where multiple objectives must be minimized or maximized simultaneously. In most multiobjective optimization problems, certain pairs of objectives have trade-off relationships, which means that no single solution exists that can simultaneously minimize or maximize all objectives. Instead, such optimization problems yield multiple optimal solutions, called non-dominated solutions or Pareto-optimal solutions. A comprehensive set of Pareto-optimal solutions is more useful than a limited set, because decision makers will have a broader range of potential solutions from which to choose the particular solution that best meets their needs.

Once a set of Pareto-optimal solutions is obtained, regardless of the method employed, the next challenging task is for a decision maker to choose a particularly apt solution, a process that often relies on personal intuition and experience. Piecemeal comparisons among a set of Pareto-optimal solutions are cumbersome and trial-and-error efforts seldom yield a solution that best meets decision makers' needs. Given such situations, data mining techniques that can glean useful knowledge from a Pareto-optimal solution set are increasingly attractive in the field of multiobjective optimization [115–117].

Data mining is a technique for extracting characteristic patterns within a large dataset, patterns that are normally not apparent, using various methods such as clustering [118–120],

principle component analysis [121, 122] and machine learning [123]. The aim of data mining is to isolate pertinent information for later use. Since Pareto-optimal solutions embody certain properties that make a particular design or system optimal with respect to a certain problem, extracting or isolating such properties will help decision makers better understand the target problem and provide information that aids decision making. Prior research efforts have proposed post-analysis methods for application to Pareto-optimal solution sets in which similar solutions are grouped together using clustering [124, 125].

Data mining techniques are also effective for the analysis of Pareto-optimal solutions in structural design problems, as can be found in the literature. Ulrich [126] proposed a clustering method and applied it to a bridge construction problem. Obayashi and Sasaki [49] applied self-organizing maps for a supersonic wing design problem for grouping similar solutions together. Oyama *et al.* [50] proposed a method to extract design modes for an airfoil shape design problem using proper orthogonal decomposition, which were extended by incorporating clustering [127]. Graening and Sendhoff [128] proposed a holistic data mining approach, namely shape mining, which consisted of clustering of shape data, the design concept extraction with machine learning, and the interaction analysis between design parameters and objectives. Thus, although data mining techniques for topology optimization results have not been developed to the best of my knowledge, they can be effective for topology optimization.

In topology optimization, since optimal configurations that include tiny substructures too complex to be efficiently manufactured are often obtained as solutions, such configurations must be modified to accommodate the relevant manufacturing capabilities and constraints. An inappropriate modification, however, may severely degrade the performance of the obtained solution, so the design engineer who modifies the solution must thoroughly understand the physical mechanism operating in the particular solution. Schemes that assist design engineers' comprehension of mechanistic factors and their interdependencies are therefore desirable. Given the potential power of data mining techniques, this chapter proposes a data mining method for extracting the physical mechanism operating in the particular solution. The proposed method sequentially applies a clustering technique and association analysis to a Pareto-optimal solution dataset such as that obtained in multiobjective topology optimization problems.

The remainder of this chapter is organized as follows. First, we briefly discuss multi-objective optimization and topology optimization, and then formulate the multiobjective

topology optimization problem considered here. The next section presents the data mining technique for treatment of multiobjective topology optimization results, using a combination of clustering and association rule analysis. We then provide four numerical examples, including two- and three-dimensional design problems, and summarize this study.

3.2 Formulation of multiobjective topology optimization problems

In this study, the proposed data mining method is applied in a multiobjective topology optimization problem in which the objective functionals are formulated as minimum mean compliances in multi-loading cases. Consider the multi-loading case in which a traction, $\mathbf{t}_i$, is applied to a boundary, Γ_{t_i} , under the condition that a fixed design domain is fixed at a boundary Γ_{u_i} for $i = 1, \dots, m$, where m is the number of loading cases. Let $\mathbf{u}_i(\mathbf{x})$ for $i = 1, \dots, m$ denote the displacement in response to traction $\mathbf{t}_i$. The minimum mean compliance problem under multi-loading conditions is then formulated as a multiobjective optimization problem as follows:

$$\inf_{\chi_{\Omega} \in L^{\infty}(D)} \mathbf{F} = [F_1, \dots, F_m] \quad (3.1)$$

$$\text{subject to:} \quad (3.2)$$

$$G = \int_D \chi_{\Omega} dD - V_{\max} \leq 0, \quad (3.3)$$

where F_i for $i = 1, \dots, m$ is the mean compliance defined as

$$F_i = \int_{\Gamma_{t_i}} \mathbf{t}_i \cdot \mathbf{u}_i d\Gamma, \quad (3.4)$$

and G represents a volume constraint with $V_{\max}$ being the upper bound of the allowable volume. The mean compliance represents the elastic compliance of the structure against the applied force and the minimization of the mean compliance yields a high stiffness structure. By assuming a linear elasticity, the displacement field $\mathbf{u}_i \in \mathcal{U}_i$ for $i = 1, \dots, m$ satisfies the following variational formulation:

$$\int_{\Gamma_{t_i}} \mathbf{t}_i \cdot \mathbf{v}_i d\Gamma - \int_D \boldsymbol{\varepsilon}(\mathbf{v}_i) : \mathbf{C} \chi_{\Omega} : \boldsymbol{\varepsilon}(\mathbf{u}_i) dD = 0, \quad (3.5)$$

for all variables $\mathbf{v}_i \in \mathcal{U}_i$ for $i = 1, \dots, m$, where $\mathbf{C}$ is the elastic tensor and $\boldsymbol{\varepsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ is a small strain tensor. The notation $\mathcal{U}_i$ represents an admissible space of a displacement and is defined as

$$\mathcal{U}_i = \{\mathbf{v} \in H^1(D)^d \mid \mathbf{v} = 0 \text{ on } \Gamma_{u_i}\}, \quad (3.6)$$

where $H^1(D)$ is a Sobolev space and d is the number of dimensions.

In the present study, the above topology optimization problem is regularized using a level set-based topology optimization method [22] and the Pareto front approximation is obtained using an extended version of a previously developed Pareto front exploration method for multiobjective topology optimization in Chapter 2, in which only a bi-objective optimization problem was considered. In this method, a number of optimization problems are scalarized, using adaptively given weighting coefficients, and then solved, starting with initial designs selected from non-dominated solutions obtained in a previous optimization loop. These initial designs are selected as adjacent pairs of non-dominated solutions that appear far apart when the currently obtained Pareto front is approximated using segments with non-dominated solutions as nodes. This method is therefore easily extended to m objective optimization problems by approximating a Pareto front by $m - 1$ -simplexes, applying the Delaunay triangulation to non-dominated solutions, and by selecting initial designs as non-dominated solutions that form the $m - 1$ -simplex as a large hypervolume. In the present study, we empirically set several optimization parameters used in the algorithm, considering the diversity of the Pareto front approximation and the computational time. Note that since this chapter focuses on data mining of a Pareto-optimal solution set obtained from a multiobjective topology optimization problem, any multiobjective topology optimization method can be employed.

3.3 Data mining in multiobjective topology optimization

3.3.1 Data mining procedure

The proposed data mining method sequentially applies clustering and association rule analysis to a Pareto-optimal solution set; Fig. 3.1 illustrates the conceptual scheme. Clustering is applied in the design space first (Fig. 3.1(a)) and the results are then visualized in the objective space (Fig. 3.1(b)). The objective space is directly visualized for problems with three or fewer objective functions, but level diagrams [129] are used in problems involving more than three

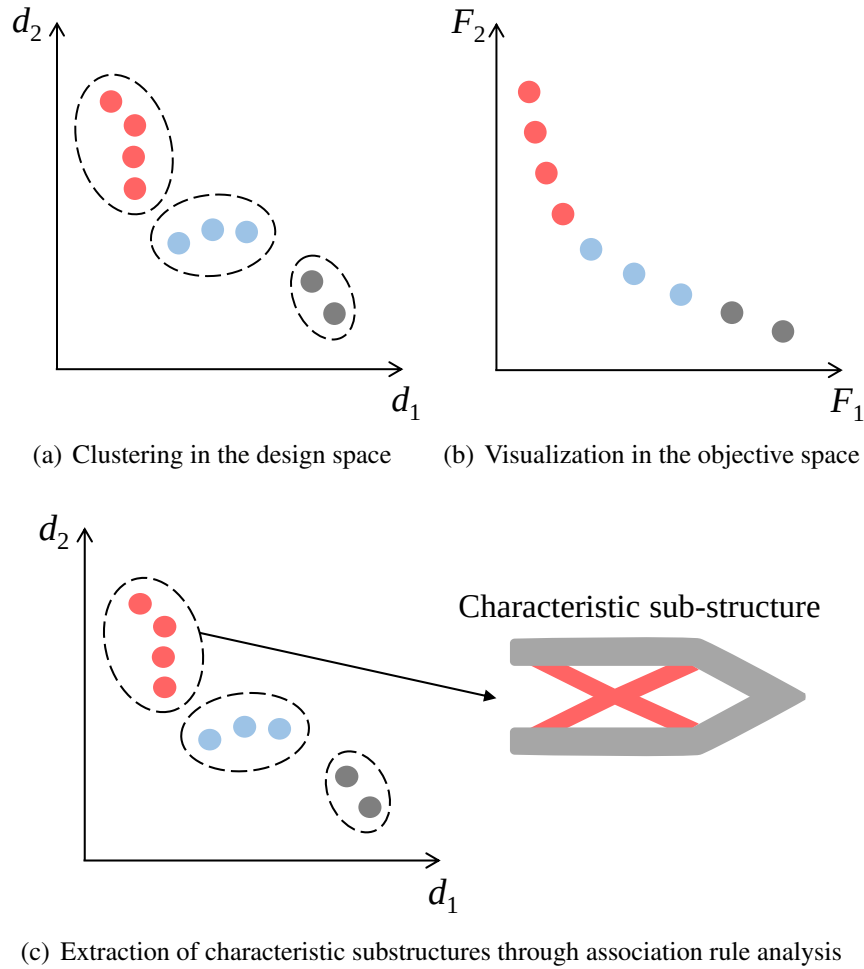


Fig. 3.1 Conceptual scheme of the proposed method

objective functions. Visualization of the clustering results in the objective space offers basic insights into the physical performances of several Pareto-optimal solutions. After clustering, detailed features in each cluster are analyzed based on the concept of association rule analysis (Fig. 3.1(c)), which enables extraction of characteristic substructures present in the clusters being examined. A result of this process is that the characteristic substructures in a particular cluster that are responsible for the position of that cluster in the objective space become known. This highlights one or more performances that may be affected from subsequent modifications which are required to accommodate the relevant manufacturing capabilities of topology optimization results at the specific design stage. As shown in Fig. 3.1(c), the data mining process gives design engineers one-to-one relationships between the key substructures and each objective, which is useful to comprehend the physical mechanism operating in the

particular solution. Details of the clustering and association rule analysis used in this study are described in the following subsections.

3.3.2 Clustering

Clustering is an unsupervised learning method for grouping a data set, so that data items within a particular cluster are more similar than they are to data in other clusters. It is a popular tool for extracting hidden features in a dataset and can be classified into two methods, hierarchical and partitional. The former constructs a tree of clusters, called a dendrogram, which is advantageous in that the number of clusters can be determined from the dendrogram after clustering. On the other hand, partitional methods partition the dataset into a prescribed number of clusters based on a certain similarity. The k -means method [130] is the most popular partitional clustering method and is often applied to Pareto-optimal solution sets [125, 127]. Metaheuristic approaches were also used for clustering: multiobjective evolutionary algorithm [126] and multiobjective particle swarm optimization [118]. The former applied clustering to Pareto-optimal solution sets. In the present study, we use the k -means method for data mining, since it is suitable for handling the large datasets that multiobjective topology optimization results typically provide.

In the k -means method, a dataset containing data, y_j for $j = 1, \dots, n$, is partitioned by solving the following optimization problem:

$$\min_{z_{jl} \in \mathcal{Z}} \sum_{j=1}^n \sum_{l=1}^k z_{jl} d(y_j, \mu_l)^2, \quad (3.7)$$

where k is the number of clusters and μ_l is the l th cluster centroid. $d(y_j, \mu_l)$ represents a non-similarity, expressed as the distance between y_j and μ_l , based on a certain metric. $\mathcal{Z}$ represents an admissible set, defined as

$$\mathcal{Z} = \{0, 1 \mid \forall j, \sum_{l=1}^k z_{jl} = 1\}. \quad (3.8)$$

That is, $z_{jl} = 1$ implies that the j th data belong to the l th cluster.

Multiobjective optimization involves two spaces, a design space and an objective space. In most previous research, clustering methods have been applied to a Pareto-optimal solution set in the objective space, since this is often of primary interest to decision makers [124, 125, 131].

On the other hand, clustering methods have also been applied in the design space, for a single-objective optimization problem [132]. In the present study, clustering is used to extract the physical mechanisms operating in the Pareto-optimal solutions, to assist design engineers' comprehension of their features. We therefore apply clustering to the topology optimization dataset in the design space and focus on the obtained structures rather than the objective values. To do this, a measure that describes the distances between configurations must be defined.

Although there are various types of topology optimization techniques and the design variables are different for each type, as briefly described in Chapter 1, the obtained optimal configurations can always be expressed using the characteristic function, χ_Ω in (1.1). Therefore, the distance between two particular configurations, A and B, for example, can be defined using their characteristic functions, χ_Ω^A and χ_Ω^B , as follows:

$$d_\chi(A,B) = \sqrt{\int_D (\chi_\Omega^A - \chi_\Omega^B)^2 dD}. \quad (3.9)$$

This distance measure represents the square root of the non-intersecting areas of configurations A and B above, and we use it to apply the k -means method to the Pareto-optimal solutions of multiobjective topology optimization problems.

The major difficulties in the k -means method are (1) its dependency on initial cluster centroids and (2) determination of an appropriate number of clusters, k , since Pareto-optimal solution set features are usually unknown prior to data mining. To mitigate the first problem and obtain more useful partitions by avoiding locally optimal partitions as far as possible, we set initial cluster centroids by using the k -means++ method [133] and perform clustering several times. On the other hand, to resolve the second problem: the estimation of the appropriate number of clusters, there exist schemes such as a maximum global silhouette index [134, 125, 131] which is suitable to a data set potentially forming meaningful clusters. However, there is no guarantee that the Pareto-optimal solutions of a multiobjective topology optimization will form meaningful clusters, and we use clustering to divide Pareto-optimal solutions into certain clusters for the sake of convenience, to isolate physical mechanisms for later scrutiny. Therefore, as for the second problem, we just set the number of clusters empirically in the present study.

3.3.3 Association rule analysis

Although the process of clustering creates groups in which geometrically similar structures in a Pareto-optimal solution set are brought into some degree of proximity in terms of the distance measure expressed in (3.9), isolating the physical mechanisms that operate in different Pareto-optimal solutions in the obtained clusters is cumbersome for design engineers. The concept of the lift index in the association rule analysis [135] is useful for extracting certain characteristic substructures in each cluster, to reveal which substructures have the most influence upon specific objectives. We focus on the following rule:

If a Pareto-optimal solution belongs to the l th cluster, point $\mathbf{x}$ in this solution is filled with material.

For the above rule, confidence and lift indexes, denoted as I_C^l and I_L^l , respectively, are defined for l th cluster as follows:

$$I_C^l(\mathbf{x}) = \frac{\sum_{i \in C_l} \chi_{\Omega}^i(\mathbf{x})}{\sum_{i \in C_l} 1}, \quad (3.10)$$

$$I_L^l(\mathbf{x}) = \frac{I_C^l(\mathbf{x})}{I_S(\mathbf{x})}, \quad (3.11)$$

with

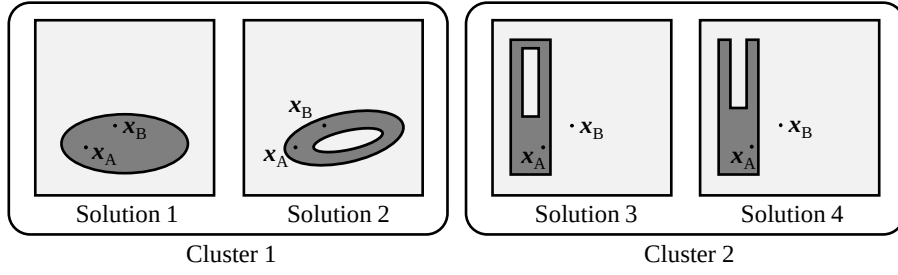
$$I_S(\mathbf{x}) = \frac{\sum_{i=1}^n \chi_{\Omega}^i(\mathbf{x})}{\sum_{i=1}^n 1}, \quad (3.12)$$

where C_l is the set of solution indexes belonging to the l th cluster. Here, $I_S(\mathbf{x})$ is the support index which represents the ratio of the number of solutions with material at point $\mathbf{x}$ to the total number of solutions. We note that $I_C^l(\mathbf{x})$ corresponds to the centroid of the l th cluster, and $I_S(\mathbf{x})$ corresponds to the centroid of all Pareto-optimal solutions.

In the following, we explain how these indexes are used and visualized using a simple example. First, we consider four pseudo solutions which are grouped into two clusters, as shown in Fig. 3.2. The dark gray regions represent structures (material), and the light gray regions are void. Now, we focus on the two rules:

If a Pareto-optimal solution belongs to the 1st cluster, point $\mathbf{x}_A$ in this solution is filled with material;

If a Pareto-optimal solution belongs to the 1st cluster, point $\mathbf{x}_B$ in this solution is filled with material.



(a) Solutions and clustering results

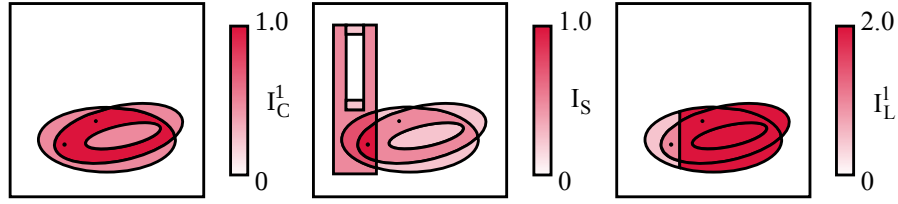
(b) Confidence index con- (c) Support index contour (d) Lift index contour for
tour for cluster 1 cluster 1

Fig. 3.2 Conceptual scheme of the association rule analysis

The confidence indexes related to the above rules, $I_C^1(x_A)$ and $I_C^1(x_B)$, can be calculated as

$$I_C^1(x_A) = I_C^1(x_B) = \frac{2}{2} = 1. \quad (3.13)$$

Next, we calculate the support indexes related to the above two rules, $I_S(x_A)$ and $I_S(x_B)$, as follows:

$$I_S(x_A) = \frac{4}{4} = 1, \quad (3.14)$$

$$I_S(x_B) = \frac{2}{4} = 0.5. \quad (3.15)$$

Finally, the lift indexes, $I_L^1(x_A)$ and $I_L^1(x_B)$, can be calculated using the confidence and support, as follows:

$$I_L^1(x_A) = \frac{1}{1} = 1, \quad (3.16)$$

$$I_L^1(x_B) = \frac{1}{0.5} = 2. \quad (3.17)$$

In the same manner, the confidence index $I_C^1(x)$, the support index $I_S(x)$, and the lift index

$I_L^l(\mathbf{x})$ can respectively be calculated over the design domain, and thus visualized by contour plots as shown in Fig. 3.2(b)–(d). As for cluster 2, these indexes can be visualized in the same manner. Actually, in the present study, these indexes are calculated at every finite element, where the characteristic function value is evaluated, and visualized by pixels whose colors correspond to the index values.

Since the regions with larger values of $I_L^l(\mathbf{x})$ represent characteristic substructures in the l th cluster, visualization of lift indexes like Fig. 3.2 and the clustering results explicitly illustrate which substructures are responsible for each objective. It is therefore extracted as knowledge that substructures with larger values of $I_L^l(\mathbf{x})$ should not be largely modified if the design engineer does not want to degrade the l th objective. Thus, index information from the association analysis will help design engineers comprehend the physical mechanisms operating in the particular solution and appropriately modify it for future production processes.

3.4 Numerical examples

In this section, we present three two-dimensional cantilever design problems and one three-dimensional cantilever design problem, to demonstrate the features and operation of the proposed data mining method for knowledge discovery in topology optimization.

3.4.1 Two-dimensional cantilever design problem 1

First considered is a simple two-dimensional cantilever design problem with the fixed design domains and boundary conditions shown in Fig. 3.3(a)–(c). Since three loading cases are considered, the optimization problem has three objective functionals. The upper limit of the total volume was set to 35% of the design domain, and the design domain was discretized using 100×200 quadrilateral first-order finite elements. Fig. 3.4 shows the obtained Pareto front approximation. It can be seen that there are several gaps in the Pareto front approximation. These gaps can be filled by adjusting some optimization parameters and performing optimization much more if the true Pareto front has sufficient diversity. There is also a possibility that the distribution of the true Pareto front is biased. For this Pareto-optimal solution set, the number of clusters was set with $k = 6$ and clustering was performed 10 times, to avoid locally optimal partitions as far as possible. In this problem, functionals F_1 , F_2 , and F_3 respectively represent mean compliances to be minimized in response to bending, tensile,

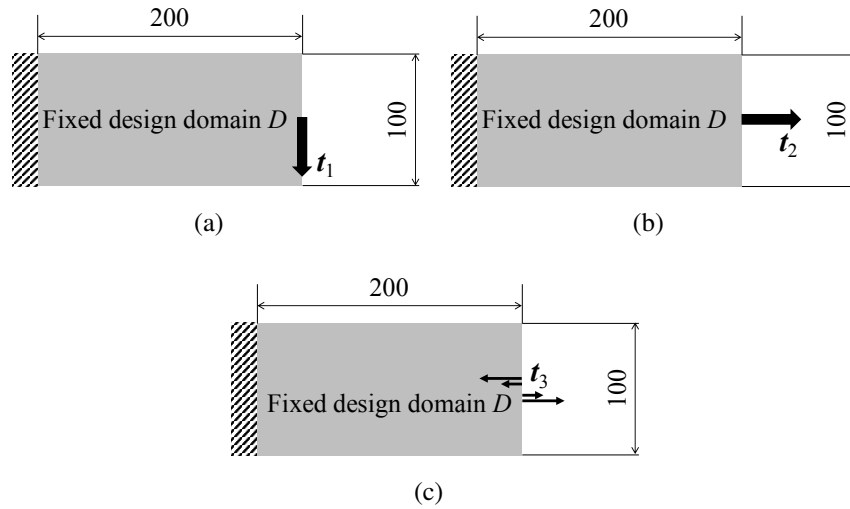


Fig. 3.3 Fixed design domains and boundary conditions for two-dimensional cantilever design problem 1

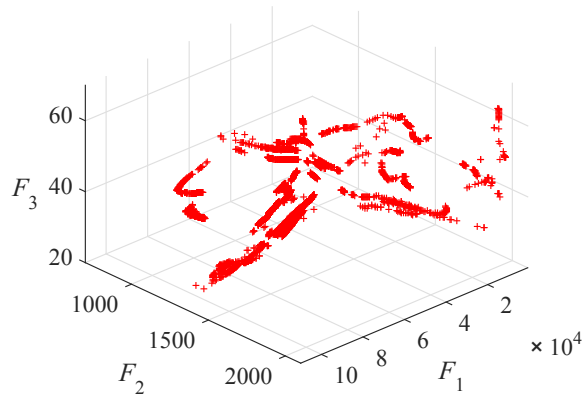


Fig. 3.4 Pareto front approximation for two-dimensional cantilever design problem 1

and torsional loading. Representative configurations for each cluster (the solution nearest each cluster centroid) and a visualization of the clustering results in the objective space are shown in Fig. 3.5 and Fig. 3.6, respectively. The distributions of clustering results (Fig. 3.6) indicate, for example, that:

- Solutions in clusters 1 and 5 have relatively low F_3 values, but F_1 values range widely, and therefore provide relatively high stiffness against torsional loading (Fig. 3.3(c)).

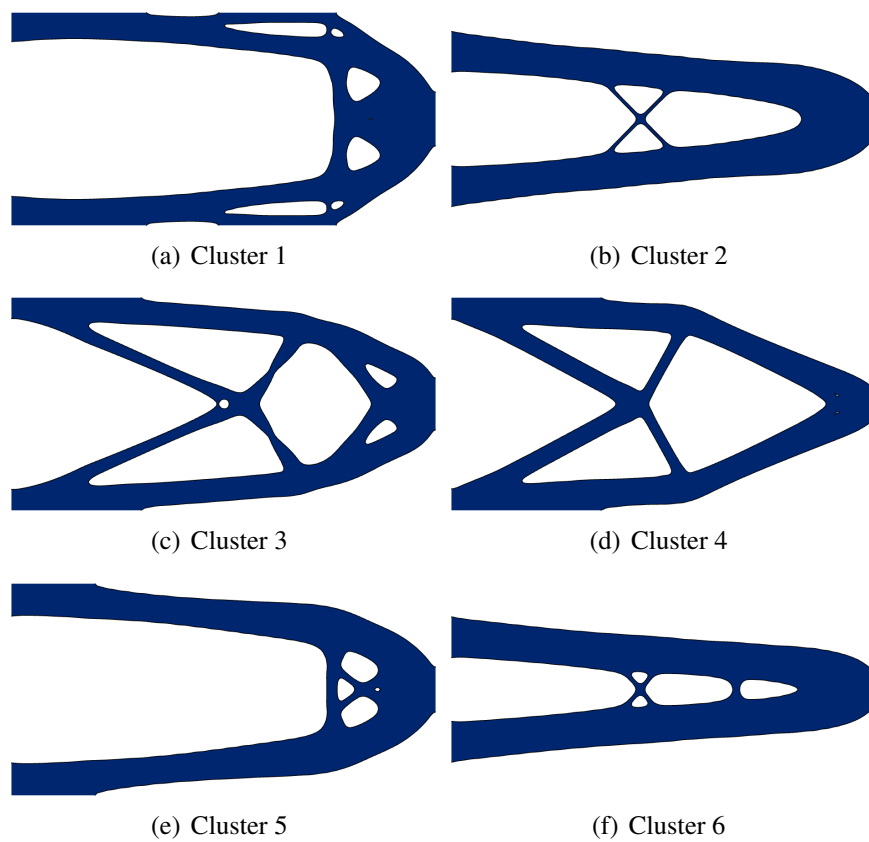


Fig. 3.5 Representative configurations for each cluster for two-dimensional cantilever design problem 1

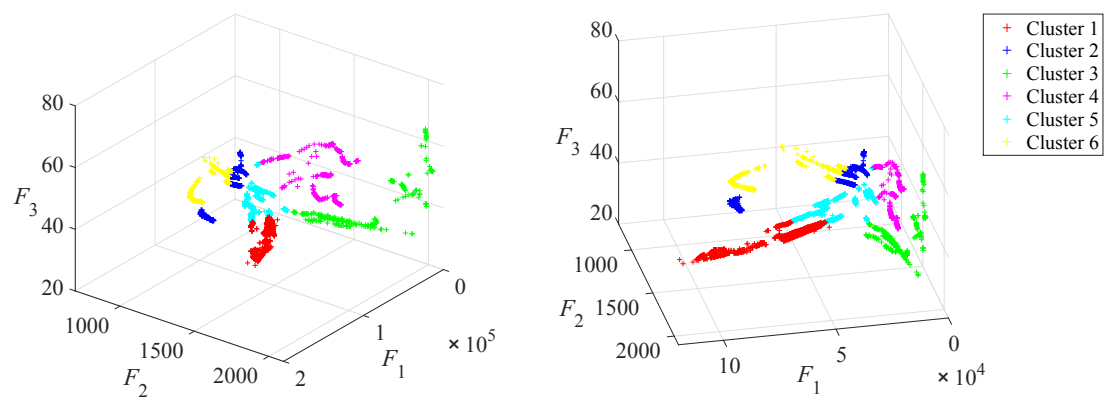


Fig. 3.6 Clustering results visualized in objective space for two-dimensional cantilever design problem 1

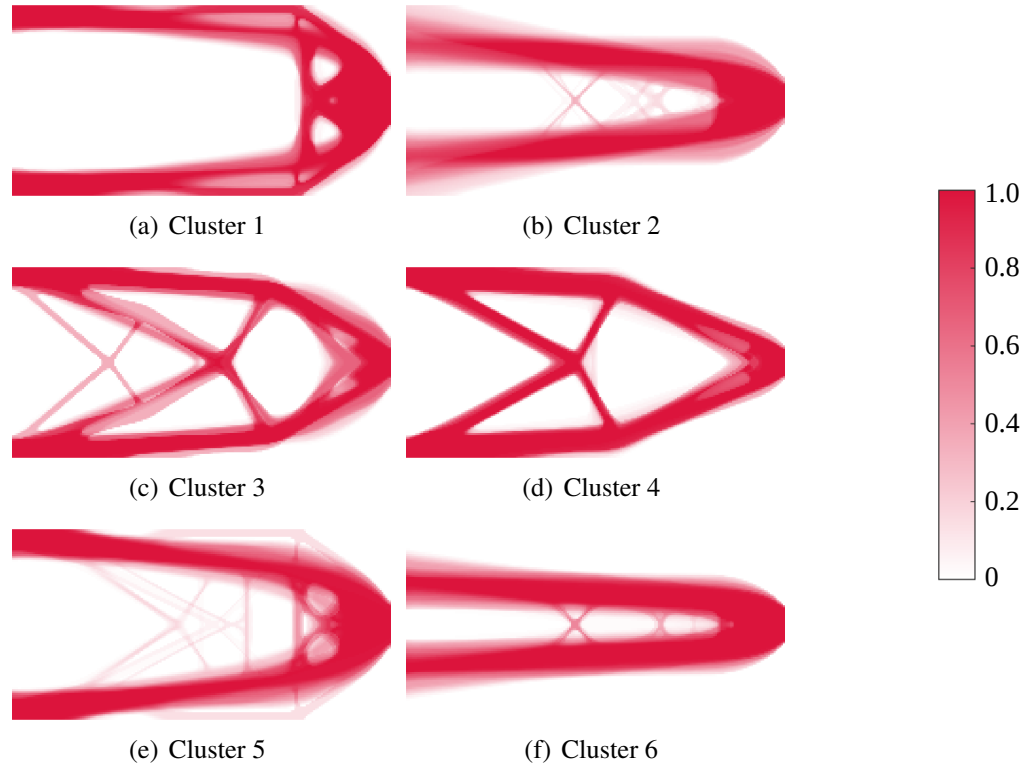


Fig. 3.7 Confidence indexes for each cluster for two-dimensional cantilever design problem 1

- Solutions in clusters 2 and 6 have relatively low F_2 values, but F_1 values range widely, and therefore provide relatively high stiffness against tensile loading (Fig. 3.3(b)).
- Solutions in clusters 3 and 4 have relatively low F_1 and F_2 values, but F_3 values range widely, and therefore provide relatively high stiffness against bending loading (Fig. 3.3(a)).
- Cluster 2 is comprised of two sub-clusters in the objective space.

We now apply association rule analysis to reveal important details within each cluster, as depicted in the confidence and lift indexes (Fig. 3.7 and Fig. 3.8, respectively). Note that lift values greater than 2 are rounded down to 2 to increase their visibility.

Fig. 3.7 shows that clusters 1 and 5 have upper and lower frame elements that are mainly open, except for substructure material located at the far right where the frames come together. This mechanical arrangement, combined with the fact that solutions in clusters 1 and 5 have relatively low F_3 values (Fig. 3.6), indicates that these relatively unbraced frames provide high stiffness against torsional loading (Fig. 3.3(c)). The major geometrical difference

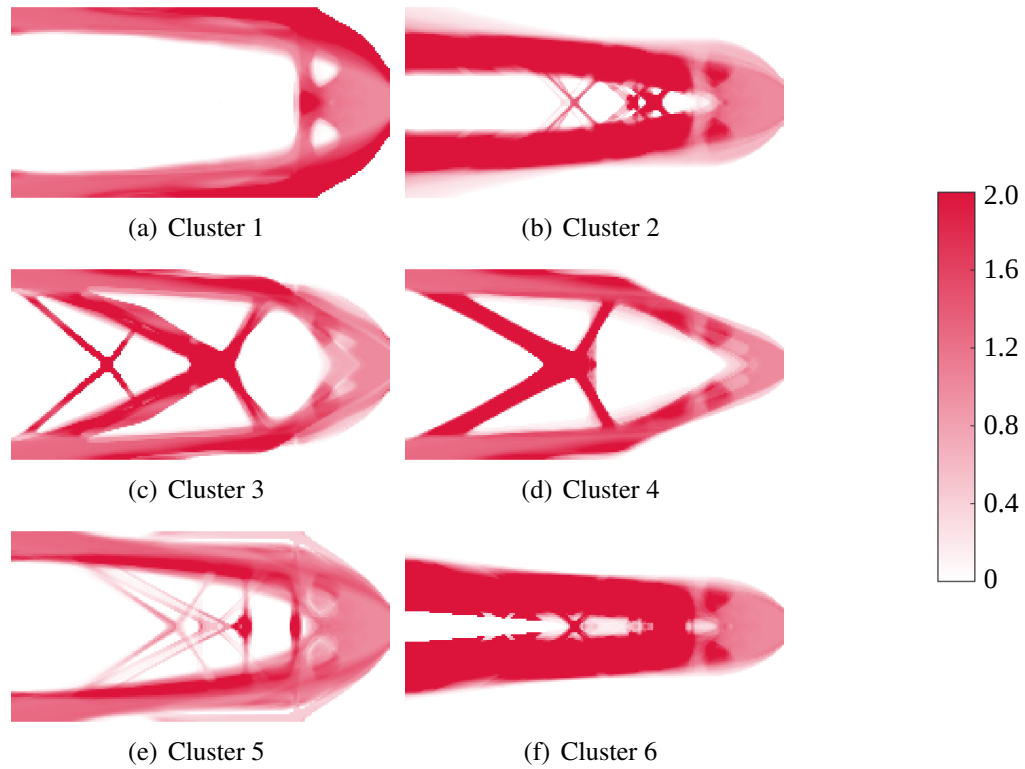


Fig. 3.8 Lift indexes for each cluster for two-dimensional cantilever design problem 1

between solutions in clusters 1 and 5 is the length of the vertical interval between the upper and lower frames; cluster 1 solutions are a little more open than those in cluster 5 (Figs. 3.7(a) and (e) and 3.8(a) and (e)). On the other hand, in terms of performances, F_3 values are lower in cluster 1 solutions than those in cluster 5, while F_1 and F_2 values are larger in cluster 1 solutions than those in cluster 5 (Fig. 3.6). A design engineer can now appreciate that, within reason, larger vertical intervals between the upper and lower frames will lead to increased stiffness against torsional loading, sacrificing stiffnesses against bending and tensile loading (Fig. 3.3(a) and (b), respectively).

The cluster 2 and 6 solutions include centrally located substructures (Figs. 3.5, 3.7 and 3.8), and have low F_2 values (Fig. 3.6). The upper and lower frames are more closely spaced in the cluster 6 solutions than those in cluster 2, and have lower F_2 values but higher F_3 values than those in cluster 2. The relatively close structural spacing thus provides high stiffness against tensile loading (Fig. 3.3(b)), at the expense of stiffness against torsional loading (Fig. 3.3(c)).

In clusters 3 and 4, interior diagonal bars are the most prominent substructures, and these configurations have correspondingly high lift indexes (Fig. 3.8(c) and (d), respectively). Since solutions in these clusters have relatively low F_1 values, these diagonal bars are likely responsible for the observed high stiffness against bending loading (Fig. 3.3(a)). Although diagonal substructures appear in clusters 2, 5 and 6, they are thinner, hence less important structurally than those in clusters 3 or 4, which is confirmed by the corresponding lift values. Thus, it appears that F_1 values are affected by the existence of diagonal substructures, and their thickness when present.

Finally, we observe that regions near the boundary where tractions are applied have relatively low lift values despite the high confidence values seen in all clusters. Therefore, it appears that the geometry of the supporting structures at the boundaries reflects all three different loading conditions (Fig. 3.3). In this way, the proposed data mining method successfully 1) extracts substructures that crucially affect the values of particular objective functionals, or all of them, 2) aids comprehension of the physical significance of geometric features, and 3) supports the choice of designs most suitable for specific loading requirements.

3.4.2 Two-dimensional cantilever design problem 2

Next, we consider another two-dimensional cantilever design problem, this time with more complex boundary conditions. In addition to applying different loading conditions (Fig. 3.9(a)–(c)), the locations of the boundaries where the displacement is fixed are different for each objective. In this three objective optimization problem considering the three loading cases, the upper limit of the total volume was set to 40% of the design domain. The design domain was discretized using 60×300 quadrilateral first-order finite elements. As with design problem 1, the number of clusters has $k = 6$ and clustering was performed 10 times to suppress locally optimal partitions. The obtained Pareto front approximation, representative configurations for each cluster, (solutions nearest each cluster centroid), and a visualization of the clustering results in the objective space, are shown in Figs. 3.10, 3.11, and 3.12, respectively. In this problem, functionals F_1 , F_2 , and F_3 respectively represent mean compliances to be minimized in response to the tractions applied in the three loading cases shown in Fig. 3.9(a)–(c). Fig. 3.12 reveals that:

- Clusters 1 and 2 solutions have relatively low F_3 values, but F_1 values range widely.
- Clusters 3 and 5 solutions have relatively low F_1 values, but F_2 values range widely.

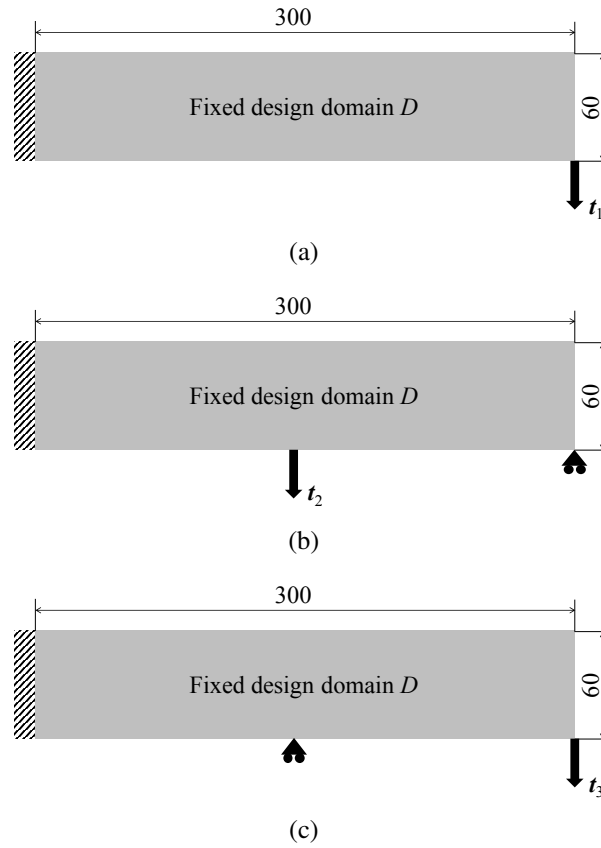


Fig. 3.9 Fixed design domains and boundary conditions for two-dimensional cantilever design problem 2

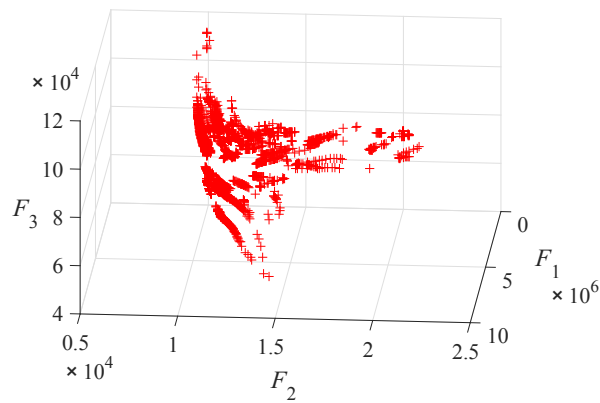


Fig. 3.10 Pareto front approximation for two-dimensional cantilever design problem 2

- Clusters 4 and 6 solutions have relatively low F_1 and F_2 values, but F_3 values range widely.

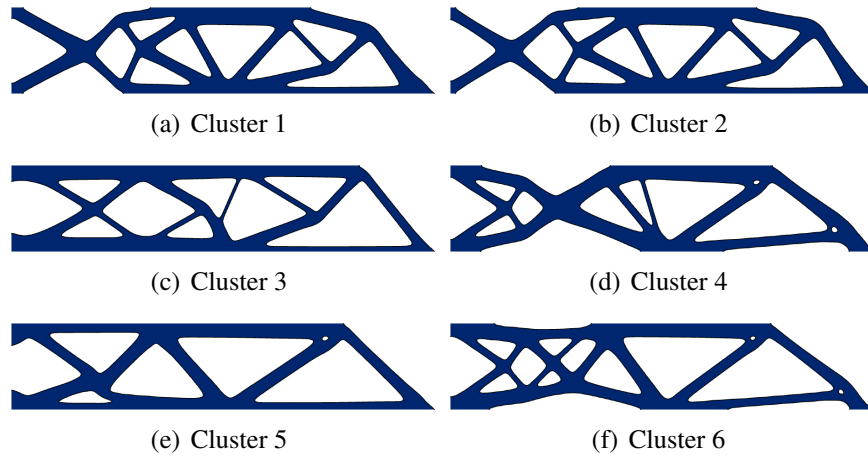


Fig. 3.11 Representative configurations for each cluster for two-dimensional cantilever design problem 2

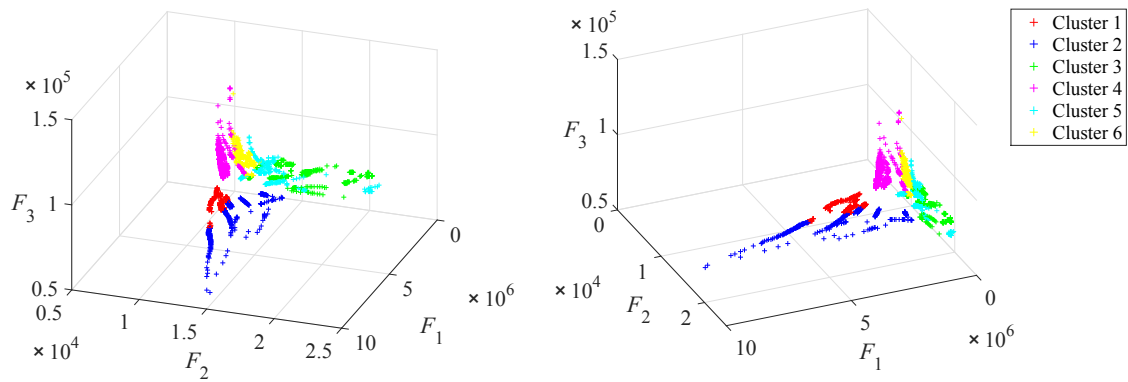


Fig. 3.12 Clustering results visualized in objective space for two-dimensional cantilever design problem 2

- Clusters 3 and 5 are intermingled in the objective space.
- Differences between clusters 1 and 2: cluster 1 solutions have lower F_2 values but cluster 2 solutions have lower F_3 values.
- Differences between clusters 4 and 6: cluster 4 solutions have lower F_2 values but cluster 6 solutions have lower F_1 values.

The relationships expressed in items one to three above imply that:

- Structures like those shown in Figs. 3.11(a) and (b) have high stiffness against the loading shown in Fig. 3.9(c).

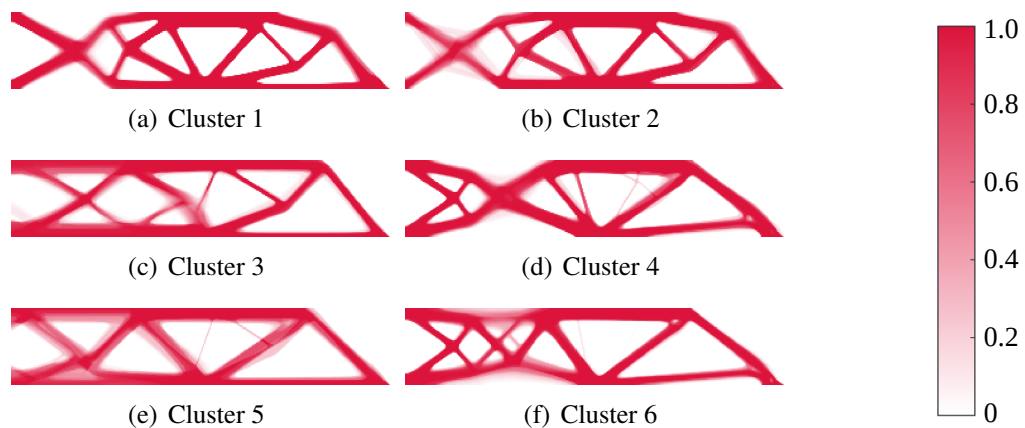


Fig. 3.13 Confidence indexes for each cluster for two-dimensional cantilever design problem 2

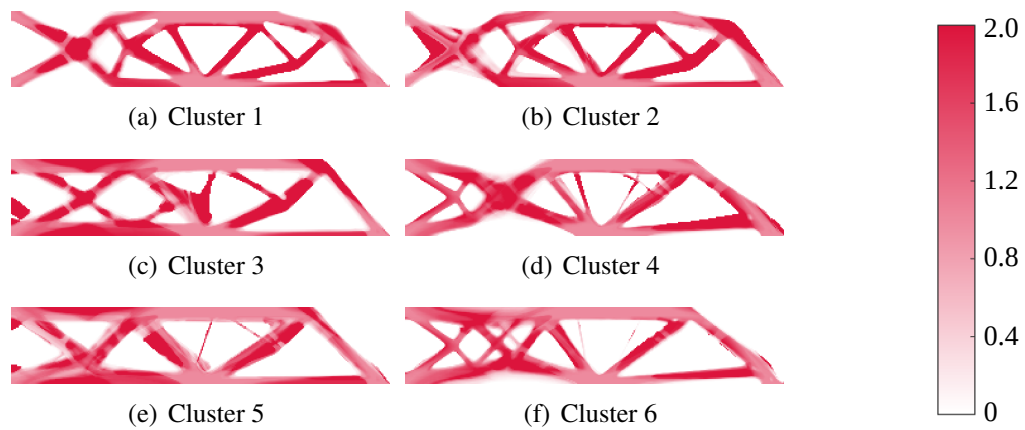


Fig. 3.14 Lift indexes for each cluster for two-dimensional cantilever design problem 2



Fig. 3.15 Overlay image accentuating the differences between representative configurations of clusters 1 and 2.

- Structures like those shown in Figs. 3.11(c) and (e) have high stiffness against the loading shown in Fig. 3.9(a).
- Structures like those shown in Figs. 3.11(d) and (f) have high stiffness against the loadings shown in Figs. 3.9(a) and (b).

On the other hand, items four to six above highlight the effects of the various geometries appearing in certain pairs of clusters in terms of the solutions' physical performances.

To analyze each cluster in more detail and clarify their differences, we serially apply the association rule analysis. Fig. 3.13 shows the confidence indexes expressed in Eq. (3.10), corresponding to each cluster's centroid. The opacities of the red regions in these figures are correlated with the confidence index values, as shown in the gradient key; values near 1.0 indicate commonality among solution substructures in such regions within each cluster. On the other hand, confidence index values in the neighborhood of 0.5 represent locations of structural differences among the solutions in a certain cluster, differences that result in widely ranging values of a particular objective function. Lift indexes for each cluster are provided to extend the analysis (Fig. 3.14). Opaque red regions where the lift index is high in these figures represent unique substructures that differentiate a certain cluster from the other clusters. Note that lift values above 2 are rounded down to 2 to enhance visibility.

As shown in Fig. 3.14(c) and (e), clusters 3 and 5 have high lift values along the upper and lower frame elements in the left portion of the structure. The high lift values in these locations indicate that these substructures are unique in clusters 3 and 5, compared to structures in other clusters, and are likely key structural elements that provide high stiffness against the loading shown in Fig. 3.9(a). On the other hand, Fig. 3.14(c) and (e) also illustrate that lift values are high in the locations of the diagonal substructures in clusters 3 and 5, but the arrangement of the structural elements in the middle and left portions of these configurations is different, indicating a lack of commonality among the interior substructures. That is, the important differences between the solutions in clusters 3 and 5 have to do with the geometries of the interior substructures, as is also the case when comparing Figs. 3.11(c) and (e). Furthermore, the fact that clusters 3 and 5 are intermingled in the objective space indicates that these geometrical differences have little impact on physical performances.

The geometrical differences between clusters 1 and 2 (Figs. 3.11(a) and (b)) are subtle but instructive. Fig. 3.15 highlights differences between representative configurations of clusters 1 and 2. The intersection of the diagonals forming an X shape near the left side in cluster 2 is slightly more to the left than that in cluster 1, and the bent T shape at the upper right corner in cluster 2 is located a little more to the right than that in cluster 1. We can appreciate that these small geometrical differences are responsible for the differences in performance between these two clusters, as reflected in their F_2 and F_3 values.

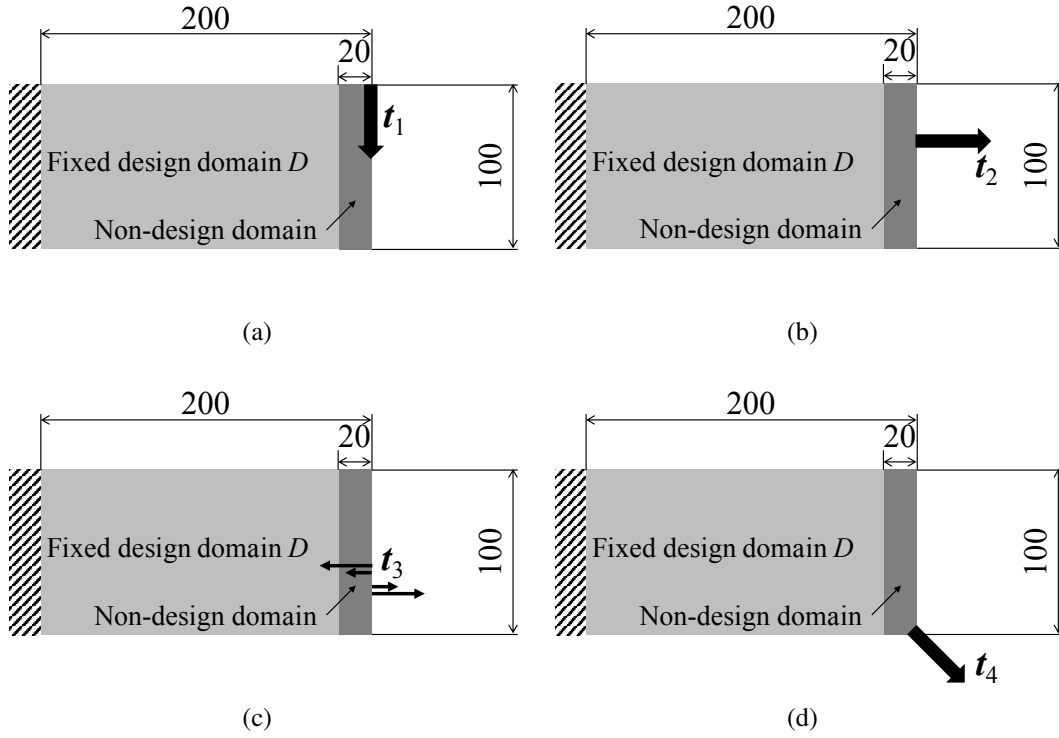


Fig. 3.16 Fixed design domains and boundary conditions for two-dimensional cantilever design problem 3

The geometrical differences between clusters 4 and 6 are much more apparent (Figs. 3.13(d) and (f), respectively). In addition to a larger number of diagonal structures in the left third of cluster 6, cluster 4 has a prominent constriction in this area, which affects the F_1 and F_2 values, although the F_3 value is affected only slightly, as shown in the objective space visualization (Fig. 3.12). In this way, the proposed data mining method extracts substructures that crucially affect the values of particular objective functionals, even for problems with more complex boundary conditions than those used in problem 1.

3.4.3 Two-dimensional cantilever design problem 3

The third two-dimensional cantilever design problem now considered has four objectives, to find minimum mean compliances for the design domains and loading conditions shown in Figs. 3.16(a)–(d). The upper limit of the total volume was set to 35% of the design domain, which was discretized into 100×200 quadrilateral first-order finite elements. The number of clusters was set with $k = 9$ this time, and clustering was again performed 10 times to suppress

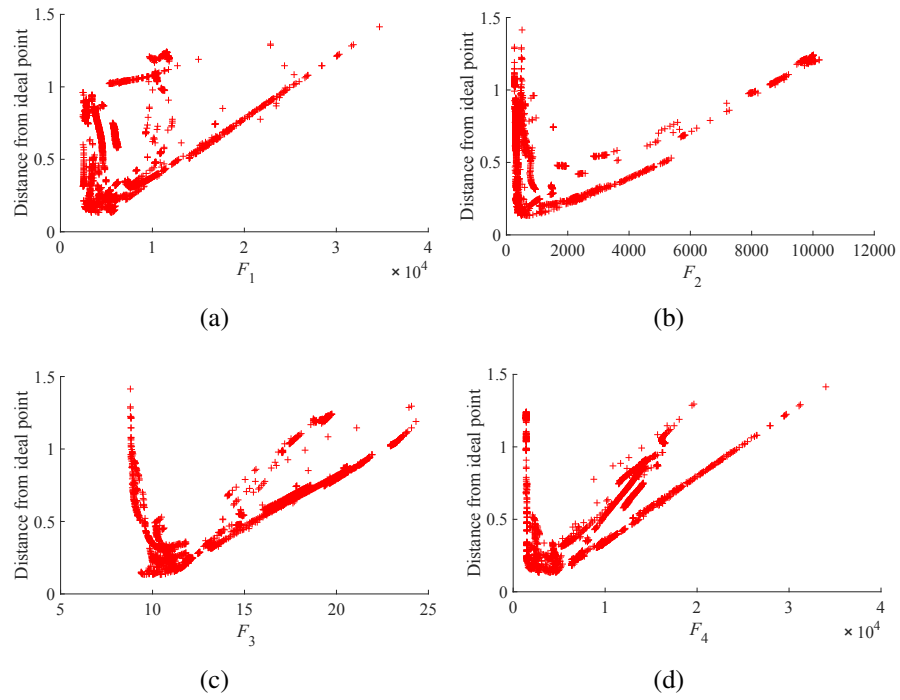


Fig. 3.17 Level diagrams of Pareto front for two-dimensional cantilever design problem 3

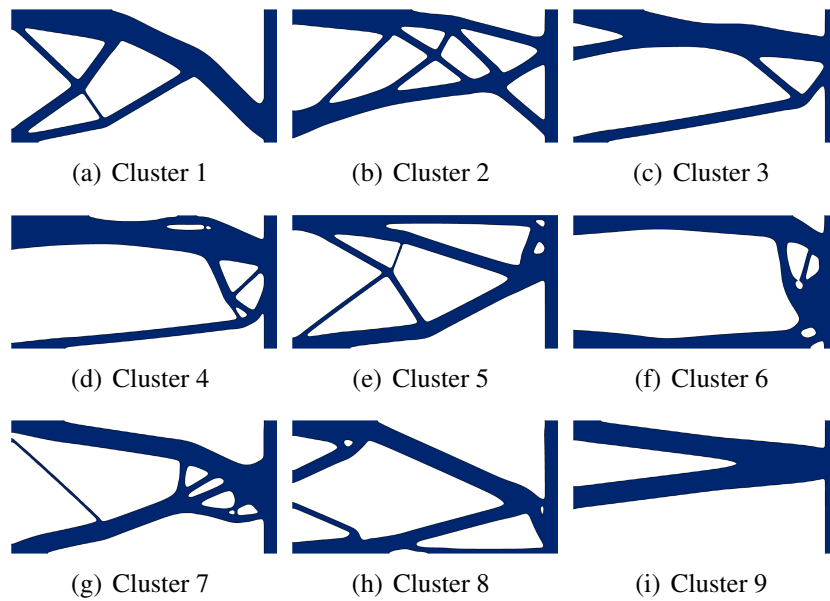


Fig. 3.18 Representative configurations for each cluster for two-dimensional cantilever design problem 3

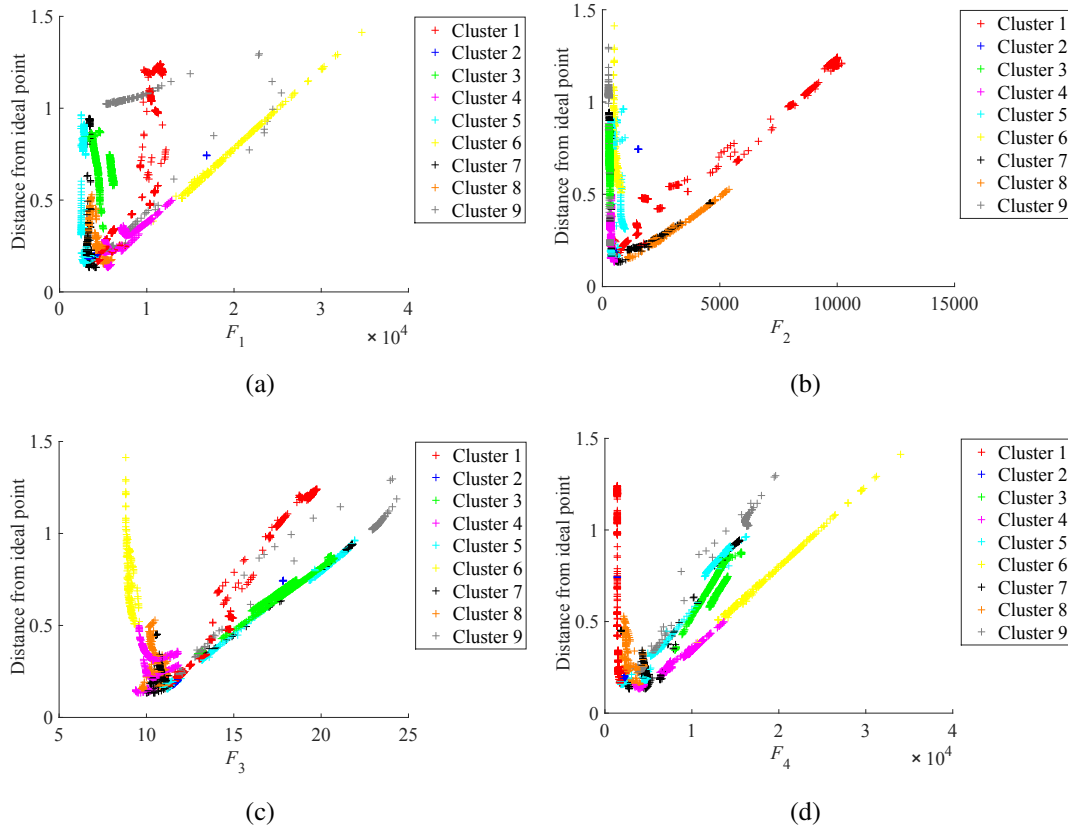


Fig. 3.19 Clustering results visualized in level diagrams for two-dimensional cantilever design problem 3

locally optimal partitions. Level diagrams for the obtained Pareto front approximation, representative configurations for each cluster (nearest solutions to each cluster centroid), and a visualization of the clustering results via level diagrams for the objective space are shown (Fig. 3.17, Fig. 3.18, and Fig. 3.19, respectively). Fig. 3.19 reveals the following cluster features:

- Cluster 5 solutions have lower F_1 values than those in the other clusters.
- Cluster 3, 4, and 9 solutions have lower F_2 values than those in the other clusters.
- Cluster 6 solutions have lower F_3 values than those in the other clusters.
- Cluster 1 solutions have lower F_4 values than those in the other clusters.

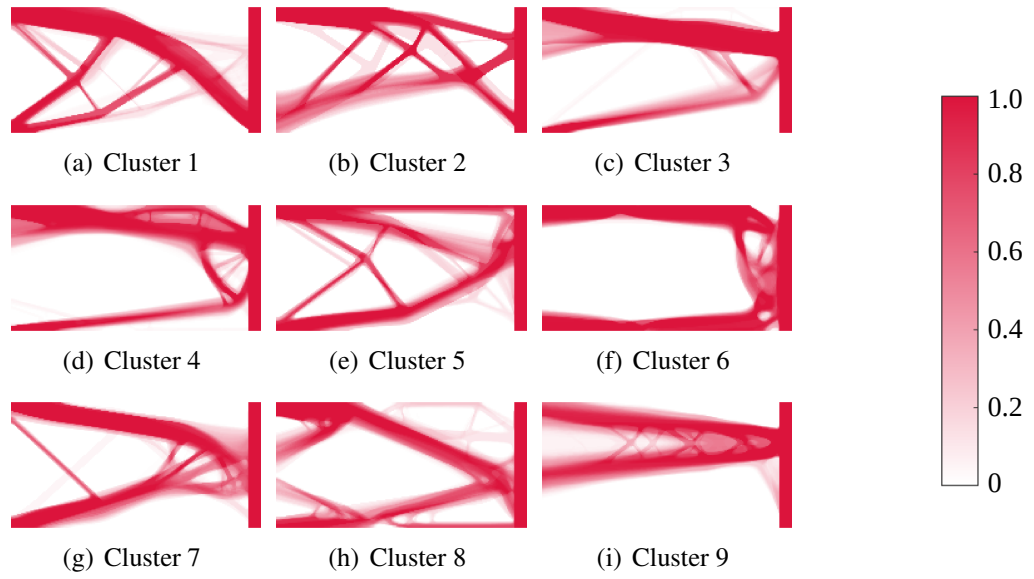


Fig. 3.20 Confidence indexes for each cluster for two-dimensional cantilever design problem 3

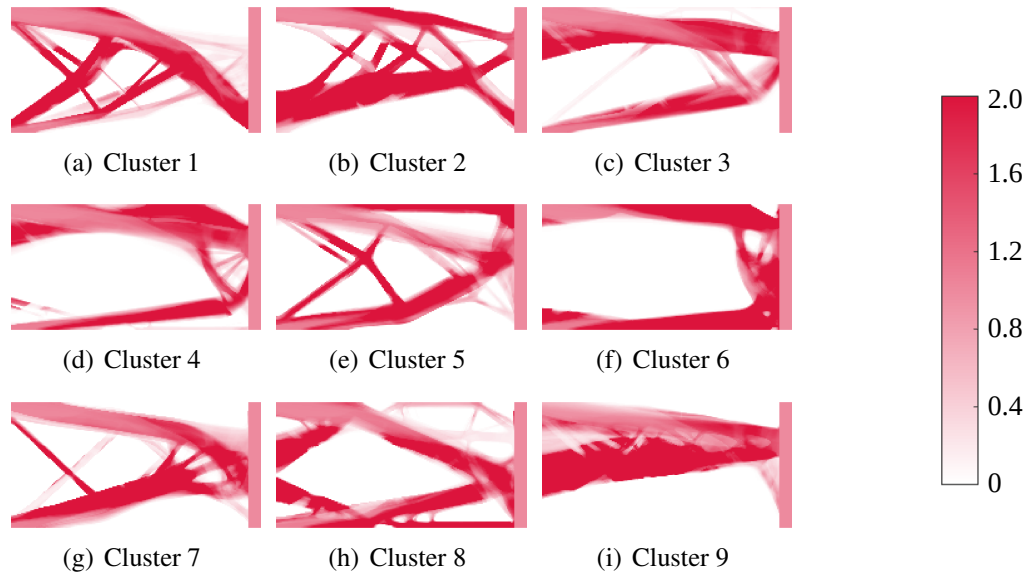


Fig. 3.21 Lift indexes for each cluster for two-dimensional cantilever design problem 3

- Cluster 8 solutions have lower values of the distance from ideal points (where the values of all objective functionals are minimized) than those in the other clusters; that is, cluster 8 solutions have relatively low values for all objectives.

We again apply the association rule analysis to each cluster to reveal details. Confidence and lift indexes for each cluster are displayed (Fig. 3.20 and Fig. 3.21, respectively), and lift values over 2 are again rounded down to 2 to enhance visibility.

Cluster 5 in cantilever design problem 3 shows a prominent structural element extending from the lower left corner diagonally upward, ending near the location where t_1 is applied. The high confidence and lift values associated with this element (Figs. 3.20(e) and 3.21(e), respectively) imply that it is a key structure that provides high stiffness against traction t_1 (Fig. 3.16(a)).

Concerning clusters 3 and 9, high confidence values are present in regions extending from the fixed boundary to the boundary where traction t_2 is applied (Figs. 3.20(c) and (f), respectively). However, some parts of these regions lack corresponding high lift values (Figs. 3.21(c) and (f)), which implies that these structures are important for providing stiffness not only against t_2 but also against other loading conditions. In fact, solutions in clusters 2 and 6 have similar structures (Figs. 3.20(b) and (g), respectively), but cluster 2 solutions have moderate values for all objectives and cluster 6 solutions have relatively high stiffness against loading t_3 in addition to t_2 (Figs. 3.19(a)–(d)). In this way, characteristic substructures can be extracted from other clusters to provide useful knowledge that facilitates the work of decision makers when choosing a particular solution to meet their needs.

3.4.4 Three-dimensional cantilever design problem

Last, we consider a three-dimensional cantilever design problem in which three loading conditions are included, hence it is a three-objective optimization problem, with the fixed design domains and loading conditions shown in Fig. 3.22. The upper limit of the total volume was set to 25% of the design domain, which was discretized into $50 \times 30 \times 30$ hexahedral first-order elements. The number of clusters was set with $k = 6$, and clustering was performed 10 times, to limit locally optimal partitions. The obtained Pareto front approximation, representative configurations for each cluster (nearest solutions to each cluster's centroid), and a visualization of the clustering results in the objective space are provided (Fig. 3.23, Fig. 3.24, and Fig. 3.25, respectively).

Based on Fig. 3.25, the following cluster features are noteworthy:

- Solutions in clusters 2, 4 and 5 have lower F_1 values than those in the other clusters, and provide relatively high stiffness against the bending loading shown in Fig. 3.22(a).

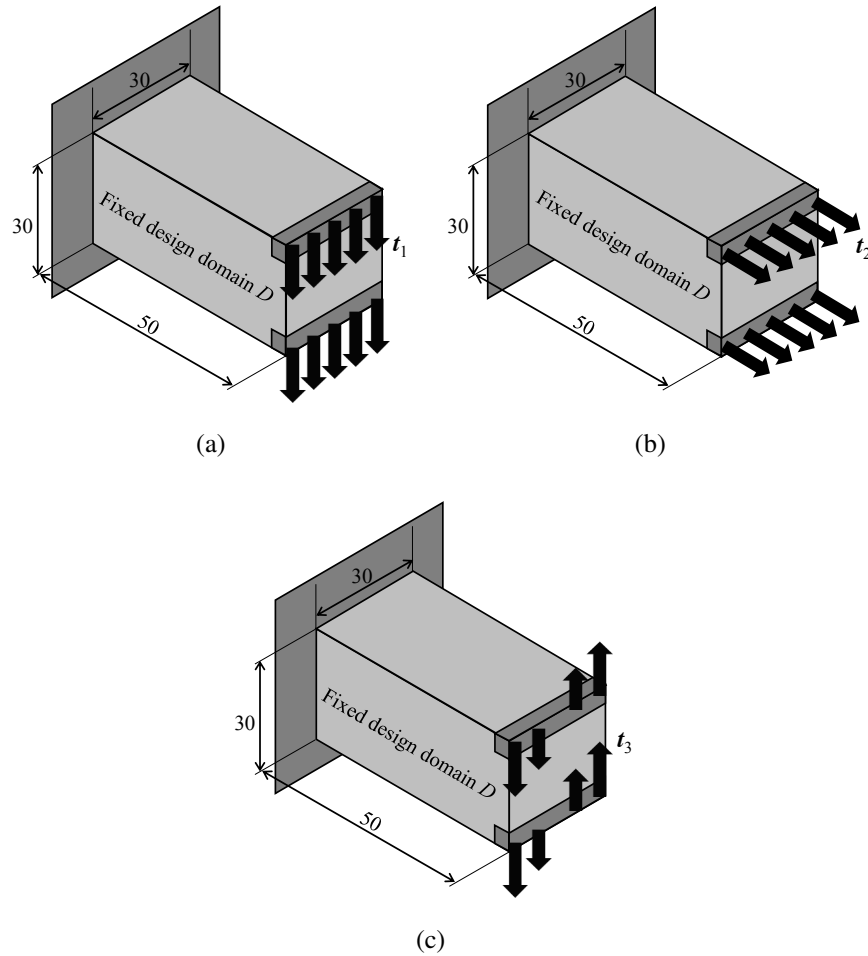


Fig. 3.22 Fixed design domains and boundary conditions for three-dimensional cantilever design problem

- Solutions in clusters 1 and 6 have lower F_2 values than those in the other clusters, and provide relatively high stiffness against the tensile loading shown in Fig. 3.22(b).
- Solutions in cluster 3 have lower F_3 values than those in the other clusters, and provide relatively high stiffness against the torsional loading shown in Fig. 3.22(c).
- Solutions in cluster 2 have lower F_3 values than those in clusters 4 or 5.
- Solutions in cluster 6 have lower F_1 values than those in cluster 1.

The association rule analysis now applied to each cluster again highlights important details. Thresholds are imposed on the confidence and lift index regions to aid visualization

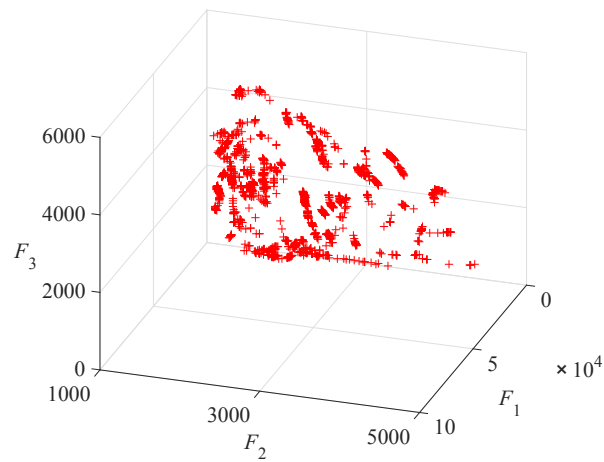


Fig. 3.23 Pareto front approximation for the three-dimensional cantilever design problem

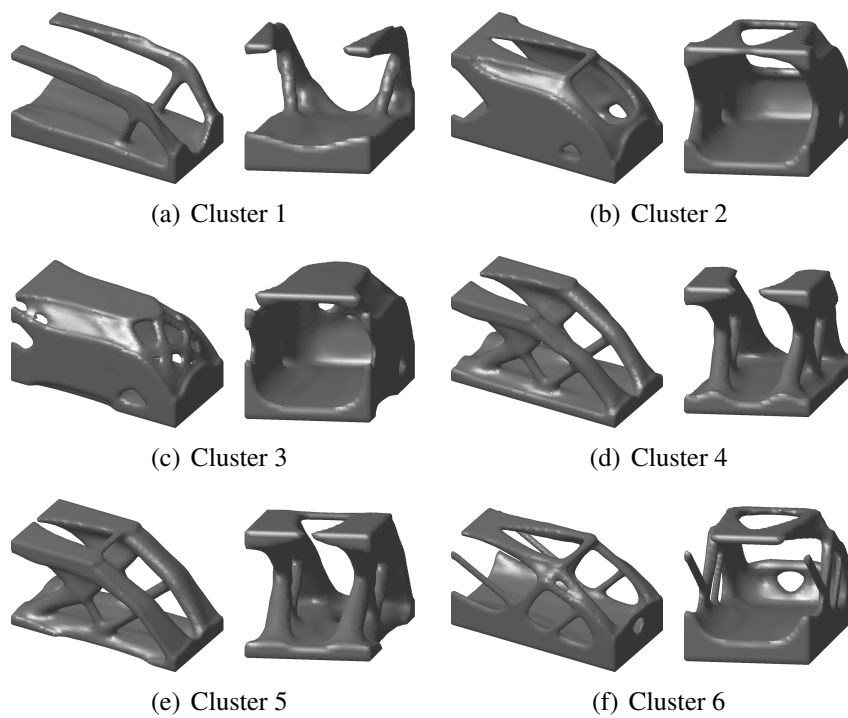


Fig. 3.24 Representative configurations for each cluster for the three-dimensional cantilever design problem

in three dimensions. For each cluster, regions with confidence indexes higher than 0.8, and those with lift indexes higher than 1.8 are shown in red (Fig. 3.26 and Fig. 3.27, respectively).

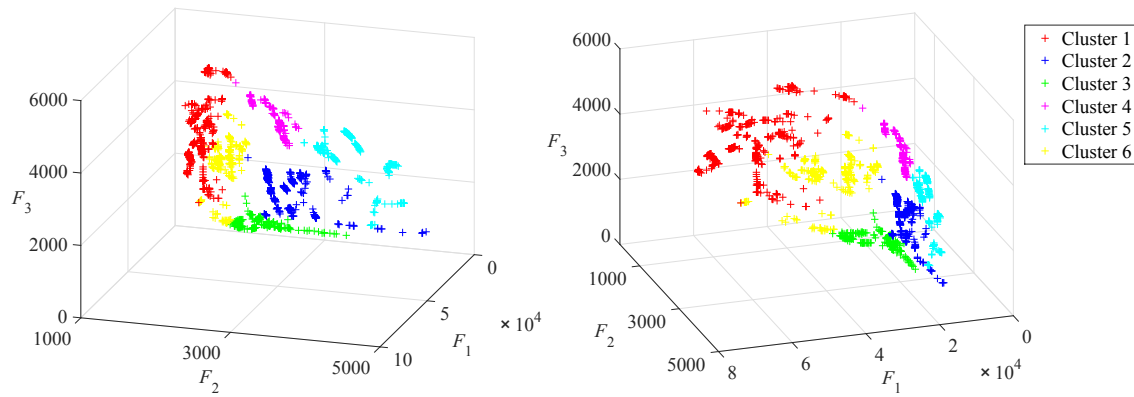


Fig. 3.25 Clustering results visualized in the objective space for the three-dimensional cantilever design problem

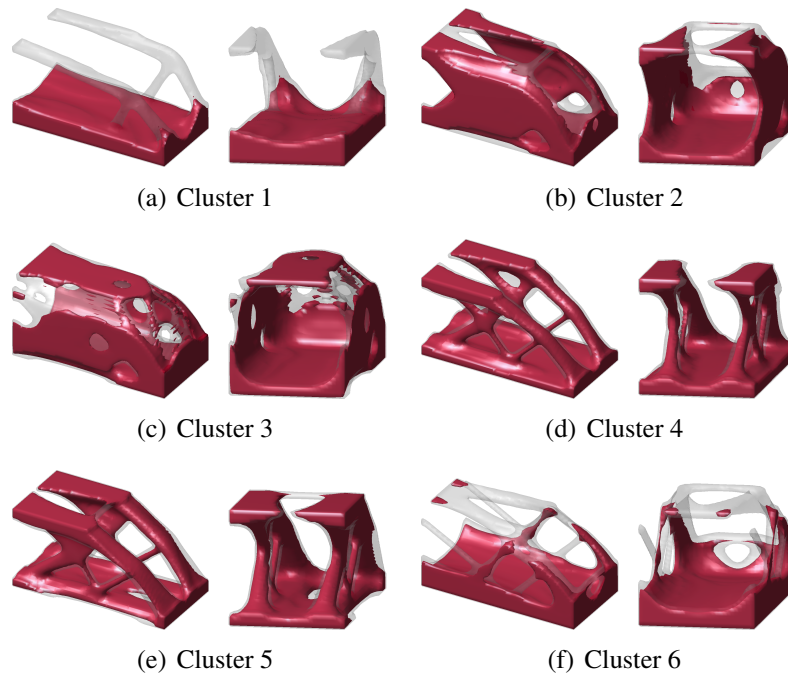


Fig. 3.26 Confidence indexes (red) and structures (semi-transparent gray) for each cluster for the three-dimensional cantilever design problem

Semi-transparent representative structural configurations for each cluster are also shown, in gray, for reference (Figs. 3.26 and 3.27).

Confidence indexes in clusters 2, 4 and 5 are high along both sides and the bottom areas (Fig. 3.26(b), (d) and (e)), but the lift indexes of these clusters are only high along both

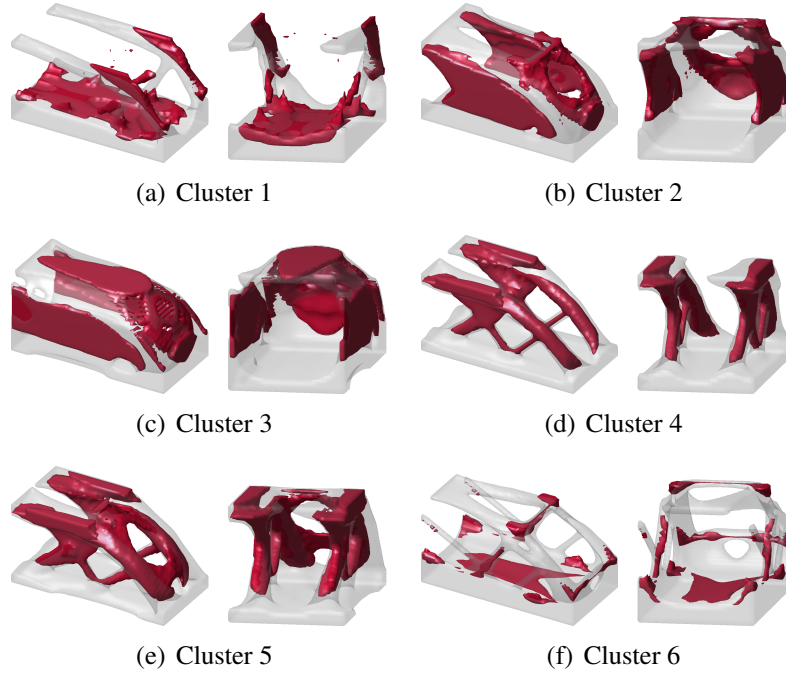


Fig. 3.27 Lift indexes (red) and structures (semi-transparent gray) for each cluster for the three-dimensional cantilever design problem

sides, not the bottom area (Fig. 3.27). This implies that the substructures along the sides are responsible for the stiffness against bending loading (Fig. 3.22(a)), and that the bottom area is a common substructure that provides stiffness against the other loadings. On the other hand, cluster 2 has high lift values along the frames appearing at the top face, and only cluster 2 among clusters 2, 4 and 5 has solid plate structures along both sides. Hence, we can grasp that these substructures result in high stiffness against torsional loading (Fig. 3.22(c)). This is further supported by the cluster 3 lift values (Fig. 3.27(c)) and the fact that cluster 3 solutions have lower F_3 values than those in the other clusters.

Focusing now on clusters 1 and 6 (Figs. 3.24(a) and (f), respectively), we find that solutions with lower F_2 values have high confidence values in the bottom areas, whereas high lift values in these two clusters only appear in relation to bottom surfaces (Figs. 3.27(a) and (f)). This indicates that the bottom parts are common substructures providing stiffness against bending and torsional loadings, and that the thickness of these bottom parts is important when high stiffness against tensile loading (Fig. 3.22(b)) is required. On the other hand, solutions in cluster 6 also have high confidence and lift values along both sides, as do clusters 2, 4 and 5, that have lower F_1 values. This reinforces the fact that solutions in cluster 6 have

lower F_1 values than those in cluster 1 because we have already extracted knowledge that the supportive substructures along the sides are responsible for the stiffness against bending loading (Fig. 3.22(a)), based on the association rule analysis applied to clusters 2, 4 and 5. Similarly, substructures affecting specific objective functionals can be extracted from other clusters and the knowledge gained can then be effectively applied during decision making for a three-dimensional design problem.

3.5 Conclusions

This chapter proposed a data mining method for knowledge discovery using the Pareto-optimal solutions of multiobjective topology optimization problems. The proposed method consists of a two-step data mining procedure which sequentially applies clustering and association rule analysis. For clustering, the distance between two solutions was defined in the design space rather than the objective space to facilitate recognition of differences between pairs of configurations and enable extraction of characteristic substructures. For association rule analysis, confidence and lift indexes for multiobjective topology optimization solutions were proposed.

In four numerical examples, the proposed method was applied to various multiobjective optimization problems, including three- and four-objective problems, and two- and three-dimensional design problems. Clustering results were visualized in the objective space for three-objective problems and illustrated using level diagrams in the four-objective problem. Confidence and lift indexes were visualized in colored plots for the two-dimensional problems and shown using isosurfaces for the three-dimensional problem. In all examples, clustering results, together with confidence and lift indexes, aided comprehension of the key substructures responsible for specific performances. Thus, the proposed data mining method may be especially useful to decision makers at the conceptual design stage, by discovering and revealing important knowledge in topology optimization problems for serviceable structural designs.

Chapter 4

Manufacturing constraints for molding and milling based on fictitious physical models

4.1 Introduction

Manufacturing methods exploiting the use of molds in casting or injection processes, and milling, are widespread in many industries. The most important manufacturing requirements when using a molding or milling process is to ensure that the shape of the product has certain geometrical features that can be manufactured, while maximizing the performances of the product under consideration [136], a design process that usually requires much trial and error and relies on the experience of design engineers. In molding, molded products must embody certain geometrical features so that mold parts can be separated, and milling cannot proceed unless the desired shape allows tool cutting faces to reach the workpiece.

In such scenarios, the design for manufacturing (DFM) process [137] is often used. The DFM concept aims to obtain product designs that are easy to manufacture and some studies incorporate CAE analysis for a casting process as a DFM tool [138, 139]. In DFM, it is important to consider the performance of products together with their manufacturing costs and manufacturability. However, conventional DFM typically focuses on a simple method for evaluating manufacturing costs [137, 140, 141] via, for example, simplification and standardization of design and manufacturing processes [142], although the lowering of performances due to such simplification has recently been considered in some research

[143, 144]. Research on DFM methods for improving product designs while ensuring their performance is relatively scarce, and reliance on design engineers' expertise to achieve product design improvements that also maintain or improve performance is still the norm. To ameliorate this situation, a new design support system that can consider product performances together with their manufacturing costs and manufacturability in the early design phase is required [145].

In this chapter, we therefore propose a manufacturability evaluation method that can be incorporated in structural optimization process as a DFM tool. To evaluate manufacturability, we introduce fictitious physical models that are described by steady-state anisotropic advection-diffusion equations. In these fictitious physical models, material domains are represented as virtual heat sources and advection directions are aligned with prescribed directions, along which mold parts are moved, or attitude in the case of a milling tool. Void regions, where the value of fictitious physical fields are high, represent either undercut geometries which would prevent the molds from being parted, interior voids that cannot be manufactured, or regions that a milling tool cannot reach. In this manner, manufacturability can be evaluated using the fictitious physical fields.

Furthermore, we incorporated the proposed method with a structural optimization method, especially topology optimization. The field of topology optimization for structural problems is essentially mature, and the results of topology optimization approaches are effectively used in many industries, such as automobile and aeronautical industries. However, the objective of topology optimization in most previous research has mainly focused on deriving optimal structures for certain devices to improve their performance. As a result, when topology optimization solutions are applied in practical manufacturing circumstances, design engineers often must interpret and modify the results to satisfy manufacturability conditions [146]. However, maintaining the performance of optimal configurations obtained during subsequent shape modification processes is often difficult for design engineers. Consequently, the performance of modified design candidates is often far below that of the originally obtained optimal solutions. This difficulty may make the use of topology optimization in real world engineering a challenging task. To overcome this problem, it is important to consider manufacturing requirements during the optimization process. How to implement manufacturing constraints, i.e., constraints due to particular manufacturing requirements, is now one of the most interesting topics in the field of topology optimization.

Manufacturing constraints are types of geometrical constraints that ensure that optimal configurations have certain desired geometrical features that permit their manufacture using certain processes. Researchers have proposed a variety of methods for imposing geometrical constraints in shape and topology optimization [147]. Length scale constraints are one of the most studied geometrical constraints in topology optimization. Imposing a minimum length scale constraint prevents the appearance in optimal configurations of excessively complex substructures and hinges that would be difficult to manufacture. Several minimum length scale geometrical constraint methods have been proposed for use in SIMP schemes [148, 26, 149].

On the other hand, maximum length scale constraints are also important in certain manufacturing processes. In die casting, for instance, a maximum length scale constraint can suppress the appearance of void shrinkage cavities that decrease fatigue strength, which may occur in large structural members. A consequence of imposing a maximum length scale constraint can also be exploited as a structural redundancy measurement, whereby loads are redistributed and load paths diversified by replacing each large structural member with a number of smaller features [150]. Several methods for imposing maximum length scale constraints have been proposed [150, 151].

Length scale control methods that can impose both minimum and maximum length scale constraints have also been proposed [152, 153] using a level set-based shape optimization scheme. Other schemes for imposing certain manufacturing constraints in shape and topology optimizations have also been proposed. For additive manufacturing (AM), Brackett *et al.* [154] summarized the issues for the application of topology optimization in AM. Leary *et al.* [155] proposed a method in which the obtained optimal configurations are modified to satisfy an overhang constraint required to avoid the use of support material in AM, and additional schemes for imposing overhang constraints during the optimization procedure have been proposed [156, 157]. Li *et al.* [158] proposed a connectivity constraint to avoid enclosed voids in structures by introducing a virtual scalar field.

As for molding constraints, Zhou *et al.* proposed a mathematical formulation of a molding constraint [159] in a SIMP scheme. Xia *et al.* proposed a molding constraint method [136] in a level set-based shape optimization scheme by limiting the advection velocity in the Hamilton-Jacobi equation, a method later extended by Allaire *et al.* [160]. Additionally, uniform cross-section surface constraints, also called extrusion constraints, have been proposed to simplify certain designs and promote manufacturability [22, 160, 161]. A

cross-section constraint can be a sufficient, but not necessary, condition for manufacturability in casting processes.

In this chapter, we incorporate the proposed manufacturability evaluation method in a topology optimization procedure to obtain optimal configurations for certain devices that provide high performance while ensuring manufacturability using molding or milling techniques. Here, molding and milling manufacturability is evaluated according to fictitious physical fields, with the manufacturing constraint imposed in the fictitious physical models.

The remainder of this chapter is organized as follows. First, we introduce the methodology for evaluating manufacturability when using molding or milling via fictitious physical models that are governed by advection-diffusion equations. Next, we formulate a geometrical constraint within a topology optimization by applying the evaluation method. Based on this formulation, we define optimization problems that not only maximize the performance of a particular device but also ensure its manufacturability. We then construct an optimization algorithm for the topology optimization using the FEM. Finally, we provide two- and three-dimensional numerical examples to confirm the applicability of the proposed method.

4.2 Evaluation of mold and milling manufacturability via fictitious physical models

4.2.1 Clarification of requirements

First, we clarify the geometrical feature requirements for manufacturability when using molding or milling techniques. Structural features that would be problematic when using casting or injection molding can be classified into two types: (1) undercut geometry that would prevent the mold from being disassembled; and (2) the presence of one or more interior voids within the structure, which would make manufacturing impractical. Figure 4.1 shows examples of obstacles in manufacturing when using molds. Fig. 4.1(a) represents undercut geometry, where the lower mold section is captured by an undercut, preventing the mold parts from being separated at the given parting line in the given parting direction, Fig. 4.1(b) represents geometry with an interior void, an empty region that is completely contained within the cast material. Manufacturing structures that include an interior void by casting or injection molding is extremely cumbersome. The direction in which a mold is disassembled is called the parting direction, denoted as $+d$ and $-d$ in these figures, and the

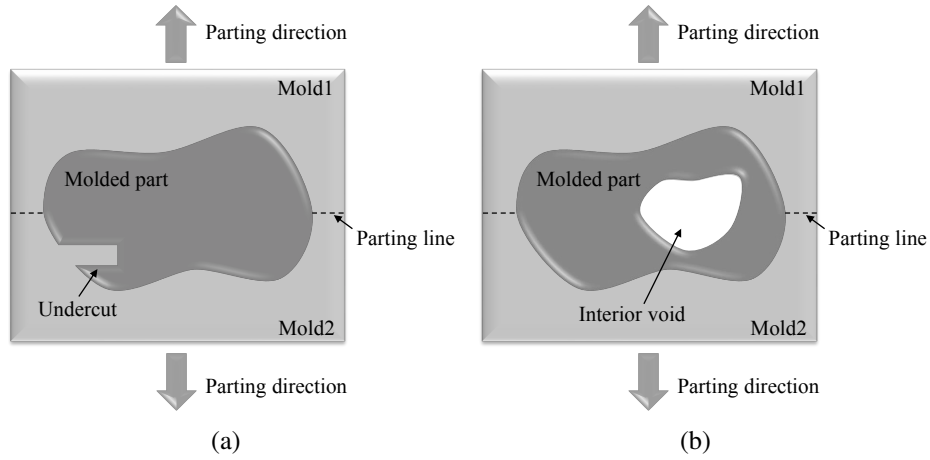


Fig. 4.1 Obstacles in manufacturing when using molds; (a) undercut; and (b) interior void.

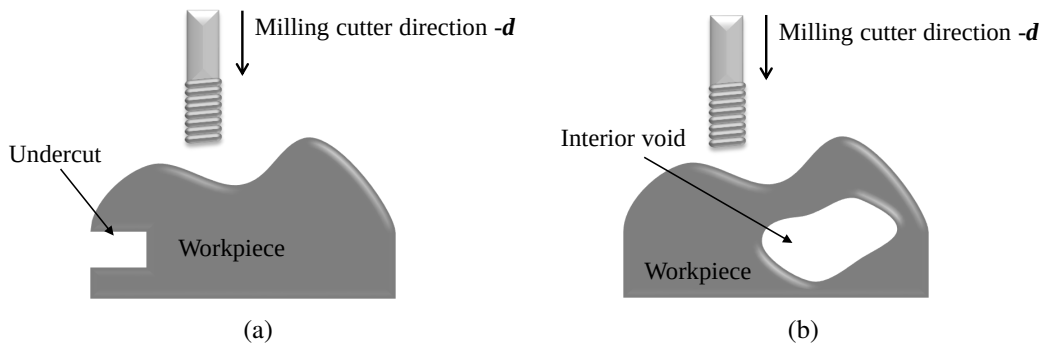


Fig. 4.2 Obstacles in manufacturing when using milling; (a) undercut; and (b) interior void.

line on which two parts of a mold make contact is called the parting line. When a product will be manufactured using casting or injection molding, design engineers must ensure that undercuts and interior voids are avoided.

On the other hand, structural features that would be problematic when using milling can also be classified into two types: (1) undercut geometry with respect to the angle of cutting tool direction, and (2) the presence of one or more interior voids within the structure. Figure 4.2 shows examples of obstacles in manufacturing when using milling. Both undercut geometry in Fig. 4.2(a) and an interior void in Fig. 4.2(b) cannot be achieved because the cutting tool cannot process such areas. Consequently, the geometrical requirements for manufacturability when using molding or milling techniques result in non-existence of

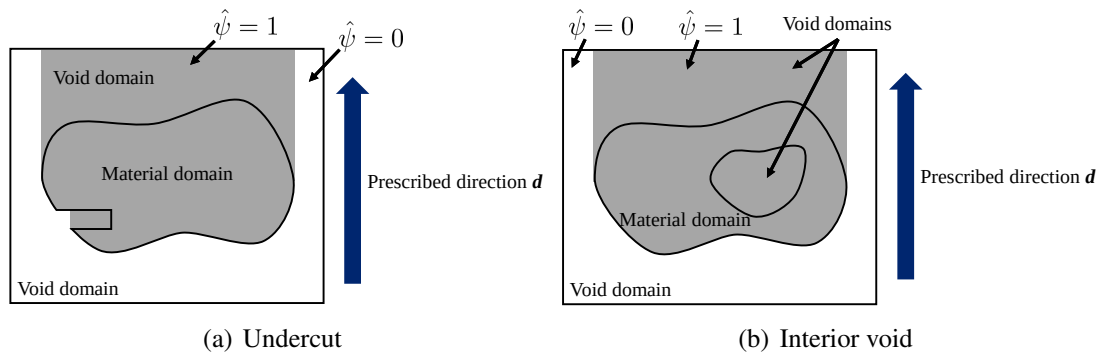


Fig. 4.3 Desired fictitious physical field $\hat{\psi}$ characteristics.

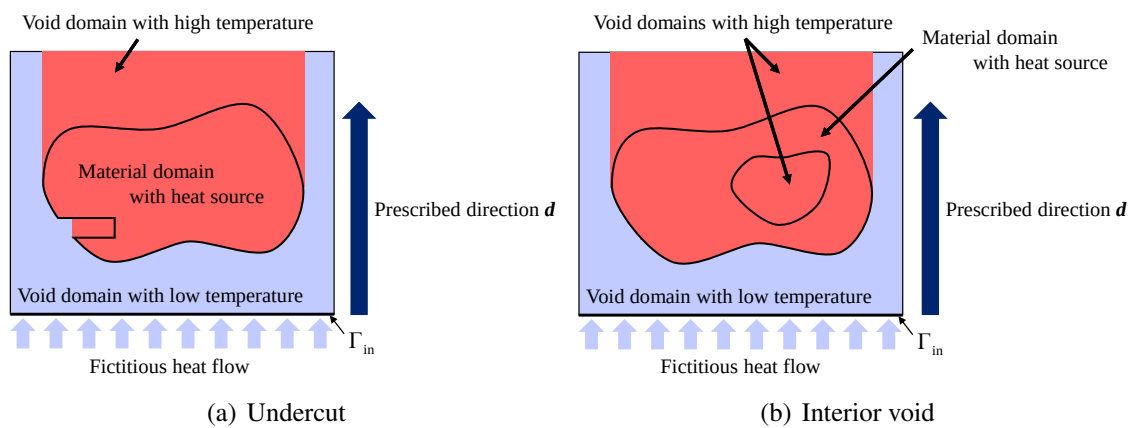


Fig. 4.4 Fictitious heat flow.

undercut geometry and interior voids. In this chapter, we propose a scheme for implicitly imposing geometrical constraints using fictitious physical models.

4.2.2 Introduction of fictitious physical models

When a designed component has a simple structure, it is easy to determine whether or not it can be manufactured using molding or milling. However, when a design engineer designs a component that has a complex structure, it may be difficult to evaluate such manufacturability. In particular, when using structural optimization methods to derive optimal structures, design engineers inevitably must interpret and modify the initially obtained results, to satisfy manufacturability requirements. Consequently, a trial and error process is required and design engineers must have broad experience when designing sophisticated components

that will be manufactured by molding or milling. To overcome these issues, we propose a manufacturability evaluation method using fictitious physical models to implicitly evaluate geometrical features.

First, we consider a fictitious state field $\hat{\psi}$, which is piecewise constant satisfying $\hat{\psi} = 0$ in the upstream side of the structure along the prescribed direction $\mathbf{d}$ and $\hat{\psi} = 1$ in the downstream side, as shown in Fig. 4.3. Such a fictitious state field let us know the presence of the undercut geometries and interior voids along the direction $\mathbf{d}$ as the presence of the void domain with $\hat{\psi} = 1$. Therefore, the governing equation whose solution become $\hat{\psi}$ should be constructed. In the present study, we construct the governing equation for the fictitious state field ψ based on an anisotropic steady-state advection-diffusion equation so that the field ψ would have the similar property to the desired field $\hat{\psi}$. That is, if the fictitious field ψ was regarded as the fictitious temperature field, a thermal conductivity tensor, an advection term and a heat generation term would be determined so that the temperature distribution could correspond to the desired field $\hat{\psi}$ at steady state.

Assume that the thermal conductivity in the analysis domain is an isotropic material and the fluid flows along the prescribed direction $\mathbf{d}$. Then, by considering the internal heat generation which is proportional to the value $(1 - \psi)$, the temperature distribution shown in Figs. 4.4(a) and (b) is expected to be obtained at steady state. Consequently, the presence of the undercut geometries and interior voids along the direction $\mathbf{d}$ can be detected by the presence of the void domains with high temperature.

Therefore, we formulate the governing equation for fictitious state field ψ , using a diffusion tensor $\mathbf{A}$ and the advection speed V , as follows:

$$\begin{cases} -L^2 \operatorname{div}(\mathbf{A} \cdot \nabla \psi) + LV\mathbf{d} \cdot \nabla \psi = \beta \chi_{\Omega}(1 - \psi) & \text{in } D \\ \psi = 0 & \text{on } \Gamma_{\text{in}} \\ \mathbf{n} \cdot (\mathbf{A} \cdot \nabla \psi) = 0 & \text{on } \partial D \setminus \Gamma_{\text{in}}, \end{cases} \quad (4.1)$$

where β is a parameter that control the degree of the heat generation, $\mathbf{n}$ is the outward unit vector normal to ∂D , and L is the length of the analysis domain along the prescribed direction for non-dimensionalization.

The diffusion tensor is set so that the components of the prescribed direction are larger than those in other directions, as follows:

$$\Lambda = \mathbf{d} \otimes \mathbf{d} + \epsilon \sum_{i=1}^{d-1} \mathbf{e}_i^\perp \otimes \mathbf{e}_i^\perp, \quad (4.2)$$

where d is the number of the spatial dimensions, $\mathbf{e}_i^\perp$ represents the orthonormal basis for the orthogonal complement of $\mathbf{d}$, and ϵ is a small constant. Γ_{in} is defined as

$$\Gamma_{\text{in}} = \{\forall \mathbf{x} \in \partial D \mid \mathbf{d} \cdot \mathbf{n} < 0\}. \quad (4.3)$$

Here, the prescribed direction is a unit vector which is opposite to the parting direction for molding and the same as the direction of processing for milling.

If we set β and V to sufficiently large values, ψ approaches 1 in the material domain and downstream side of the material along the prescribed direction. Consequently, the void regions where the value of the fictitious state field, ψ , is high correspond to either undercuts or interior void regions. Therefore, the presence of undercut and interior void regions can be evaluated by visualizing the fictitious state field in void domains by the term $\psi(1 - \chi_\Omega)$

The above discussion can easily be generalized to a process using molds consisting of multiple parts or multi-axis milling process via multiple fictitious physical models, each of which corresponds to each of multiple prescribed directions. Let m denote the number of mold parts or axis for milling. The fictitious state field corresponding to the prescribed direction $\mathbf{d}_i$ is denoted by ψ_i for $i = 1, \dots, m$. In this case, the void regions where the values of all fictitious state fields, ψ_i ($i = 1, \dots, m$), are high correspond to either undercuts or interior void regions. Therefore, the presence of undercut and interior void regions can be evaluated by visualizing the term $(1 - \chi_\Omega) \prod_{i=1}^m \psi_i$ that represents the intersection of the void regions where the value of each fictitious state field, ψ_i , is high. The validity of these fictitious physical models is confirmed in Section 4.4. The proposed method solves physical models described with partial differential equations, similar to the method used in existing CAE tools, so the proposed method is highly compatible.

Application to structural optimization

We can incorporate the manufacturability evaluation method described above with a structural optimization to obtain optimal structures for certain product parts or components that provide

high performance while ensuring manufacturability for molding and milling. In the structural optimization procedure, undercut and interior void regions can be nullified by minimizing the following functional:

$$F_M = \int_D (1 - \chi_\Omega) \prod_{i=1}^m \psi_i dD. \quad (4.4)$$

That is, by minimizing F_M together with objective functional F , which aims to improve a physical performance of a certain device, the manufacturing constraint is incorporated in the structural optimization.

Application to mold design

Furthermore, once the optimization procedure is finished, appropriate mold designs for manufacturing the structurally optimized product components can be created using the fictitious physical models. Let the domain M_i be defined as

$$M_i = \{\forall \mathbf{x} \in D \mid \psi_i < c\}, \quad (4.5)$$

for all indices $i = 1, 2, \dots, m$ where $c \in (0, 1)$ is a real constant. M_i then represents domain filled with the i th mold part. If there is an intersection of multiple domains, it can be incorporated into any convenient mold part.

Predetermination of parting lines in the structural optimization

In the above method for structural optimization, the parting lines are determined according to the mold design after the optimization procedure. However, in practical engineering, it is often attractive to be able to predetermine parting lines, based on the cost of fabricating the mold. The proposed method can be extended to allow predetermination of mold parting lines in a structural optimization.

Predetermining mold parting lines is comparable to predetermining certain parts of the analysis domain that is included in a certain mold part. Let M_i^{pre} for $i = 1, 2, \dots, m$ denote a sub-domain of the analysis domain that is predetermined to be filled with the i th mold part, and let D^{und} represent a sub-domain of the analysis domain for which the particular mold part it is to be included in is undetermined, as shown in Fig. 4.5. In this case, shadow regions in M_i^{pre} viewed from Γ_i represent either undercuts or interior voids, since M_i^{pre} should be included in the i th mold part. Consequently, the molding constraint for this case can be

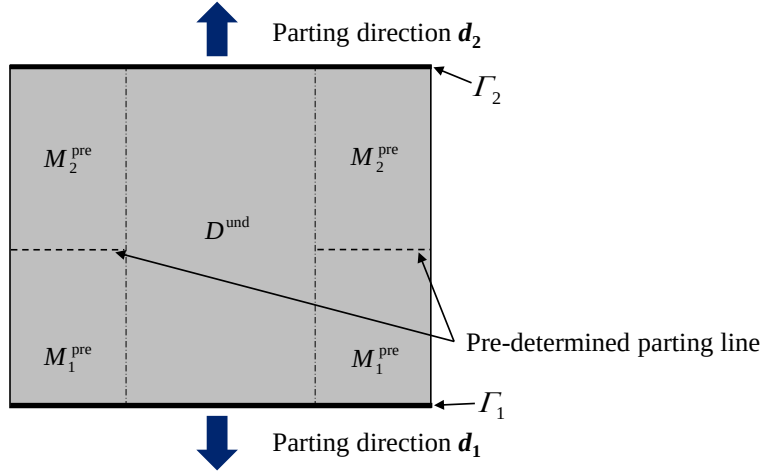


Fig. 4.5 Predetermination of a parting line.

imposed in the structural optimization procedure by minimizing the following functional:

$$F_M^{\text{pre}} = \sum_{i=1}^m \int_{M_i^{\text{pre}}} (1 - \chi_{\Omega}) \psi_i dD + \int_{D^{\text{und}}} (1 - \chi_{\Omega}) \prod_{i=1}^m \psi_i dD. \quad (4.6)$$

4.2.3 Minimum mean compliance problem

Now, we formulate a minimum mean compliance problem considering molding or milling manufacturability, using the fictitious physical models presented in Section 4.2.2.

Consider an elastic structure occupying a material domain Ω that is fixed at boundary Γ_u , with a traction $\mathbf{t}$ applied at Γ_t . Let $\mathbf{u}$, $\mathbf{C}$ and $\boldsymbol{\varepsilon}$ respectively denote the displacement field, the elastic tensor, and the strain tensor, represented as $\boldsymbol{\varepsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$. Using the level set-based structural representation expressed in (1.10) and (1.11), the optimization problem to determine an optimal configuration of the material domain Ω that has a minimum mean compliance and appropriate manufacturability features under a volume constraint can be

formulated as follows:

$$\inf_{\chi_\phi} F = \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{u} d\Gamma + \bar{\gamma} F_M \quad (4.7)$$

subject to:

$$G = \int_D \chi_\phi dD - V_{\max} \leq 0, \quad (4.8)$$

where $\bar{\gamma}$ is a weighting coefficient applied to the manufacturing constraint. Note that the proposed method can also be applicable to the density approaches. $\mathbf{u} \in \mathcal{U}$ and $\psi_i \in \mathcal{T}^i$ satisfy the following variational formulations:

$$E_1 = \int_{\Gamma_t} \mathbf{t} \cdot \tilde{\mathbf{u}} d\Gamma - \int_D \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{C} \chi_\phi : \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) dD = 0 \quad (4.9)$$

$$E_i^{\text{FPM}} = \int_D \beta \chi_\phi (1 - \psi_i) \tilde{\psi}_i dD - \int_D L_i^2 \nabla \tilde{\psi}_i \cdot \Lambda_i \cdot \nabla \psi_i dD - \int_D \tilde{\psi}_i L_i V d\mathbf{i} \cdot \nabla \psi_i dD = 0, \quad (4.10)$$

for all variables $\tilde{\mathbf{u}} \in \mathcal{U}$ and $\tilde{\psi}_i \in \mathcal{T}^i$, where

$$\mathcal{U} = \{\tilde{\mathbf{u}} \in H^1(D)^d \mid \tilde{\mathbf{u}} = \mathbf{0} \text{ on } \Gamma_u\}, \quad (4.11)$$

$$\mathcal{T}^i = \{\tilde{\psi} \in H^1(D) \mid \tilde{\psi} = 0 \text{ on } \Gamma_i\}, \quad (4.12)$$

for all indices $i = 1, 2, \dots, m$. In the above formulation, the first term of the objective functional represents the mean compliance and the second term is the objective functional expressing the manufacturing constraint. G_1 represents the volume constraint and $V_{\max}$ is the upper limit of the allowable material volume. E_1 is a weak form equilibrium equation for the displacement field, $\mathbf{u}$. E_i^{FPM} for $i = 1, 2, \dots, m$ are the weak forms of the governing equations of the fictitious physical models formulated in (4.1). $\tilde{\mathbf{u}}$ and $\tilde{\psi}_i$ are the test function of the weak forms of (4.9) and (4.10), and $H^1(D)$ is a Sobolev space. The above optimization problem is converted into a non-constrained problem using Lagrange's method for undetermined multipliers.

4.2.4 Optimum design problem for a compliant mechanism

Next, we formulate an optimum design problem for a compliant mechanism [162, 163] considering molding or milling manufacturability, using the fictitious physical models described in Section 4.2.2.

Consider a material domain Ω , fixed at boundary Γ_u , with a traction $\mathbf{t}_{\text{in}}$ applied at Γ_{in} . Let $\mathbf{e}$ denote the the direction of the specified deformation at output port Γ_{out} . An optimum design problem for a compliant mechanism can then be formulated as the following mutual mean compliance maximization problem:

$$\inf_{\chi_\phi} F = - \int_{\Gamma_{\text{out}}} \mathbf{e} \cdot \mathbf{u} d\Gamma + \bar{\gamma} F_M^m \quad (4.13)$$

subject to:

$$G = \int_D \chi_\phi dD - V_{\text{max}} \leq 0. \quad (4.14)$$

$\mathbf{u} \in \mathcal{U}$ and $\psi_i \in \mathcal{T}^i$ satisfy the following variational formulations:

$$E_2 = \int_{\Gamma_{\text{out}}} \mathbf{e} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_{\text{out}}} k_{\text{out}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_{\text{in}}} k_{\text{in}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma - \int_D \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{C} \chi_\phi : \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) dD = 0 \quad (4.15)$$

$$E_i^{\text{FPM}} = \int_D \beta \chi_\phi (1 - \psi_i) \tilde{\psi}_i dD - \int_D L_i^2 \nabla \tilde{\psi}_i \cdot \Lambda_i \nabla \psi_i dD - \int_D \tilde{\psi}_i L_i V \mathbf{d}_i \cdot \nabla \psi_i dD = 0, \quad (4.16)$$

for all variables $\tilde{\mathbf{u}} \in \mathcal{U}$ and $\tilde{\psi}_i \in \mathcal{T}^i$ and all indices $i = 1, 2, \dots, m$. In the above formulation, the first term of the objective functional represents the mutual mean compliance and the second term is the objective functional that imposes the manufacturing constraint. E_2 is the weak form equilibrium equation of the displacement field, $\mathbf{u}$. The second and the third terms of E_2 represent Robin boundary conditions, for which parameters k_{out} and k_{in} allow the setting of reaction forces, due to deformation at boundaries Γ_{out} and Γ_{in} , that automatically ensure appropriate structural stiffness.

4.3 Numerical implementation

4.3.1 Optimization algorithm

In the optimization algorithm, the initial level set function is set in the first step and the governing equations are solved using the finite element method (FEM) in the second step. In the third step, the objective functional is evaluated using (4.7) or (4.13). If the objective functional is converged, the optimization procedure is halted, otherwise the adjoint equations are solved using the FEM. In the fourth step, the sensitivities are evaluated. In the fifth step,

the level set function is updated using the reaction-diffusion equation and the optimization procedure then returns to the second step. Sensitivity analysis for the manufacturing constraint via fictitious physical models is discussed in Appendix A.3.

4.3.2 Approximated characteristic function

In the present study, the characteristic function χ_ϕ is replaced with a smoothed Heaviside function H_ϕ , since χ_ϕ is discontinuous and numerical oscillations occur during the optimization procedure, as follows:

$$H_\phi = \begin{cases} 1 & \text{for } \phi > w \\ \frac{1}{2} + \frac{\phi}{w} \left(\frac{15}{16} - \frac{\phi^2}{w^2} \left(\frac{5}{8} - \frac{3}{16} \frac{\phi^2}{w^2} \right) \right) & \text{for } -w \leq \phi \leq w \\ 0 & \text{for } \phi < -w, \end{cases} \quad (4.17)$$

where w represents the width of the transition.

Furthermore, we use the ersatz material approach [20]. That is, the equilibrium equations (4.9) and (4.15) are respectively approximated with the following equations:

$$\begin{aligned} E_1 &= \int_{\Gamma_i} \mathbf{t} \cdot \tilde{\mathbf{u}} d\Gamma - \int_D \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{C} \left(H_\phi(1 - \varepsilon_{\text{mat}}) + \varepsilon_{\text{mat}} \right) : \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) dD = 0, \\ E_2 &= \int_{\Gamma_{\text{out}}} \mathbf{e} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_{\text{out}}} k_{\text{out}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_{\text{in}}} k_{\text{in}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma \\ &\quad - \int_D \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbf{C} \left(H_\phi(1 - \varepsilon_{\text{mat}}) + \varepsilon_{\text{mat}} \right) : \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) dD = 0, \end{aligned} \quad (4.18)$$

where ε_{mat} represents the ratio of the Young's modulus for the two materials, one structural and the other void. Parameter ε_{mat} is introduced to avoid singularities in the stiffness matrix.

4.3.3 Normalization for sensitivity scaling

The scale of the sensitivity F'_C for the mean compliance or the mutual mean compliance is significantly influenced by the scale of the fixed design domain and the setting of the boundary conditions, whereas the scale of the sensitivity F'_M for the manufacturing constraint is relatively constant, due to the non-dimensional definition of the fictitious physical models. This makes it difficult to set appropriate values for the weighting coefficient, $\bar{\gamma}$. In the present

study, we therefore normalize the sensitivity F'_C , as follows:

$$\bar{F}'_C = \frac{F'_C \int_D dD}{\int_D |F'_C| dD}. \quad (4.19)$$

Then, we define the total sensitivity F' , so that

$$F' = \bar{F}'_C + \gamma F'_M, \quad (4.20)$$

where γ is a weighting coefficient.

4.4 Numerical examples

4.4.1 Evaluation of manufacturability

We first examine the validity of the manufacturability evaluation method using the two fictitious physical models. We consider two structures, Case 1 that has undercut geometry, and Case 2 that has appropriate manufacturability, as respectively shown in Figs. 4.6(a) and (b). We evaluate the manufacturability of these structures when two prescribed directions are aligned with the vertical axis. ϵ for the diffusion tensor Λ in (4.2) was set to 10^{-2} and advection speed V was set to 100. Parameter β in (4.1) was set to 10^4 . Figures 4.7(a) and (b) show the fictitious physical fields ψ_1 and ψ_2 obtained by solving (4.1) for two prescribed directions opposite to each other, and Fig. 4.8(a) shows the distribution of $\psi_1\psi_2(1 - \chi)$ for Case 1. Figure 4.8(b) shows the distribution of $\psi_1\psi_2(1 - \chi)$ for Case 2. As shown, regions with high values of $\psi_1\psi_2(1 - \chi)$ indicate a geometry that would be problematic to manufacture. We can confirm that such regions are successfully highlighted using the proposed fictitious physical models incorporating advection-diffusion equations, indicating that our proposed method can function effectively as a DFM tool.

4.4.2 Dependency of ψ on advection speed and parameter β value

To determine appropriate parameter settings, we first examine the dependency of the fictitious physical field, ψ , with respect to different settings of values V and β , defined in (4.1). In this example, we use the same model as that shown in Fig. 4.6(a). That is, we assume two opposed vertical prescribed directions. To ensure that the value of the fictitious physical field,

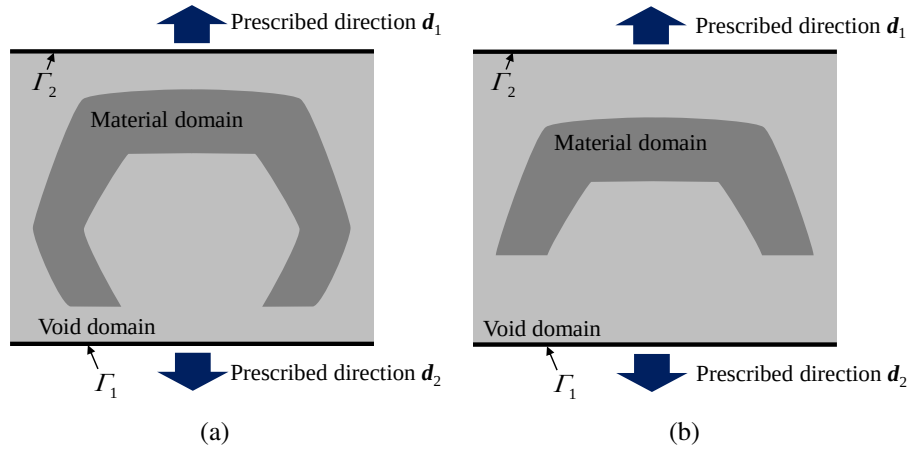


Fig. 4.6 Evaluation models: (a) with undercut (Case 1); (b) manufacturable (Case 2).

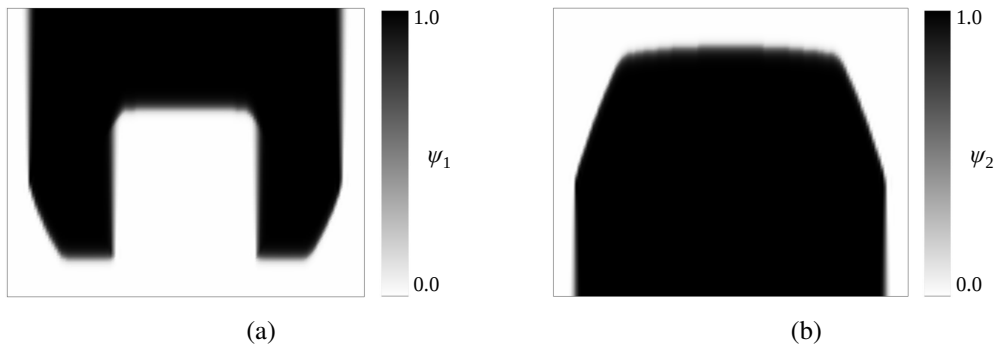


Fig. 4.7 Fictitious physical fields: (a) ψ_1 ; (b) ψ_2 .

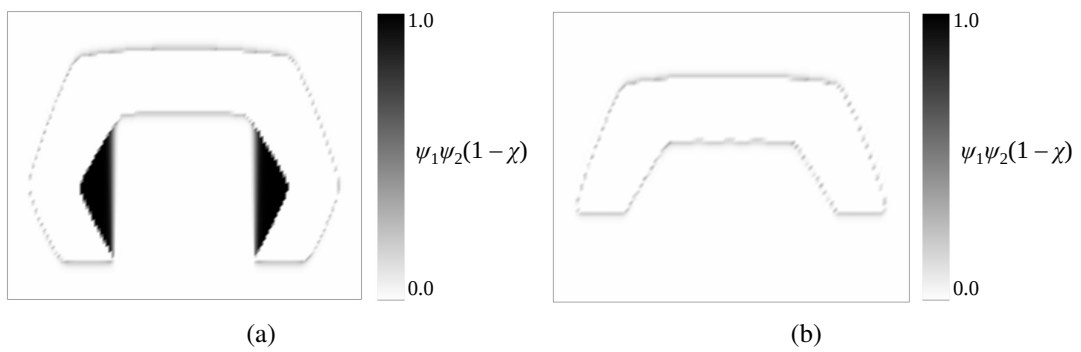
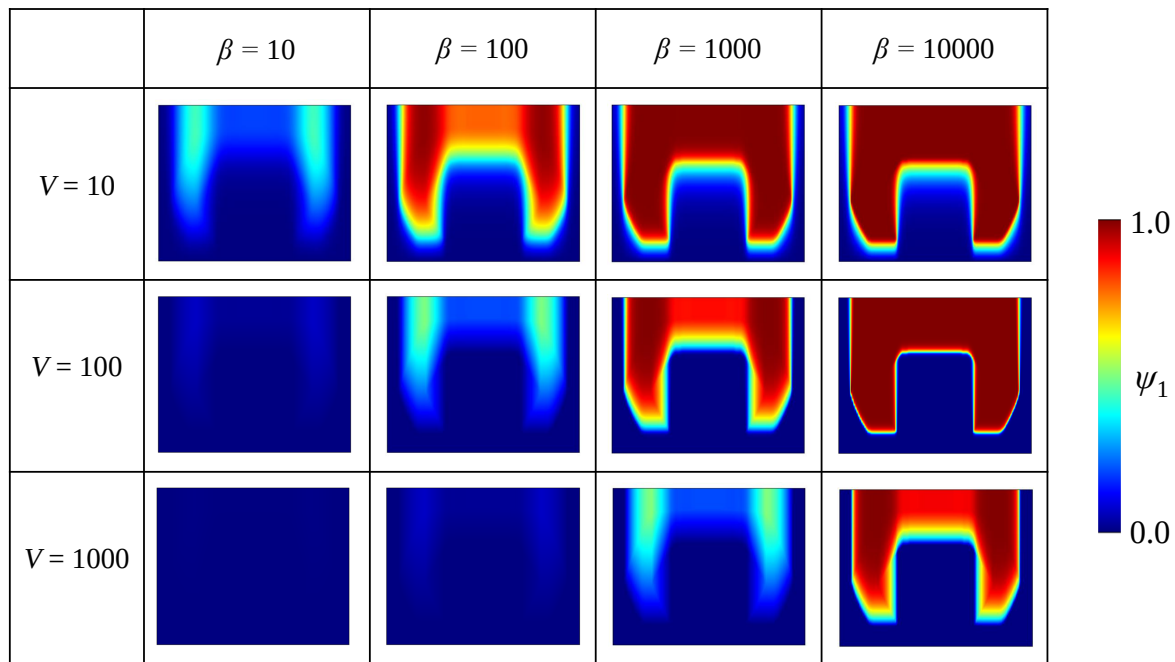


Fig. 4.8 The distribution of $\psi_1\psi_2(1-\chi)$ for the structures: (a) with undercut (Case 1); (b) that can be manufactured (Case 2).

Fig. 4.9 Fictitious physical field ψ .

ψ , correctly represents high and low fictitious temperature areas, namely that ψ is nearly 0 in upstream side of the structure and 1 in the downstream side, appropriate values for V and β must be set. Figure 4.9 shows fictitious physical field ψ for various settings of V and β , and indicates that β should be set to values at least 10 times larger than that of the advection velocity magnitude, V .

4.4.3 Topology optimization for two-dimensional minimum mean compliance problem 1

We now combine the proposed method with the level set-based topology optimization. First, the proposed method is applied to a two-dimensional minimum mean compliance problem to confirm the validity and utility of the proposed manufacturing constraint. Figure 4.10 shows the fixed design domain and boundary conditions. The isotropic linearly elastic material employed has Young's modulus = 210 GPa and Poisson's ratio = 0.31, respectively. The upper limit of the allowable volume was set to 40% of the volume of the fixed design domain. The regularization parameter τ was set to 1×10^{-4} . We assume two prescribed direction opposed along vertical axis for this two-dimensional problem. In all of the following examples of the

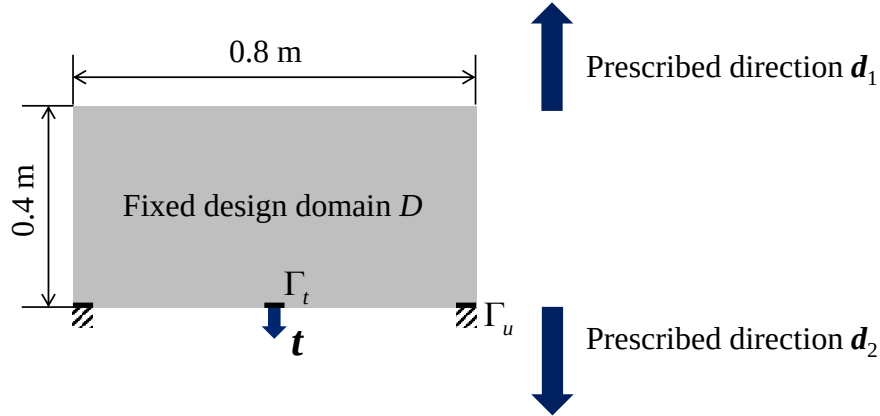


Fig. 4.10 Fixed design domain and boundary conditions of the two-dimensional problem 1.

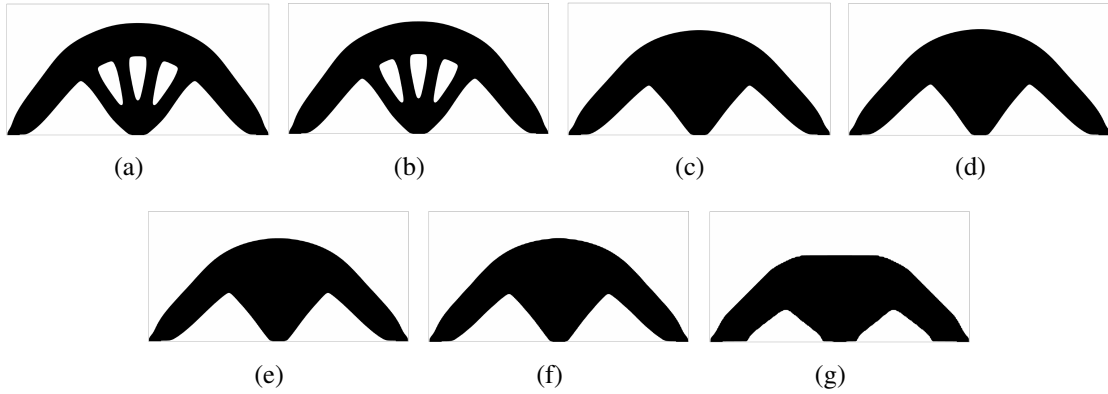


Fig. 4.11 Optimal configurations: (a) without manufacturing constraint (2.90×10^{-8} J); (b) $\gamma = 0.1$, (2.91×10^{-8} J); (c) $\gamma = 0.5$, (2.97×10^{-8} J); (d) $\gamma = 1.0$, (2.97×10^{-8} J); (e) $\gamma = 5.0$, (2.97×10^{-8} J); (f) $\gamma = 10$, (2.97×10^{-8} J); (g) $\gamma = 50$, (3.17×10^{-8} J). Values in parentheses indicate the mean compliance values.

two-dimensional problem, parameters of the fictitious physical models were set as $\epsilon = 10^{-2}$, $V = 100$, and $\beta = 1000$. In the following examples, we examine the dependency of the optimal configurations on the value of parameter γ and on the initial configuration.

Dependency of optimal configurations on parameter γ

First, we examine the dependency of the optimal configurations with respect to different settings of parameter γ . In this example, the fixed design domain was filled with material for the initial configuration.

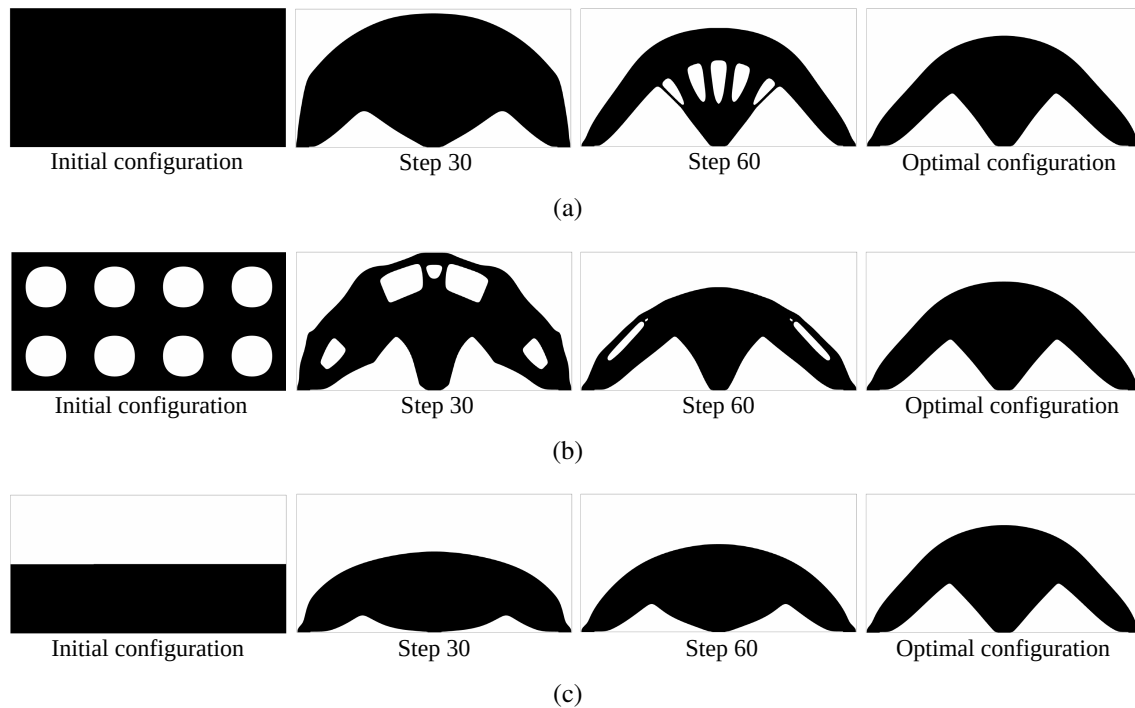


Fig. 4.12 Initial configurations, intermediate results and optimal configurations: (a) Case 1; (b) Case 2; (c) Case 3.

Various obtained optimal configurations are depicted in Figs. 4.11(a)–(g). The optimal configuration obtained in the absence of a manufacturing constraint is shown in Fig. 4.11(a), for comparison, and we observe that several interior voids are present, indicating that this configuration cannot be manufactured by molding and milling. On the other hand, the optimal configurations in Fig. 4.11(c)–(g) show geometrical features that are appropriate for manufacturing when the prescribed directions are set along the y -axis. However, as shown in Fig. 4.11(b), when γ is set to a relatively small value, the manufacturing constraint fails to prevent the inclusion of void areas in the optimal configuration. When γ is set to too large a value, the performance of the obtained optimal configuration (Fig. 4.11(g)) is considerably below that of the other configurations (Fig. 4.11(a)–(f)). However, the obtained optimal configurations are almost identical when γ is set in the range of 0.5–10. Consequently, we can confirm that optimal configurations with appropriate manufacturability show little dependency on the value of weighting coefficient γ .

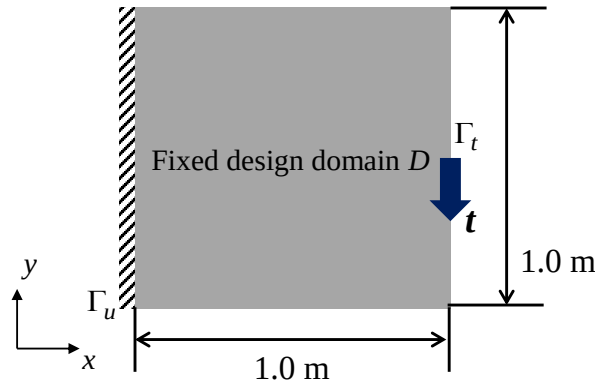


Fig. 4.13 Fixed design domain and boundary conditions of the two-dimensional problem 2.



Fig. 4.14 Prescribed directions for the two-dimensional design problem: (a) Prescribed directions along the x -axis; (b) Prescribed directions along the y -axis; (c) Prescribed directions with the angle between them being 90° ; (d) Prescribed directions with the angle between them being 135° .

Dependency of optimal configurations on the initial configuration

Next, we examine the dependency of the optimal configurations with respect to different setting of the initial configurations, using three different configurations. The initial configuration for Case 1 has material filling the fixed design domain, a configuration of eight holes for Case 2, and material filling only the lower half of the fixed design domain for Case 3. In this example, γ was set to 1, respectively.

Initial, intermediate, and obtained optimal configurations are shown in Fig. 4.12. The obtained optimal configuration are almost identical in these three cases, so we confirm that the dependency of the optimal configurations on the initial configuration is extremely low. Furthermore, the results shown in Fig. 4.12 demonstrate that intermediate results during the optimization procedure can violate the manufacturing constraint, although it is satisfied in the final optimal configurations. This advantageous behavior occurs because the proposed

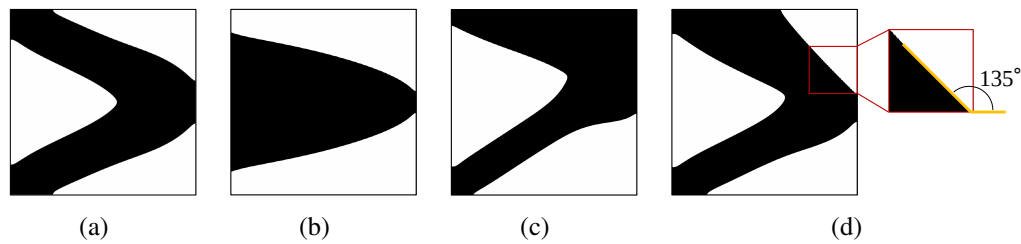


Fig. 4.15 Optimal configurations obtained for various settings of the prescribed directions; (a) Prescribed directions along the x -axis; (b) Prescribed directions along y -axis; (c) Prescribed directions with the angle between them being 90° ; (d) Prescribed directions with the angle between them being 135° .

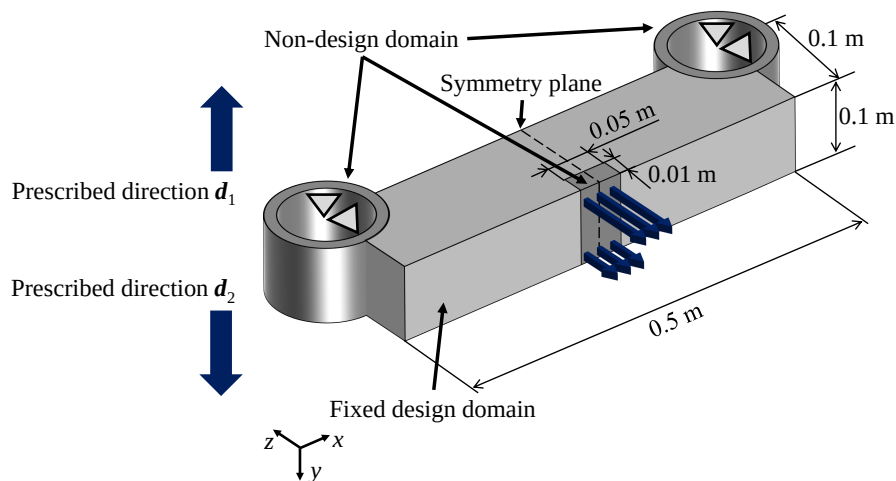


Fig. 4.16 Fixed design domain and boundary conditions of the three-dimensional minimum mean compliance problem.

method does not restrict the design space, but imposes the manufacturing constraint via the fictitious physical models.

4.4.4 Topology optimization for two-dimensional minimum mean compliance problem 2

Here we examine the effect of the prescribed directions on the optimal configurations. Figure 4.13 shows the fixed design domain and boundary conditions. The isotropic linearly elastic material employed has Young's modulus = 210 GPa and Poisson's ratio = 0.31, respectively. The upper limit of the allowable volume was set to 50% of the volume of the

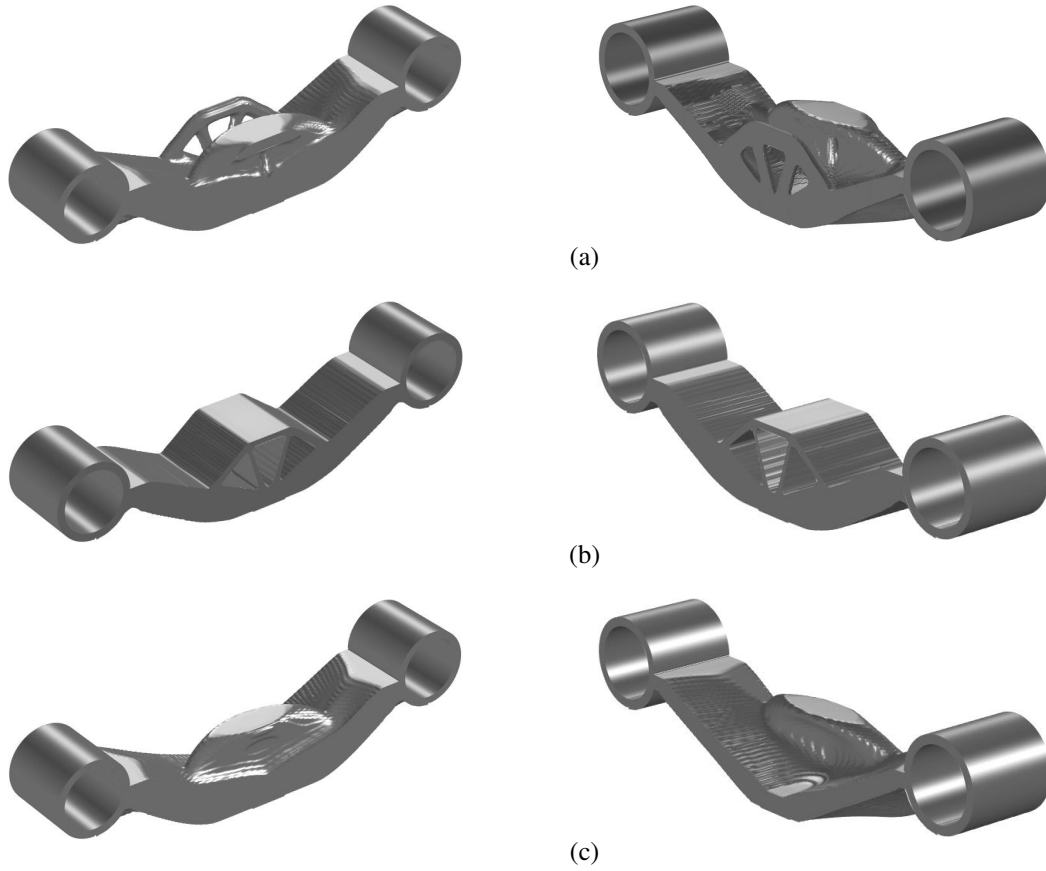


Fig. 4.17 Optimal configurations for the three-dimensional minimum mean compliance problem: (a) non-geometrical constraint, (8.05×10^{-10} J); (b) uniform cross-section surface constraint, (8.64×10^{-10} J); (c) proposed manufacturing constraint imposed, (8.19×10^{-10} J). Values in parentheses indicate the mean compliance values.

fixed design domain. The regularization parameter τ was set to 1×10^{-4} . The weighting coefficient γ was set to 5. In this example, the fixed design domain was filled with material for the initial configuration.

Figure 4.14 illustrates the prescribed direction considered in this example, and Fig. 4.15 shows the optimal configurations obtained for each prescribed direction settings. As shown in this figure, we can confirm that the proposed method successfully obtain the optimal configurations depending on the setting of the prescribed direction.

4.4.5 Topology optimization for three-dimensional minimum mean compliance problem

We now apply the proposed method to a three-dimensional minimum mean compliance problem. Figure 4.16 shows the fixed design domain and the boundary conditions. Since the design model is symmetrical, the fixed design domain is defined as only the left half of the illustrated design domain. The inner surfaces of the cylindrical shapes are fixed and the applied traction $\mathbf{t}$ is described as follows:

$$\mathbf{t} = \begin{cases} 1000 \text{ N} & 0 \leq y \leq 0.25 \\ 500 \text{ N} & 0.75 \leq y \leq 1.0 \\ 0 \text{ N} & \text{otherwise,} \end{cases} \quad (4.21)$$

where $y = 0$ at the upper surface of the design model. The isotropic linearly elastic material has Young's modulus = 210 GPa and Poisson's ratio = 0.31, respectively. The upper limit of the allowable volume was set to 40% of the volume of the fixed design domain. We again assume two prescribed directions opposed along the y -axis. In this problem, to demonstrate the effectiveness of the proposed method, we compare the optimal configurations obtained without a geometrical constraint, when using a uniform cross-section surface constraint, and when using the geometrical constraint. The regularization parameter τ was set to 1×10^{-4} except for the case of the uniform cross-section surface constraint, where the x and z components of τ were both set to 1×10^{-4} and the y component of τ was set to 1×10^{-1} . In the fictitious physical models, parameters were set as $\epsilon = 10^{-2}$, $V = 100$, and $\beta = 1000$. The weighting coefficient γ was set to 1.

Figure 4.17 shows the obtained optimal configurations. The optimal solution shown in Fig. 4.17(a) that was obtained only by focusing on improvement of the physical performance has the smallest mean compliance among these three solutions, although manufacturing this configuration by molding or milling might be difficult since an undercut is included no matter where the parting surface is set. On the other hand, the optimal configuration shown in Fig. 4.17(b), obtained by imposing a uniform cross-section surface constraint, is simple enough to be manufactured. As is obvious, however, the physical performance, i.e. the mean compliance, of this result is not as good as that of the optimal solution shown in Fig. 4.17(a). The optimal configuration shown in Fig. 4.17(c) also has favorable manufacturability and the mean compliance is lower than that for Fig. 4.17(b). Therefore, the optimal solution

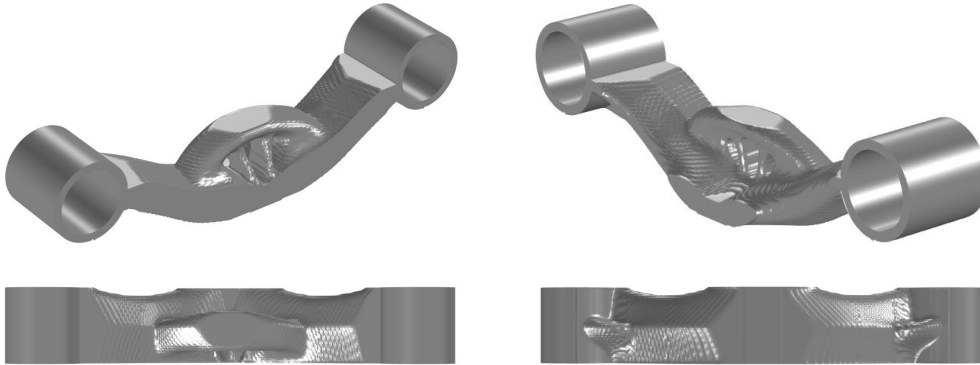


Fig. 4.18 Optimal configuration for the three-dimensional minimum mean compliance problem with predetermined mold parting line, mean compliance = 8.37×10^{-10} J.

obtained when imposing the manufacturing constraint is a better design candidate when manufacturability is a prerequisite.

Predetermination of parting line location for molding

Next, we examine the effectiveness of predetermining the location of the parting line for a two-part mold. We assume a two-part mold with opposed parting directions along the y -axis, with the parting line predetermined on the surface $y = 0.05$, i.e., at middle of the design domain, based on the formulation in Section 4.2.2. All parameters are the same as those used in Section 4.4.5.

Figure 4.18 shows the optimal configuration. The mean compliance of the optimal configuration here is lower than that of the optimal configuration shown in Fig. 4.17(b), although it is higher than that of the optimal configuration shown in Fig. 4.17(c), where the manufacturing constraint is imposed but the parting line is not predetermined. This result indicates that the optimal configuration with the parting line location preset at $y = 0.05$ can be manufactured, and that setting the location of the mold parting line prior to the optimization procedure is a useful alternative to allowing the proposed method to determine the location.

4.4.6 Topology optimization for an optimum design problem of a compliant mechanism

The proposed method is now applied to an optimum design problem for a compliant mechanism. In this example, the molds for manufacturing the optimized structure will also be

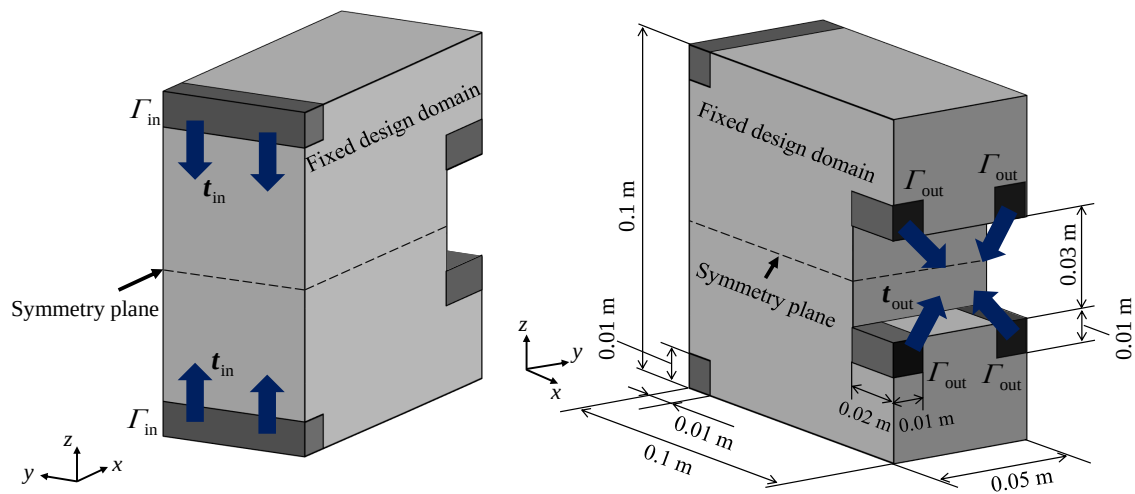


Fig. 4.19 Fixed design domain and boundary conditions of the optimum design problem for compliant mechanism.

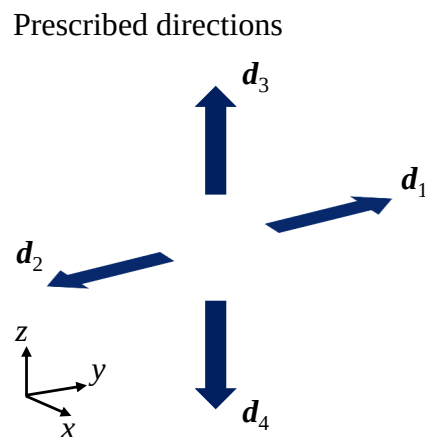


Fig. 4.20 Prescribed directions for the optimum design problem of compliant mechanism.

designed. Figure 4.19 shows the fixed design domain and the boundary conditions. Since the design model is symmetrical, the fixed design domain is defined as the upper half of the design domain. A traction, t_{in} , is applied at boundaries t_{in} that are fixed along the x and y axes. The isotropic linearly elastic material has Young's modulus = 210 GPa and Poisson's ratio = 0.31, respectively. The upper limit of the allowable volume was set to 20% of the volume of the fixed design domain. We assume that four prescribed directions will be considered to manufacture the obtained compliant mechanism design, and let the prescribed directions be denoted as d_1, d_2, d_3 and d_4 , as shown in Fig. 4.20. The regularization parameter τ was

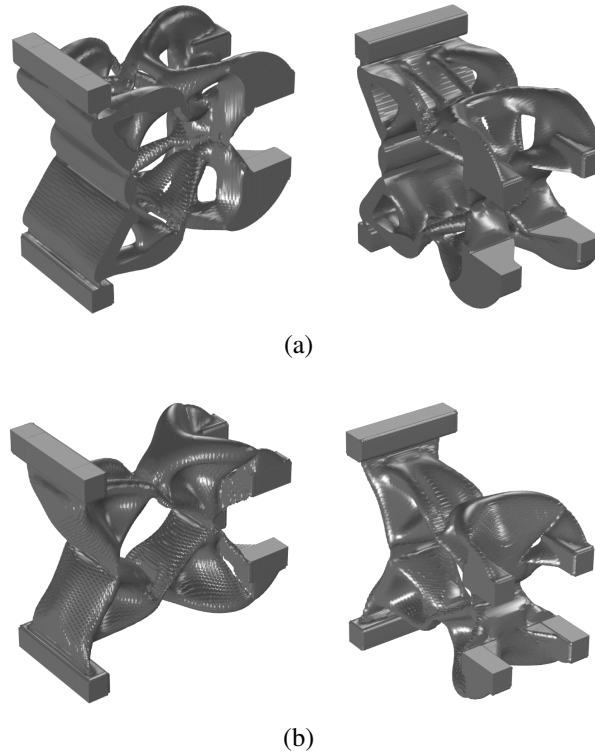


Fig. 4.21 Optimal configurations for the optimum design problem of a compliant mechanism obtained (a) without the manufacturing constraint (2.66×10^{-10} J); and (b) with manufacturing constraint imposed (2.43×10^{-10} J). Values in parentheses indicate the mutual mean compliance values.

set to 1×10^{-4} . Due to the symmetry of the design model and the definition of the fixed design domain, we introduce three fictitious physical models that correspond to prescribed directions $\mathbf{d}_1$, $\mathbf{d}_2$, and $\mathbf{d}_3$. In the fictitious physical models defined in (4.1), parameters were set as $\epsilon = 10^{-2}$, $V = 100$, and $\beta = 1000$. The weighting coefficient γ was set to 5.

Figure 4.21 shows the obtained optimal configurations. The optimal solution shown in Fig. 4.21(a) obtained when focusing only on improvement of the physical performance has a larger mutual mean compliance than that of the result shown in Fig. 4.21(b) that was obtained considering the manufacturability. However, the optimal solution obtained when considering the manufacturability has a simpler structure than that obtained without the manufacturing constraint imposed, which facilitates manufacturing by molding and milling.

Figure 4.22 shows the mold parts for manufacturing the optimal configuration shown in Fig. 4.21(b). *Mold part 4*, whose parting direction is $\mathbf{d}_4$, is identical to that shown in Fig. 4.22(c) due to the symmetry of the fixed design domain. The shapes of the mold parts

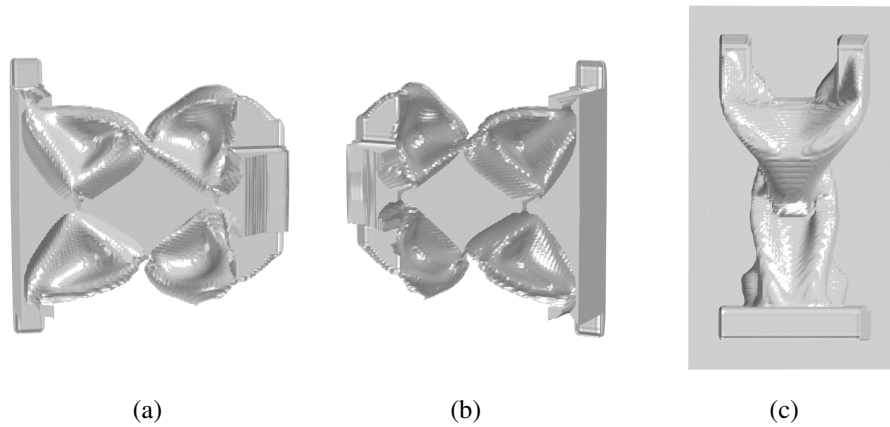


Fig. 4.22 Mold parts and parting directions for manufacturing the optimal configuration obtained with manufacturing constraint imposed: (a) d_1 (*Mold part 1*); (b) d_2 (*Mold part 2*); (c) d_3 (*Mold part 3*).

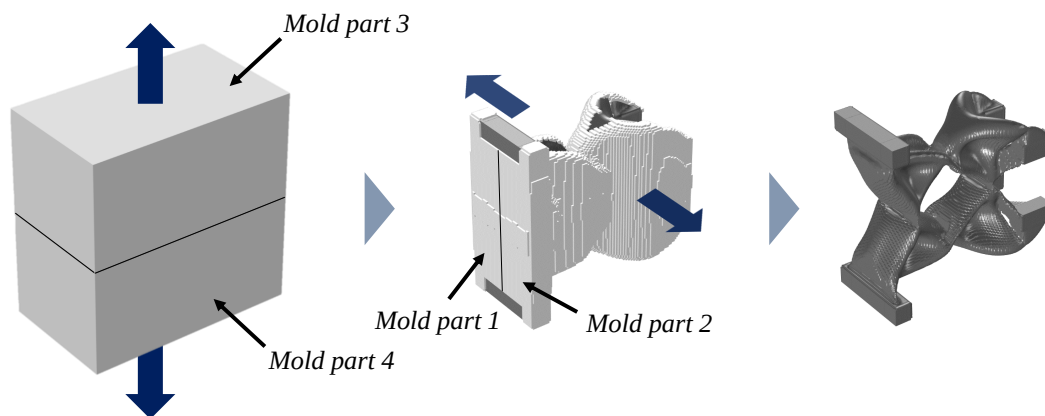


Fig. 4.23 Sequential separation of molds parts.

are obtained using (4.5). As mentioned in Section 4.2.2, when certain domains intersect, such domains can be included in any relevant mold part. Here, the order in which the mold parts are separated depends on which intersecting domains are included in particular mold parts. In the example shown in Fig. 4.22, *Mold part 3* consists of M_3 , *Mold part 1* consists of $(M_1 \cap D_{y^+}) \setminus M_3$, and *Mold part 2* consists of $(M_2 \cap D_{y^-}) \setminus M_3$, where D_{y^+} and D_{y^-} are

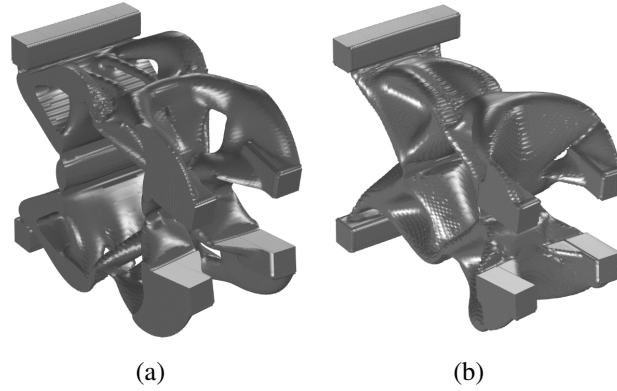


Fig. 4.24 Deformed shapes of optimal configurations for the optimum design problem for a compliant mechanism obtained (a) without the manufacturing constraint; (b) with the manufacturing constraint.

defined as follows:

$$D_{y^+} = \{\mathbf{V}\mathbf{x} \in D \mid y \geq 0\}, \quad (4.22)$$

$$D_{y^-} = \{\mathbf{V}\mathbf{x} \in D \mid y < 0\}, \quad (4.23)$$

where $y = 0$ at the center of the design model. In the current case, the order in which the mold parts are parted from the cast object is illustrated in Fig. 4.23. First, *Mold part 3* and *Mold part 4* are parted and then *Mold part 1* and *Mold part 2* are parted. That is, *Mold part 1* and *Mold part 2* operate as casting cores, and the optimal configuration obtained considering the manufacturing constraint is appropriate for manufacture by molding. Note that this mold part design does not include gates, through which molten material enters the mold.

Figure 4.24 shows the deformed shapes of the two examples of the compliant mechanism three-dimensional design problem. As shown, the optimal configuration obtained when the manufacturing constraint is imposed deforms in the specified direction, confirming the utility of the proposed method.

4.5 Summary

This chapter presented a method for evaluating the manufacturability of designs when using molding and milling, based on the use of fictitious physical models, and extended it to a

scheme for imposing a manufacturing constraint within a topology optimization procedure. We achieved the following:

1. The geometrical requirements for manufacturability using molding and milling were clarified, so that design engineers could ensure that the components do not incorporate undercuts or interior voids.
2. Fictitious physical models were introduced to implicitly represent the manufacturability when using molding and milling techniques. The fictitious physical models were mathematically described using advection-diffusion equations. A manufacturing constraint for use in a structural optimization process was then formulated using the fictitious physical models.
3. In the numerical implementation, an optimization algorithm was constructed and the non-dimensional sensitivity was used to enable simple adjustment of a weighting coefficient.
4. Two- and three-dimensional numerical examples were provided. The dependencies of the distribution of the fictitious physical fields on the setting of advection velocity V and parameter β were examined. The proposed method was then applied to topology optimization design problems and obtained manufacturable optimal configurations.
5. In two-dimensional design problems, optimal configurations obtained for each numerical example demonstrated a very low dependency on the setting of the weighting coefficient (parameter γ), and the initial configurations. Also, we confirmed that the proposed method can obtain optimal configurations depending on the setting of the prescribed directions.
6. In the minimum mean compliance problem, the proposed method provided an optimal configuration that was manufacturable and had the lowest mean compliance except for the optimal configuration where a manufacturing constraint was not imposed, which could not be manufactured. Furthermore, we demonstrated that the proposed method can set the location of the parting line relative to mold parts prior to the optimization procedure.
7. An optimal design for a compliant mechanism to be manufactured using a four-part mold was obtained. The obtained optimal configuration deformed in the specified direction even though the manufacturing constraint was imposed.

Chapter 5

Reliability-based topology optimization under geometrical uncertainty

5.1 Introduction

The industrial application of topology optimization methodologies has attracted much attention for at least a decade. In a topology optimization, consideration of uncertainties in attributes such as load magnitudes and directions, material properties, and shapes, seeks to take into account particular manufacturing situations or usage environments. Geometrical uncertainties arising from manufacturing errors and operational wear may directly affect the physical performance of various devices. Geometrical uncertainties can cause particularly large effects in micro fabrication processes for micro electro mechanical systems (MEMS), due the small geometrical scale. However, since the physical performance of a device depends on the details of its shape in implicit and highly non-linear ways, design engineers can seldom predict the effects of geometrical variations and therefore must modify a design manually to improve it, a time-consuming process. Thus, there is a great need for structural design methods that efficiently consider geometrical uncertainties during the optimization stage.

Optimizations considering uncertainty are mainly classified into robust optimizations and reliability-based optimizations. In robust approaches, the mean and the variance of the response of a device or system is usually minimized so that the response becomes less sensitive to the particular uncertainty. Previous research related to robust topology optimization has considered uncertainties in load directions [164], and the load magnitudes

and location where a load is applied [165]. [166] proposed a topology optimization method that takes into account the spatially varying uncertainty in a material property in addition to uncertainty in the direction of an applied load, based on the Karhunen-Loève (K-L) expansion, and this work was extended to topology optimization under geometrical uncertainty as mentioned below.

Robust topology optimization methods under geometrical uncertainty have also been proposed. Sigmund [167] proposed a robust optimization formulation that considered two uniform geometrical variations, i.e., eroded and dilated, using projections with different thresholds. This method was extended to accommodate non-uniform variations by Schevenels *et al.* [168], with spatially varying thresholds used in a Heaviside projection and thresholds generated with a Monte Carlo method. Lazarov *et al.* [169] also proposed a method considering non-uniform variations, in which a K-L expansion was used to represent a random field for a threshold, using a finite number of random variables so that the perturbation with respect to these variables yielded additional linear systems amenable to solution without relying on a Monte Carlo method. In these methods, geometrical variations are represented relatively easily as spatially varying thresholds, with the magnitude of erosion or dilation depending on the length scale and radius of an applied density filter.

On the other hand, Jansen *et al.* [170] proposed a geometrical uncertainty modeling by shifting the center of the density filter kernel using the random perturbation vector, in which the mean and the standard deviation of the performance and their sensitivities were computed by the Monte Carlo method. This method has an advantage, compared to the above threshold based schemes, of the ability to model relatively large uncertain geometrical variations, owing to the Eulerian description. The research group also proposed a Lagrangian approach for sufficiently small geometrical variations by representing them as shifts of the finite element nodes, incorporating geometric non-linearities in the robust topology optimization [171]. This Lagrangian approach makes the analytical derivation of the sensitivities much more complex, so they incorporated a semi-analytical approach in which the derivatives of the finite element matrices are computed using finite differences. In a level set-based approach, Guo *et al.* [172] proposed a level set-based structural optimization method considering boundary uncertainties by assuming that the boundary perturbations are small enough to allow approximation of the objective function using a first-order Taylor expansion. Chen and Chen [173] proposed a level set-based robust shape and topology optimization in which geometrical variations were modeled by advection of the level set function with random

normal velocities applied on the boundaries extracted as a zero level set, and the statistical moments of performance were evaluated using a Gauss quadrature formula, with evaluation of the objective function required at each quadrature point. Zhang and Kang [174] proposed a robust shape and topology optimization with stochastic level set perturbation in which geometrical variations were represented by the finite random perturbation applied to the level set function. This method can consider the geometrical variations that create a new hole. The perturbation approaches in the level set method were also applied with the extended finite element method (X-FEM) [175, 176].

Reliability-based design optimization (RBDO) is another powerful approach for considering uncertainties, and is applied in a topology optimization [177] in which external loads and geometric dimensions are considered as random variables. In RBDO, limit state functions describing safe and failure states are introduced and the failure probability calculated with these functions is minimized. There are several methods to evaluate failure probabilities, including Monte Carlo simulation (MCS) [178, 179], surrogate models [180, 181], the first-order reliability method (FORM) [182], and the second-order reliability method (SORM) [183]. A MCS is relatively accurate but computationally expensive; the FORM is the most popular method for estimating failure probability, due to its simplicity and efficiency.

Based on such reliability analyses, RBDO problems are usually formulated as two-level nested optimization problems. The FORM uses the reliability index approach (RIA), in which probabilistic constraints are evaluated at the most probable failure point (MPFP), searched for in the inner loop of the optimization procedure. On the other hand, the performance measure approach (PMA) [184] is more stable and efficient than the RIA for evaluating probabilistic constraints [185, 186]. In the PMA, probabilistic constraints are evaluated at the minimum performance target point (MPTP), searched for in the inner loop of the optimization procedure.

One difficulty with the RBDO approach stems from its inherent double-loop structure that incurs high computational cost. Single-loop approaches offer alternatives, such as the single-loop single-vector (SLSV) method [187, 188] in which the probabilistic constraint is replaced by an equivalent deterministic constraint. These methods are very efficient for solving RBDO problems that have linear or moderately non-linear limit state functions. On the other hand, in PMAs, several methods have been proposed to improve the robustness and efficiency of MPTP searches, even for problems that have non-linear performance functions [189–191].

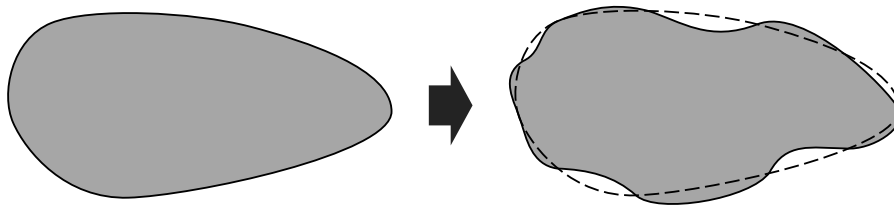


Fig. 5.1 Schematic of unperturbed and perturbed shapes.

Recently, a reliability-based topology optimization method under geometrical uncertainty has also been proposed [192]. This method was based on the PMA, incorporating the random threshold projection and the polynomial chaos expansion to represent the geometrical variations and then to evaluate the stochastic structural response, and successfully obtained the optimized solutions according to the target reliability settings. However, only relatively small geometrical variations were allowed in this method due to the use of the random threshold projection, as pointed out in [170].

In this chapter, we propose a method for reliability-based topology optimization under geometrical uncertainties that employs an inverse reliability method based on a PMA and a two-level nested algorithm in the optimization procedure. The proposed method uses an Eulerian description for geometrical variations that does not require the assumption that shape variations are sufficiently small. Consequently, we model geometrical variations with an advection equation in which the advection velocity is given as a random field and represents the magnitude and direction of the variations. Therefore, the advection equation used in the optimization problems here is applied to geometrical variations in addition to physical equilibrium equations, which now depend on the advection equation because physical equilibrium states for perturbed shapes are the focus. Although this yields a complicated dependency of the objective function on design variables, sensitivities for both MPTP searches and the topology optimization can be derived systematically using the adjoint variable method, owing to the implicit description of the geometrical variations in the advection equation.

5.2 Formulation of reliability for shape uncertainty

5.2.1 Shape uncertainty modeled in an Eulerian description

To formulate a reliability topology optimization problem considering geometrical uncertainties, they must first be modeled mathematically. Figure 5.1 is a schematic representation of geometrical variation. Lagrangian and Eulerian descriptions are two possible candidates for modeling such variation. In a Lagrangian description, variations are represented as trajectories of points, such as the nodes of a finite element mesh, and an assumption that variations are sufficiently small is usually required to avoid mesh distortions. On the other hand, in an Eulerian description, the variations are represented by a variation field observed at spatially fixed points. Since a structural configuration is implicitly represented by the characteristic function in a topology optimization, the Eulerian description is especially suitable for modeling geometrical variations, so we use it here. We considered the material derivative of the normalized density in Eulerian description. Shape variations are then formulated with a fictitious advection equation for a normalized density θ with a random velocity $\mathbf{V}(\mathbf{x})$ as follows:

$$\frac{D\theta}{Dt} = \frac{\partial\theta(\mathbf{x},t)}{\partial t} + \mathbf{V}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x},t) = 0, \quad (5.1)$$

where $D\theta/Dt$ represents the material derivative and $\mathbf{V}(\mathbf{x})$ corresponds to the motion of the material coordinates, $\partial\mathbf{x}/\partial t$. The magnitude of the variations in shape can therefore be evaluated according to the magnitude of $\mathbf{V}(\mathbf{x})$ velocity. Considering the initial and boundary conditions for this fictitious advection equation, the uncertain shape variations are modeled as

$$\begin{cases} \frac{\partial\theta(\mathbf{x},t)}{\partial t} + \mathbf{V}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x},t) = 0 & \text{for } (\mathbf{x},t) \in D \times [0,T] \\ \mathbf{n}(\mathbf{x}) \cdot \nabla\theta(\mathbf{x},t) = 0 & \text{for } (\mathbf{x},t) \in \Gamma_- \times [0,T] \\ \theta(\mathbf{x},0) = \bar{\theta}(\mathbf{x}) & \text{for } \mathbf{x} \in D, \end{cases} \quad (5.2)$$

where T is a final time, $\mathbf{n}$ is a normal vector pointing outward and $\Gamma_- = \partial D|_{\mathbf{V} \cdot \mathbf{n} < 0}$. In the present study, we assume that the components of random velocity field $\mathbf{V}(\mathbf{x})$ are independent of each other and are Gaussian with a zero average. The Gaussian function is usually used to model a random error and has been applied to shape uncertainty modeling in the previous research [170, 171, 173]. Even though the Gaussian function is unbounded, it can also be used to model truncated normal distributions which are bounded, when the truncation occurs at the tail region [193]. On the other hand, another assumption can be found in literature

[168, 169, 192] in which the geometrical variations are represented by the random threshold projection and the probability density is assumed to be uniformly distributed in an interval.

5.2.2 Karhunen-Loève expansion

To express the random velocity field using uncorrelated random variables, we apply the Karhunen-Loève (K-L) expansion [194], a series expansion method that represents a continuous random field, $Y(\mathbf{x}, \vartheta)$, as follows:

$$Y(\mathbf{x}, \vartheta) = \mu(\mathbf{x}) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \psi_i(\mathbf{x}) \xi_i(\vartheta), \quad (5.3)$$

where $\mathbf{x} \in D$ is a spatial coordinate, $\vartheta \in \Theta$ is a coordinate in the sample space Θ , $\mu(\mathbf{x})$ is the mean function of the random field, and ξ_i are standard normal mutually uncorrelated random variables. λ_i and ψ_i are the eigenvalue and eigenfunctions of the autocovariance function of the random field, obtained by solving the following homogeneous Fredholm integral equation of the second kind:

$$\int_D \text{Cov}(\mathbf{x}, \mathbf{x}') \psi_i(\mathbf{x}') d\mathbf{x}' = \lambda_i \psi_i(\mathbf{x}), \quad (5.4)$$

where $\text{Cov}(\mathbf{x}, \mathbf{x}')$ is an autocovariance function, modeled in this study using a Gaussian function as follows:

$$\text{Cov}(\mathbf{x}, \mathbf{x}') = \sigma(\mathbf{x}) \sigma(\mathbf{x}') \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{l_C^2}\right), \quad (5.5)$$

where l_C is the correlation length and $\sigma(\mathbf{x})$ is the standard deviation at coordinate $\mathbf{x}$. Numerical methods for discretization of the continuous form of the eigenvalue problem in (5.4) were discussed in detail by [194]. We use the finite element method to solve the problem, projecting the autocovariance function onto the space spanned by the shape function N as

$$\text{Cov}(\mathbf{x}, \mathbf{x}') \approx N(\mathbf{x})^T \mathbf{K} N(\mathbf{x}'), \quad (5.6)$$

where $\mathbf{K}$ is the matrix whose components $k_{ij} = \text{Cov}(\mathbf{x}_i, \mathbf{x}_j)$ with $\mathbf{x}_i$ and $\mathbf{x}_j$ denoting the coordinates of the finite element nodes.

The above K-L expansion can then be approximated using a finite number of terms by sorting the eigenvalues λ_i and their corresponding eigenfunctions ψ_i in a descending order

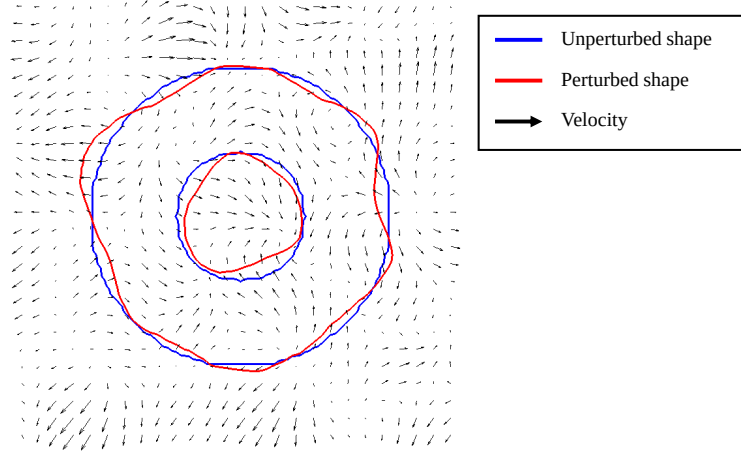


Fig. 5.2 A schematic of a perturbed shape by advection.

and truncating the series as follows:

$$Y(\mathbf{x}, \vartheta) = \mu(\mathbf{x}) + \sum_{i=1}^M \sqrt{\lambda_i} \psi_i(\mathbf{x}) \xi_i(\vartheta), \quad (5.7)$$

where M is the number of terms of the truncated K-L expansion. The error due to the truncation can be evaluated as

$$\varepsilon_{\text{KL}} = 1 - \frac{1}{\int_D \sigma(\mathbf{x})^2 dD} \sum_{i=1}^M \lambda_i, \quad (5.8)$$

and set ε_{KL} is set as 0.1 in this study. Using the K-L expansion, the random velocity field can be approximated as

$$\mathbf{V}(\mathbf{x}, \vartheta) = \sum_{j=1}^d V_j(\mathbf{x}, \vartheta) \mathbf{e}_j = \sum_{j=1}^d \sum_{i=1}^M \sqrt{\lambda_i} \psi_i(\mathbf{x}) \xi_i^j(\vartheta) \mathbf{e}_j, \quad (5.9)$$

where $\mathbf{e}_j$ represents the basis vectors of the canonical coordinate and d is the number of spatial dimensions. Figure 5.2 illustrates a perturbed shape by the proposed geometrical uncertainty modeling using Eulerian description where the circular shape is perturbed by advection whose velocity is given by (5.9).

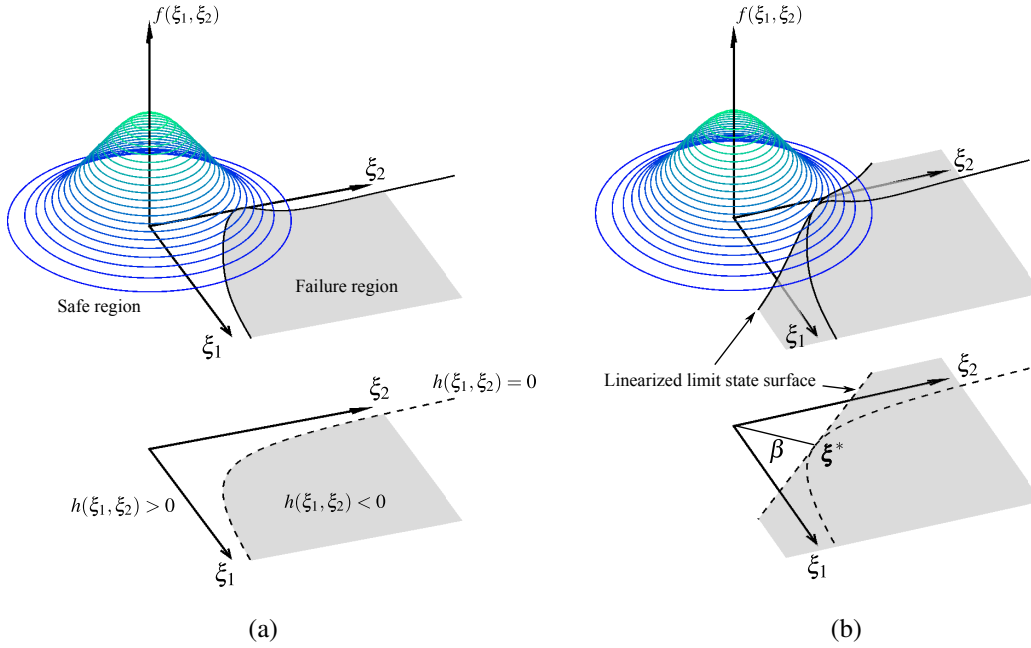


Fig. 5.3 Standard Gaussian probability density function: (a) limit state function; (b) linearized limit state function.

5.2.3 Inverse reliability method

Reliability can be theoretically defined as the probability of a desired state continuing in time, i.e., the probability of non-failure. The limit state of failure is represented as a function, g , called the limit state function, of stochastic variables $\mathbf{z}$ in which the safe state is represented as $g(\mathbf{z}) > 0$ and the failure state is $g(\mathbf{z}) < 0$. The isosurface of $g(\mathbf{z}) = 0$ is called the limit state surface. The probability of failure, P_f , can be evaluated using the joint probability density function $f(\mathbf{z})$ and the limit state function $g(\mathbf{z})$ as follows:

$$P_f = P(g(\mathbf{z}) < 0) = \int_{g(\mathbf{z}) < 0} f(\mathbf{z}) d\mathbf{z}. \quad (5.10)$$

Reliability P_r is evaluated as $P_r = 1 - P_f$. However, the complexity of $f(\mathbf{z})$ and $g(\mathbf{z})$ makes it computationally expensive to evaluate (5.10), so the first order reliability method (FORM) is often used, in which the limit state function is linearly approximated.

Reliability index approach

The FORM is usually used in a RIA. In a FORM, stochastic variables $\mathbf{z}$ are converted into independent standard Gaussian stochastic variables $\boldsymbol{\xi}$, and the limit state function in $\boldsymbol{\xi}$ -space is then linearized at the design point, also called the most probable failure point (MPFP) $\boldsymbol{\xi}^*$, which is the nearest point on the limit state surface from the origin of $\boldsymbol{\xi}$ -space. Figure 5.3 illustrates an example of a linearized limit state function in 2-D $\boldsymbol{\xi}$ -space where $h(\boldsymbol{\xi})$ is the limit state function in $\boldsymbol{\xi}$ -space. The probability of failure is then approximated using the standard Gaussian function, namely,

$$P_f = \Phi(-\beta) = \int_{-\infty}^{-\beta} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\xi^2\right) d\xi, \quad (5.11)$$

where β , called a reliability index, is the distance from the origin to the design point, obtained by solving the following problem:

$$\beta = \min_{\boldsymbol{\xi}} \|\boldsymbol{\xi}\| \quad \text{subject to } h(\boldsymbol{\xi}) = 0. \quad (5.12)$$

The reliability constraint can then be imposed via β as

$$\beta \geq \Phi^{-1}(\bar{P}_r), \quad (5.13)$$

where $\bar{P}_r$ is the lower limit of reliability.

Performance measure approach

In contrast to a RIA, a performance measure approach (PMA) replaces a probabilistic constraint with a constraint with respect to the minimum performance on the hypersphere in $\boldsymbol{\xi}$ -space, which represents the target reliability index. That is, the point, called the minimum performance target point (MPTP), on a hypersphere of radius β_T where the limit state function is minimized, is searched using

$$h_{\min} = \min_{\boldsymbol{\xi}} h(\boldsymbol{\xi}) \quad \text{subject to } \|\boldsymbol{\xi}\| = \beta_T = \Phi^{-1}(\bar{P}_r), \quad (5.14)$$

with the reliability constraint imposed as

$$h_{\min} \geq 0. \quad (5.15)$$

If reliability index β corresponds to target reliability index β_T , the most probable failure point (MPFP) corresponds to the MPTP.

In this study, shape uncertainty is represented using independent Gaussian random variables via an advection equation and K-L expansion, as mentioned previously in sections 5.2.1 and 5.2.2. Therefore, ξ -space is formed by setting

$$\xi = [\xi_1^1, \xi_2^1, \dots, \xi_M^1, \xi_1^2, \dots, \xi_M^d]. \quad (5.16)$$

5.3 Formulation of optimization problems

5.3.1 Minimum mean compliance problem

Consider that a traction $\mathbf{t}$ is applied to boundary Γ_t of a fixed design domain and displacement $\mathbf{u}$ is fixed at boundary Γ_u . We first consider a reliability-based topology optimization for a mean compliance problem. That is, based on the mean compliance, the limit state function must be defined as

$$h(\xi) = c - \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{u} d\Gamma, \quad (5.17)$$

where c is the threshold distinguishing a safe state from failure and the second term is the mean compliance. However, the lack of local information such as stress makes it difficult to determine this threshold according to the mean compliance. In the previous study [192], this threshold was empirically determined. In the present study, on the other hand, we set the threshold as the objective function, instead of setting it in advance. The smaller the threshold value c is, the more the state is likely to become failure. Consequently, minimizing c under the reliability constraint yields the solution with maximum performance ensuring the target reliability index. Therefore, the optimization problem under a volume constraint can be formulated, as follows:

$$\inf_{\hat{\varphi} \in L^\infty(D; [-1, 1])} F = c \quad (5.18)$$

subject to:

$$\min_{\xi \in \mathcal{S}} h(\xi, \mathbf{u}, \hat{\varphi}) \geq 0, \quad (5.19)$$

$$\int_D \theta(\mathbf{x}, 0) dD - V_{\max} \leq 0, \quad (5.20)$$

with

$$h(\xi, \mathbf{u}, \hat{\varphi}) = c - \int_{\Gamma_t} \mathbf{t} \cdot \mathbf{u} d\Gamma, \quad (5.21)$$

where S represents a hypersphere of radius β_T and $V_{\max}$ is the upper limit of the allowable volume. Assuming a linear elasticity for elastic tensor $\mathbf{C}$ and small strain tensor $\boldsymbol{\varepsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$, the displacement $\mathbf{u} \in \mathcal{U}$ satisfies the following variational formulation:

$$\int_{\Gamma_t} \mathbf{t} \cdot \tilde{\mathbf{u}} d\Gamma - \int_D \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}) : \mathbf{C} \theta(\mathbf{x}, T)^p : \boldsymbol{\varepsilon}(\mathbf{u}) dD = 0, \quad (5.22)$$

for all variables $\tilde{\mathbf{u}} \in \mathcal{U}$, with space $\mathcal{U}$ defined as

$$\mathcal{U} = \{\tilde{\mathbf{u}} \in H^1(D)^d \mid \tilde{\mathbf{u}} = 0 \text{ on } \Gamma_u\}, \quad (5.23)$$

where H^1 is a Sobolev space.

5.3.2 Optimum design problem for a compliant mechanism

Consider again that a traction $\mathbf{t}$ is applied to boundary Γ_t of the fixed design domain and displacement $\mathbf{u}$ is fixed at boundary Γ_u . We now formulate a reliability-based topology optimization problem for the optimum design of a compliant mechanism. As was the case for the minimum mean compliance problem, the optimization problem is formulated by setting the threshold of the limit state function as the objective function, as follows:

$$\inf_{\hat{\varphi} \in L^\infty(D; [-1, 1])} \quad F = -c \quad (5.24)$$

subject to:

$$\min_{\xi \in S} h(\xi, \mathbf{u}, \hat{\varphi}) \geq 0, \quad (5.25)$$

$$\int_D \theta(\mathbf{x}, 0) dD - V_{\max} \leq 0, \quad (5.26)$$

with

$$h(\xi, \mathbf{u}, \hat{\varphi}) = \int_{\Gamma_{\text{out}}} \mathbf{e} \cdot \mathbf{u} d\Gamma - c, \quad (5.27)$$

where Γ_{out} denotes the location where the displacement is to be maximized and $\mathbf{e}$ the direction in which the displacement is to be maximized. The first term in (5.27) is a mutual mean compliance which represents the elastic compliance of the structure for the desired direction

e and is maximized in usual deterministic optimization. The larger the threshold value c in (5.27) is, the more the state is likely to become failure. Consequently, maximizing c under the reliability constraint yields the solution with maximum performance ensuring the target reliability index. Therefore, the optimization problem is formulated as a maximization problem by adding the minus sign to the objective function. Assuming a linear elasticity, displacement $\mathbf{u} \in \mathcal{U}$ satisfies the following variational formulation,

$$\int_{\Gamma_i} \mathbf{t} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_i} k_{\text{in}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma - \int_{\Gamma_{\text{out}}} k_{\text{out}} \mathbf{u} \cdot \tilde{\mathbf{u}} d\Gamma - \int_D \varepsilon(\tilde{\mathbf{u}}) : \mathbf{C}\theta(\mathbf{x}, T)^p : \varepsilon(\mathbf{u}) dD = 0, \quad (5.28)$$

for all variables $\tilde{\mathbf{u}} \in \mathcal{U}$, where k_{in} and k_{out} are parameters for Robin boundary conditions imposed to ensure the stiffness of the obtained configurations.

5.3.3 Filtering of the standard deviation function

The proposed method expresses shape variations using an advection scheme. If locations where loads are applied are allowed to be perturbed, the influence of shape variations on the loading conditions must be considered. For simplicity in the present study, we assume that variations in the boundaries where the loads are applied are very small, i.e., the standard deviation $\sigma(\mathbf{x})$ is sufficiently small at these boundaries. For numerical stability, the standard deviation $\sigma(\mathbf{x})$ for the entire domain is calculated using the Helmholtz-type of PDE filter, as follows:

$$\int_D (\tilde{\sigma} \sigma_0 - l_\sigma^2 \nabla \tilde{\sigma} \cdot \nabla \sigma - \tilde{\sigma} \sigma) dD = 0, \quad (5.29)$$

for $\sigma \in \mathfrak{S}$ and all variables $\tilde{\sigma} \in \tilde{\mathfrak{S}}$, with

$$\mathfrak{S} = \{\sigma \in H^1(D) \mid \tilde{\sigma} = \sigma_0 \epsilon \text{ on } \Gamma_\sigma\} \quad (5.30)$$

$$\tilde{\mathfrak{S}} = \{\tilde{\sigma} \in H^1(D) \mid \tilde{\sigma} = 0 \text{ on } \Gamma_\sigma\}, \quad (5.31)$$

where l_σ is a parameter determining the degree of smoothing, σ_0 is the characteristic standard deviation, and ϵ is a sufficiently small positive number, set as 10^{-4} in this study. Since the magnitude of $\sigma(\mathbf{x})$ is determined by that of σ_0 , the parameter σ_0 determines the degrees of the standard deviation for the shape uncertainty. Consequently, this value should be adjusted to represent the standard deviation in the certain manufacturing process or usage environment which is focused on. However, this chapter focuses on the construction of a reliability-based topology optimization under shape uncertainty and does not focus on the particular manufac-

turing process or usage environment. Therefore, this parameter is empirically determined to $\sigma_0 = 2$ in the present study. The parameter l_σ is also empirically set to $0.1L$ where L is the characteristic length of the design domain. $\Gamma_\sigma = \Gamma_t$ for the minimum mean compliance problem, and $\Gamma_\sigma = \Gamma_t \cup \Gamma_{\text{out}}$ for the compliant mechanism optimum design problem.

5.4 Numerical implementation

5.4.1 MPTP search algorithm

Several methods have been proposed to search for the MPTP during the inner loop of the optimization procedure, such as the advanced mean value, conjugate mean value, and hybrid mean value methods [195], the conjugate gradient method [190], and hybrid chaos control method [189]. In the present study, to stably handle geometrical uncertainties that yield highly non-linear limit state functions, we introduce a step size, s , into the advanced mean value method, in a manner similar to the scheme adopted in previous research [191], and use the following update formula:

$$\xi^n = \beta_T \frac{\tilde{\xi}^n}{\|\tilde{\xi}^n\|_{L^2}}, \quad (5.32)$$

with

$$\tilde{\xi}^n = (1-s)\xi^{n-1} - s\beta_T \frac{\nabla_\xi h(\xi^{n-1}, \mathbf{u}, \hat{\phi})}{\|\nabla_\xi h(\xi^{n-1}, \mathbf{u}, \hat{\phi})\|_{L^2}}, \quad (5.33)$$

where ξ^n represents ξ at the n th inner iteration. When $s = 1$, the above update formula corresponds to that used in the advanced mean value method. The following is the MPTP search algorithm we employ:

- **Step 1:** Set the initial value of ξ as $\xi^0 = \mathbf{0}$ and the iteration counter with $n = 1$.
- **Step 2:** Set the step size as $s = 1$.
- **Step 3:** Solve the advection equation in (5.2) with the finite difference method.
- **Step 4:** Solve the governing equation with the finite element method.
- **Step 5:** Compute a new value for performance function h^{n+1} .
- **Step 6:** If $h^{n+1} > h^n$, then set $s \leftarrow 0.5s$ and proceed to Step 8. Otherwise set $s = 1$, $n \leftarrow n + 1$ and proceed to Step 7.

- **Step 7:** Compute the sensitivities of the performance function based on the adjoint variable method, as explained in Appendix A.4.
- **Step 8:** Update ξ using the update formula in (5.32).
- **Step 9:** If the change in ξ is sufficiently small and satisfies

$$\frac{\|\xi^n - \xi^{n-1}\|_{L^2}}{\beta_T} \leq \varepsilon_{\text{inner}}, \quad (5.34)$$

the MPTP search halts, otherwise return to Step 3.

Due to the local search strategy, this algorithm can obtain only one solution even if there are several MPTP points. However, the local search-based reliability analysis is still a powerful approach to obtain a candidate of the MPTP efficiently and has widely been used in previous research [191, 192]. We hope to address the issue in our future research.

5.4.2 Optimization algorithm

The optimization algorithm is now described:

- **Step 1:** Perform the K-L expansion with the finite element method to obtain ψ_i and λ_i for $i = 1, 2, \dots, M$, where M is determined as the minimum value satisfying $\varepsilon_{\text{KL}} \leq \overline{\varepsilon_{\text{KL}}}$. $\overline{\varepsilon_{\text{KL}}}$ is the allowable error of the truncated K-L expansion.
- **Step 2:** Set initial values for $\hat{\phi}$.
- **Step 3:** Apply the PDE filter to $\hat{\phi}$ with the finite element method.
- **Step 4:** Perform the MPTP search in the inner loop as described above.
- **Step 5:** Compute the design sensitivity based on the adjoint variable method as described in Appendix A.4.
- **Step 6:** Update the design variables $\hat{\phi}$ using the method of moving asymptotes (MMA) [31].
- **Step 7:** If the change in the design variables is sufficiently small and satisfies

$$\frac{\|\hat{\phi}^n - \hat{\phi}^{n-1}\|_{L^2(D)}}{\|\hat{\phi}^n\|_{L^2(D)}} \leq \varepsilon_{\text{opt}}, \quad (5.35)$$

where $\hat{\phi}^n$ represents $\hat{\phi}$ at the n th outer iteration, the optimization procedure halts, otherwise return to Step 3.

In the present study, to achieve an almost 0–1 density in the optimized solutions, the continuation scheme is applied. In the continuation scheme, parameter α_h for the Heaviside projection was initially set to 10. Once the optimization procedure converged, the parameter was increased by 5 and the optimization procedure restarted. This continuation scheme was applied until the parameter α_h reached 25. The convergence criteria for the inner and outer loops were set with $\varepsilon_{\text{inner}} = 1 \times 10^{-4}$ and $\varepsilon_{\text{opt}} = 1 \times 10^{-3}$, respectively.

5.5 Numerical examples

5.5.1 Verification by Monte Carlo Simulation

First, the accuracy of the PMA is examined by comparing the failure probability estimated by the proposed method and the Monte Carlo Simulation (MCS), via the minimum mean compliance problem formulated in Section 5.3.1. To make the failure probability estimated by the MCS be sufficiently close to the true value, more random samples are required as the true failure probability gets smaller. That is, the larger the target reliability index is in the PMA, the more iterations in the MCS would be required to verify the accuracy of the PMA by the MCS. In terms of the computational cost of the MCS, we set β_T up to 3 for comparison, and 10^5 samples were used for each MCS.

Figure 5.4 shows the fixed design domain and boundary conditions. Since the design model is symmetrical, only the right half was considered as the design domain. For application of the finite element method, the design domain was discretized into 200×100 first-order quadrilateral elements. When applying the finite difference method, the Lax-Wendroff method was used, which is an explicit scheme and is suitable for straightforward parallel computation. For application of the Lax-Wendroff scheme, the fixed design domain was discretized into a 201×101 grid, with spatial steps in both directions of $\Delta x = 1.0$ and time steps of $\Delta t = \min(0.2, 0.5 \Delta t_{\text{CFL}})$, where Δt_{CFL} is the maximum time step satisfying the CFL condition. The minmod function was adopted as the flux limiter. The upper limit of the allowable volume was set to 40% of the volume of the fixed design domain. The PDE filter parameter was set to $R = 1.5$. The final time for the advection was set to $T = 1$, which implies that the magnitude of velocity $V(\mathbf{x})$ represents the magnitude of the shape variations.

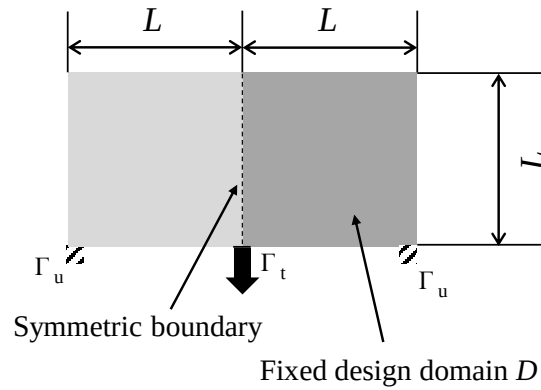


Fig. 5.4 Fixed design domain and boundary conditions for bridge design problem.

	$l_C = L$	$l_C = 0.5L$	$l_C = 0.1L$
$\beta_T = 1$			
$\beta_T = 3$			

Fig. 5.5 Obtained optimized configurations.

Table 5.1 Comparison between PMA and MCS.

β_T values for optimization	Case 1 where $l_C = L$		Case 2 where $l_C = 0.5L$		Case 3 where $l_C = 0.1L$	
	β_{MCS}	$\widehat{Cov}$	β_{MCS}	$\widehat{Cov}$	β_{MCS}	$\widehat{Cov}$
1.0	0.50	4.8×10^{-3}	0.29	4.0×10^{-3}	-0.60	1.9×10^{-3}
1.5	1.08	7.9×10^{-3}	0.88	6.6×10^{-3}	-0.10	2.9×10^{-3}
2.0	1.61	1.3×10^{-2}	1.38	1.0×10^{-2}	0.36	4.2×10^{-3}
2.5	2.00	2.1×10^{-2}	1.79	1.6×10^{-2}	0.82	6.2×10^{-3}
3.0	2.32	3.1×10^{-2}	2.11	2.4×10^{-2}	1.30	9.7×10^{-3}

In other words, the standard deviation of the shape variation at each point is approximately $\sigma(\mathbf{x})$.

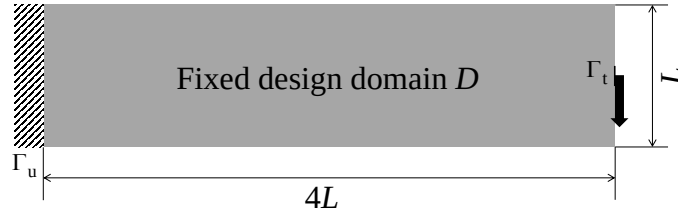


Fig. 5.6 Fixed design domain and boundary conditions for cantilever design problem.

Figure 5.5 illustrates some of the optimized configurations obtained for various values of β_T and l_C . All configurations have the same topology, but the size of the interior voids is different depending on the parameter settings. Table 5.1 lists the reliability index β_{MCS} calculated by the MCS performed to the optimized configurations obtained by the proposed method, and the coefficient of variation on the estimated failure probability, $\widehat{Cov}$. Since the coefficient of variation on the estimated failure probability, $\widehat{Cov}$, is sufficiently small, it is confirmed that the failure probability calculated by the MCS is close to the true value. This table implies that the PMA overestimates the reliability. This would be resulted from high nonlinearity of the limit state function on the geometrical variations. However, the relative relation of the reliability index between the PMA and the MCS agrees with each other. Therefore, the proposed method using the the PMA can efficiently and qualitatively consider the reliability. More accurate reliability would be obtained by using a higher order analysis such as the second-order reliability method (SORM).

The computational time in the reliability analysis is investigated in this example. The finite element analysis to compute the limit state value was dominant in the reliability analysis. On the other hand, that of the advection equation was only up to 11%.

5.5.2 Cantilever design problem

Now, the proposed method is applied to the cantilever design problem based on the formulation in Section 5.3.1. Figure 5.6 shows the fixed design domain and boundary conditions. For application of the finite element method, the fixed design domain was discretized into 320×80 first-order quadrilateral elements. For application of the Lax-Wendroff scheme, the fixed design domain was discretized into a 321×81 grid, with spatial steps in both directions of $\Delta x = 1.0$ and time steps of $\Delta t = \min(0.2, 0.5\Delta t_{CFL})$, where Δt_{CFL} is the maximum time step satisfying the CFL condition. The upper limit of the allowable volume was set to 50%

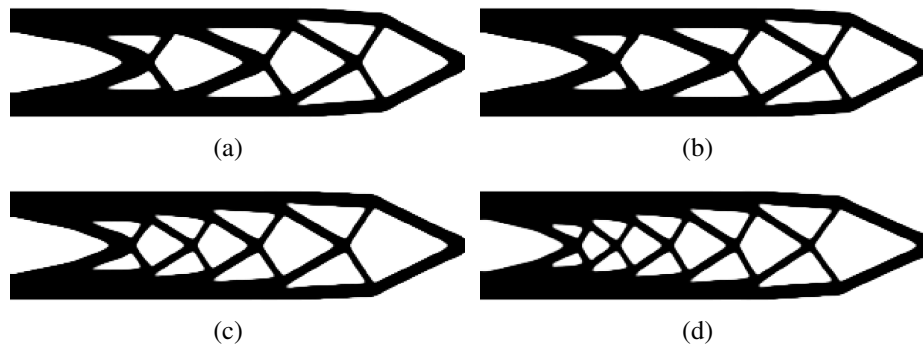


Fig. 5.7 Obtained optimized configurations for (a) $\beta_T = 0$ (deterministic solution); (b) $\beta_T = 1$; (c) $\beta_T = 3$; and (d) $\beta_T = 5$.

Table 5.2 Mean compliance values ($\times 10^4$) at MPTP calculated by setting various values of β_T for optimized configurations shown in Fig. 5.7 after optimization.

β_T values for analysis	β_T values for optimization			
	0	1	3	5
0	3.50	3.50	3.50	3.52
1	3.68	3.66	3.66	3.67
3	4.04	4.02	3.99	3.99
5	4.58	4.52	4.41	4.34

of the volume of the fixed design domain. The PDE filter parameter was set to $R = 2.5$. The final time for the advection was set to $T = 1$.

Dependency of optimal configuration on parameter β_T

Here, we examine the dependency of obtained optimized configurations on parameter β_T that represents the target reliability index. In these examples, parameter l_C in (5.5) that determines the autocorrelation in the K-L expansion was set to $0.1L$, resulting in $M = 325$. This value is relatively large due to the small correlation length setting.

Figure 5.7 shows the obtained optimized configurations for various values of β_T . As β_T is increased, the obtained optimized configurations include thicker elements near the fixed boundary and an increasing number of linear elements, which implies that considering geometrical variations in topology optimization is more important when the target reliability is large. Table 5.2 lists the mean compliance values at MPTPs calculated after optimization by setting various values for β_T for each optimized configuration obtained when $\beta_T = 0, 1, 3,$

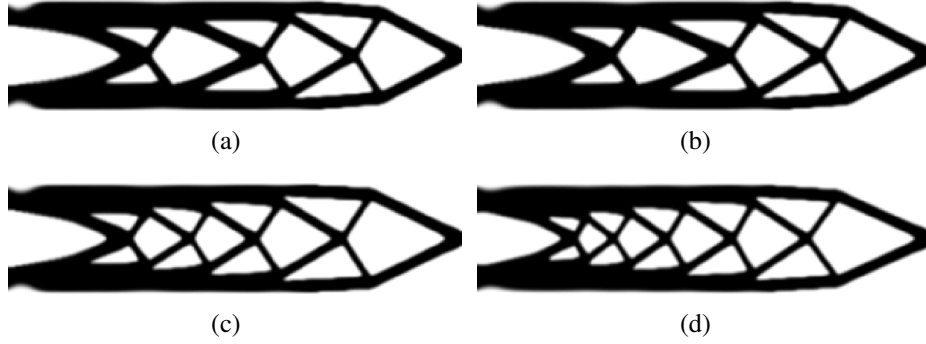


Fig. 5.8 Perturbed shapes at MPTP when setting $\beta_T = 5$ for optimized configurations obtained with (a) $\beta_T = 0$; (b) $\beta_T = 1$; (c) $\beta_T = 3$; and (d) $\beta_T = 5$.



Fig. 5.9 Obtained optimized configurations for (a) $l_C = 0.5L$; and (b) $l_C = L$.

and 5. The data show that when $\beta_T \leq 1$ for post-analysis, the values of the objective function are almost the same as those for optimized configurations obtained when $\beta_T = 0, 1, 3$, and 5. On the other hand, as β_T for post-analysis is increased, optimized configurations obtained for each β_T are superior to those obtained for other β_T values in this optimization. This indicates that the proposed method can effectively obtain local optima that have some degree of reliability for geometrical variations, depending on the β_T setting.

Figure 5.8 shows the perturbed shapes at MPTPs calculated by setting $\beta_T = 5$ after optimization for each of the optimized configurations shown in Fig. 5.7. The linear elements near the fixed boundary become very thin when $\beta_T \leq 3$, whereas this thinning was alleviated when $\beta_T = 5$, which results in a high stiffness for shape variations (Fig. 5.8).

Dependency of optimal configuration on parameter l_C

Next, we examine the dependency of obtained optimized configurations on parameter l_C in (5.5), which determines the spatial width of the autocorrelation function for geometrical variations. In this example, parameter β_T was set to 5 and two cases were examined, with $l_C = 0.5L$ resulting in $M = 17$, and $l_C = L$ resulting in $M = 6$.

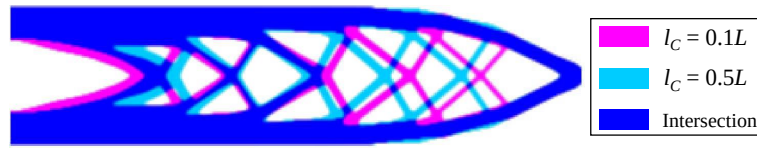


Fig. 5.10 Overlay image highlighting differences between optimized configurations obtained for $l_C = 0.1L$ and $0.5L$.

Table 5.3 Mean compliance values ($\times 10^4$) at MPTPs calculated with $l_C = 0.1L, 0.5L$, and L for optimized configurations shown in Fig. 5.9 after optimization.

l_C values for analysis	l_C values for optimization		
	$0.1L$	$0.5L$	L
$0.1L$	4.34	4.65	4.84
$0.5L$	5.03	5.02	5.24
L	4.99	4.99	4.91

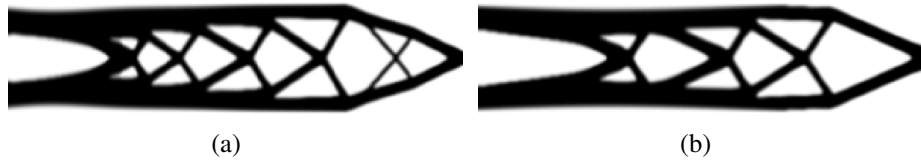


Fig. 5.11 Perturbed shapes at MPTPs when setting $\beta_T = 5$ for optimized configurations obtained with (a) $l_C = 0.5L$; and (b) $l_C = L$.

Figure 5.9 shows the optimized configurations obtained for $l_C = 0.5L$ and L . Although the optimized configurations for $l_C = 0.5L$ (Fig. 5.9(a)) and $l_C = 0.1L$ (Fig. 5.7(d)) have the same topology, there are geometrical differences. The optimized configuration when $l_C = 0.1L$ has thicker elements near the boundary where the design domain is fixed than when $l_C = 0.5L$, as shown in Fig. 5.10. On the other hand, the optimized configuration with $l_C = L$ has fewer linear elements than when $l_C = 0.1L$ or $0.5L$, and is similar to the deterministic solution, which implies that considering geometrical uncertainty in topology optimization is more important when the correlation length of the variations is small.

Table 5.3 lists mean compliance values at the MPTPs calculated after optimization, with settings of $l_C = 0.1L, 0.5L$, and L for each optimized configuration obtained when $l_C = 0.1L, 0.5L$, and L . Here, the data show that the optimized configuration obtained for a certain value of l_C has the lowest mean compliance among the optimized configurations

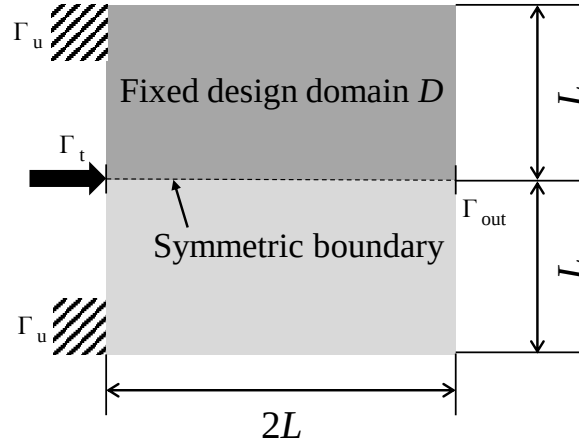


Fig. 5.12 Fixed design domain and boundary conditions for compliant mechanism optimum design problem.

obtained for other values of l_C with respect to a given l_C setting used for post-analysis. This demonstrates that the proposed method effectively obtains solutions when various l_C settings are applied.

Figure 5.11 illustrates the perturbed shapes at MPTPs for optimized configurations obtained when $l_C = 0.5L$ and L (Fig.5.9). Compared with the perturbed shapes for the optimized configurations when $l_C = 0.1L$, the upper and lower frames have become uniformly thin, reflecting the larger width of the autocorrelation function when $l_C = 0.5L$ and L . Thus, parameter l_C values have a significant effect on considered shape variations and resulting optimal configurations, and therefore should be carefully set to harmonize with a particular manufacturing situation or usage environment.

5.5.3 Optimum design problem for a compliant mechanism

Last, the proposed method is applied to an optimum design problem for the compliant mechanism problem formulated in Section 5.3.2. Figure 5.12 shows the fixed design domain and boundary conditions. Since the design model is symmetrical, only the upper half was considered as the design domain. For the finite element method analysis, the fixed design domain was discretized into 200×100 first-order quadrilateral elements. The Lax-Wendroff scheme was used for the finite difference method analysis, with the fixed design domain discretized into a 201×101 grid, with spatial steps of $\Delta x = 1.0$ in both directions, and a time step of $\Delta t = \min(0.2, 0.5 \Delta t_{CFL})$. The minmod function was adopted as the flux limiter.

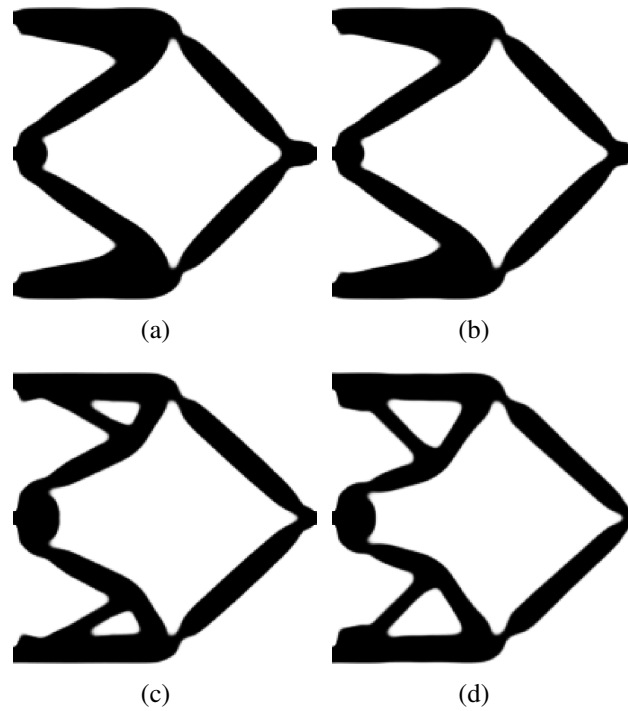


Fig. 5.13 Obtained optimized configurations for (a) $\beta_T = 0$ (deterministic solution); (b) $\beta_T = 1$; (c) $\beta_T = 3$ and (d) $\beta_T = 5$.

Table 5.4 Mutual mean compliance values at MPTPs calculated with various values of β_T for optimized configurations shown in Fig. 5.13 after optimization.

β_T values for analysis	β_T values for optimization			
	0	1	3	5
0	1.22	1.21	1.20	1.20
1	1.14	1.14	1.14	1.13
3	0.84	0.84	0.88	0.87
5	0.35	0.34	0.40	0.53

The upper limit of the allowable volume was set to 30% of the fixed design domain volume. The PDE filter parameter was set to $R = 5.0$. The final time for the advection was set to $T = 1$, which implies that the magnitude of velocity $V(\mathbf{x})$ represents the magnitude of shape variations. Parameters for the Robin boundary conditions were set with $k_{\text{in}} = 1.0$ and $k_{\text{out}} = 0.01$.

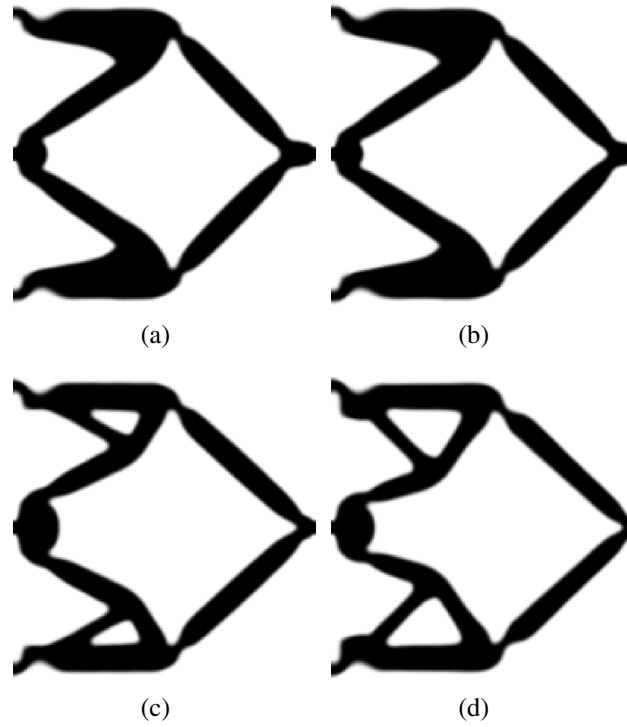


Fig. 5.14 Perturbed shapes at MPTPs when setting $\beta_T = 5$ for optimized configurations obtained when (a) $\beta_T = 0$ (deterministic solution); (b) $\beta_T = 1$; (c) $\beta_T = 3$ and (b) $\beta_T = 5$.

Dependency of optimal configuration on parameter β_T

In this subsection, we again examined the dependency of obtained optimized configurations on parameter β_T that represents the target reliability index. The parameter for the K-L expansion was set to $l_C = l_\sigma = 0.1L$, which resulted in $M = 162$.

Figure 5.13 shows the obtained optimized configurations for the various values of β_T . These configurations have different topologies, and as the value of β_T is increased, the corresponding optimized configurations have thicker elements near the boundaries where the displacement is fixed or the traction is applied. This behavior is similar to that in the minimum mean compliance problem. Again, we confirmed that considering geometrical variations in topology optimization is important when the target reliability is large. Table 5.4 lists the mutual mean compliance values at MPTPs calculated after optimization, having set various values of β_T for each optimized configuration shown in Fig. 5.13. The data indicate that the optimized configuration obtained for a certain value of β_T has the highest mutual mean compliance, i.e., a lower value of the objective function, among the optimized

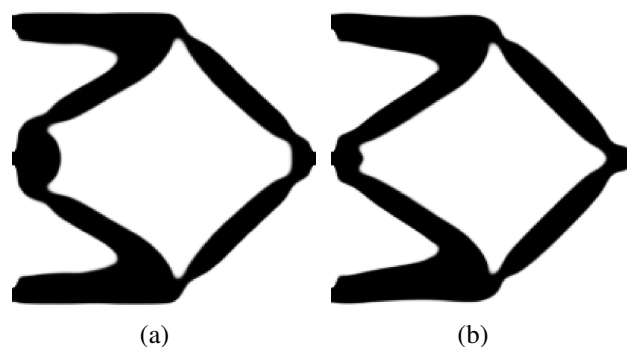


Fig. 5.15 Obtained optimized configurations for (a) $l_C = 0.5L$; and (b) $l_C = L$.

configurations obtained for other values of β_T with respect to a given β_T setting for post-analysis. The proposed method thus can obtain optimal configurations with higher reliability for geometrical variations, depending on the β_T setting, although the deterministic value of the mutual mean compliance is degraded.

Figure 5.14 shows the perturbed shapes at MPTPs calculated by setting $\beta_T = 5$ after optimization for each of the optimized configurations shown in Fig. 5.13. The results show that the elements near the fixed boundary have become much thinner, for all configurations, and the optimized configuration obtained when $\beta_T = 3$, and 5 has an additional supporting structure that provides increased reliability for shape variations. Note that shape variations illustrated in Figs. 5.14(a)–(d) mainly occurred at the elements near the fixed boundary, and these variations did not make any hinges in compliant mechanism designs. This means that the proposed method works similarly to the deterministic one for hinges, in this example. Consequently, the proposed method does not ensure the hinge-less designs, and the appropriate settings of parameters for the Robin boundary conditions, corresponding to the spring stiffness, prevented hinges from appearing in the optimized solutions.

Dependency of optimal configuration on parameter l_C

Here, we examine the dependency of obtained optimized configurations on parameter l_C . In this example, parameter β_T was set to 5 and two cases were examined, with $l_C = 0.5L$ resulting in $M = 9$, and $l_C = L$ resulting in $M = 4$.

Figure 5.15 illustrates the optimized configurations obtained for $l_C = 0.5L$ and L . The optimized configurations for $l_C = 0.5L$ (Fig. 5.15(a)) and $l_C = L$ (Fig. 5.15(b)) have the same topology, but it is different from that for $l_C = 0.1L$ (Fig. 5.13(d)). The optimized

Table 5.5 Mutual mean compliance values at MPTPs calculated with $l_C = 0.1L, 0.5L$, and L for optimized configurations shown in Fig. 5.15 after optimization.

l_C values for analysis	l_C values for optimization		
	$0.1L$	$0.5L$	L
$0.1L$	0.88	0.72	0.74
$0.5L$	0.81	0.90	0.90
L	0.98	0.93	1.04

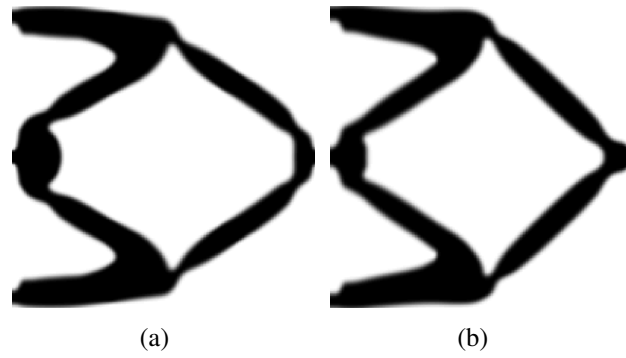


Fig. 5.16 Perturbed shapes at MPTPs when setting $\beta_T = 5$ for optimized configurations obtained with (a) $l_C = 0.5L$; and (b) $l_C = L$.

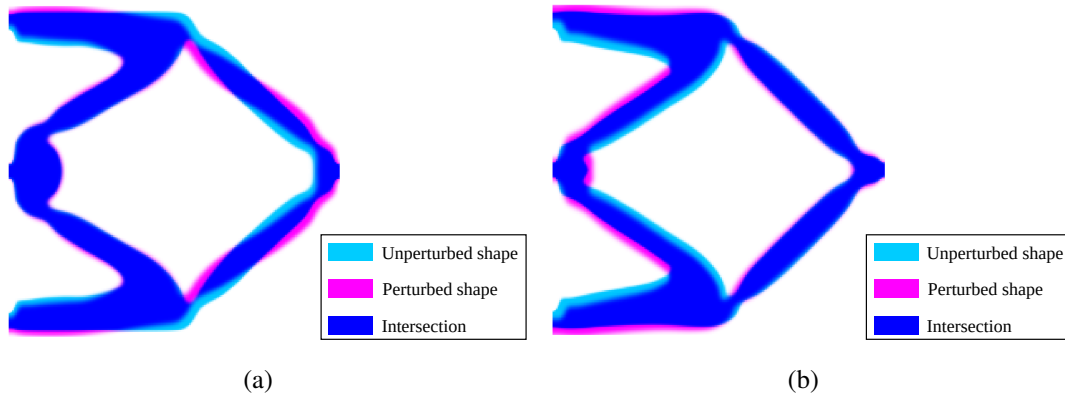


Fig. 5.17 Overlay image highlighting differences between unperturbed and perturbed shapes for optimized configurations obtained by $l_C = 0.5L$ and L .

configurations when $l_C = 0.5L$, and L have fewer linear elements than when $l_C = 0.1L$, and are similar to the deterministic solution, which again implies that geometrical uncertainty should be considered more when l_C is small.

Table 5.5 lists mutual mean compliance values calculated after optimization at the MPTPs of $\beta_T = 5$, with analysis settings of $l_C = 0.1L, 0.5L$, and L for each optimized configuration obtained for optimization settings of $l_C = 0.1L, 0.5L$, and L , respectively. This data indicates that diagonal components are higher than or equal to the other components in the same row, as is the same in all previous tables. This demonstrates that the proposed method effectively considers the effect of l_C settings on the solutions.

Figure 5.16 shows the perturbed shapes at MPTPs for optimized configurations obtained with $l_C = 0.5L$ and L (Fig. 5.15). Figure 5.17 highlights the differences between unperturbed (Fig. 5.15) and perturbed shapes (Fig. 5.16) for $l_C = 0.5L$ and L . Different from the case when $l_C = 0.1L$, linear elements change in their position and angle rather than their thickness when $l_C = 0.5L$ and L , which reflects the larger width of the autocorrelation function. Thus, we confirmed again that parameter l_C values have a significant effect on considered perturbation and obtained solutions, and therefore should be carefully set, depending on a particular manufacturing situation or usage environment.

5.6 Summary

This chapter proposed a new reliability-based topology optimization method that operates under geometrical uncertainty. We achieved the following:

1. Geometrical variations were modeled with an advection equation in which stochastic velocity was expressed using the K-L expansion. Based on this model, we formulated reliability-based topology optimization problems with a performance measure approach for inverse reliability.
2. Based on the optimization formulations, we constructed an iterative two-level optimization algorithm that uses an inner iteration to search for MPTPs and an outer iteration that updates the design variables. In both optimization levels, sensitivities were systematically derived using the adjoint variable method.
3. The proposed method was applied to two numerical examples to confirm its validity and utility. In the minimum mean compliance problem, we examined the dependencies of the optimal configurations on parameters β_T and l_C and confirmed that the proposed method successfully obtains optimized configurations reflecting these parameter settings. With increasing values of β_T , additional linear elements appeared in the

optimized configurations, alleviating the influence of the shape perturbation on the objective function. On the other hand, with increasing values of l_C , the increasing width of the autocorrelation function reflected a relatively uniform shape perturbation, resulting in uniformly thicker structures, which are similar to the deterministic solution. Consequently, it is important to consider the geometrical uncertainty in topology optimization particularly when the magnitude of the variations is large and the correlation length of the variations is small.

4. In the mutual mean compliance problem, the proposed method also effectively obtains optimal configurations, with geometries that reflect parameter β_T settings. With increasing values of β_T , linear structural elements in the corresponding optimized configurations were thicker near the boundaries where displacement was fixed or traction was applied, and supporting elements appeared near the boundary where the displacement was fixed, providing improved reliability against shape uncertainties.

Chapter 6

General conclusions

This thesis focused on a topology optimization methodology incorporating Pareto front exploration, manufacturing constraints and reliability designs for the realization of streamlining production processes. The following is the summary of achievements.

In Chapter 2, a Pareto front exploration method for multiobjective topology optimization problems was proposed. The proposed method incorporated adaptive weighting and point selection schemes in which the weighting coefficients and the initial designs are adaptively determined considering the current distribution of the Pareto front approximation. Based on this concept, multiobjective topology optimization methods for stiffness maximization problems, design problems of a no-moving-part valve and a micro-channel heat sink were constructed. In the stiffness maximization problem, the proposed method provides Pareto-optimal solution sets that clearly represent the trade-off relationship between the objectives and are useful to understand the physical mechanism operated in the optimal configurations. In the optimum design problem of a no-moving-part valve, an optimization problem was formulated as a bi-objective optimization problem, with one objective functional to minimize the total potential energy in the forward flow, and the other to maximize the total potential energy in the reverse flow. In the numerical example, the obtained Pareto-optimal solutions were discussed in terms of their diodicity values, commonly used for comparing the performance of NMP valves. The proposed method can obtain different Pareto-optimal solutions that had almost the same diodicity values, while these solutions cannot be distinguished by the conventional approach based on the diodicity, which implies the advantage of the proposed method. In the optimum design problem of a micro-channel heat sink, an optimization problem was formulated as a bi-objective optimization problem in which maximal heat exchange and minimal pressure drop were the objectives. In numerical examples, Pareto-optimal solutions

were obtained and clearly illustrated the trade-off relationships between heat exchange and pressure drop. A comparison of results obtained by the proposed method with those from a conventional weighted sum method allow us to confirm that the new scheme for adaptively setting weighting coefficients effectively avoids undesirable trapping in low-quality local Pareto fronts. We can confirm that the proposed Pareto front exploration method enables design engineers to choose a particularly suitable solution from the Pareto-optimal solution set, depending on the requirements of the design problem under consideration.

In Chapter 3, a data mining method for knowledge discovery using the Pareto-optimal solutions of multiobjective topology optimization problems was constructed. The proposed method consists of a two-step data mining procedure which sequentially applies clustering and association rule analysis. For clustering, the distance between two solutions was defined in the design space rather than the objective space to facilitate recognition of differences between pairs of configurations and enable extraction of characteristic substructures. For association rule analysis, confidence and lift indexes for multiobjective topology optimization solutions were proposed. In numerical examples, clustering results were visualized in the objective space for three-objective problems and illustrated using level diagrams in the four-objective problem. Confidence and lift indexes were visualized in colored plots for the two-dimensional problems and shown using isosurfaces for the three-dimensional problem. In all examples, clustering results, together with confidence and lift indexes, aided comprehension of the key substructures responsible for specific performances. Thus, the proposed data mining method may be especially useful to decision makers at the conceptual design stage, by discovering and revealing important knowledge in topology optimization problems for serviceable structural designs.

In Chapter 4, a scheme for imposing a geometrical constraint within a topology optimization procedure was proposed, using on fictitious physical models. The geometrical requirements for manufacturability using molding and milling were first clarified. Fictitious physical models were then introduced to implicitly represent the manufacturability of a design. The fictitious physical models were constructed using advection-diffusion equations, via which the geometrical constraint was formulated. In numerical examples, the dependencies of the fictitious physical fields on parameters in the source and advection terms were examined. The proposed method was then applied to topology optimization problems and obtained manufacturable optimal configurations. Optimal configurations demonstrated a very low dependency on the setting of the weighting coefficient and the initial configurations.

Also, we confirmed that the proposed method can obtain optimal configurations depending on the setting of the prescribed directions which correspond to the parting directions for molding, or cutter directions for milling. Furthermore, it is demonstrated that the proposed method can set the location of the parting line relative to mold parts prior to the optimization procedure.

In Chapter 5, a reliability-based topology optimization method that operates under geometrical uncertainty was proposed. First, geometrical variations were modeled with an advection equation in which stochastic velocity was expressed using the K-L expansion. Based on this model, we then formulated reliability-based topology optimization problems with a performance measure approach for inverse reliability. To solve the problem, an iterative two-level optimization algorithm that uses an inner iteration to search for MPTPs and an outer iteration to update the design variables was constructed. In both optimization levels, sensitivities were systematically derived using the adjoint variable method. In numerical examples, the dependencies of the optimal configurations on the target reliability index and the correlation length of geometrical uncertainties were examined. The results indicated that with increasing values of the target reliability index, additional linear elements appeared in the optimized configurations, alleviating the influence of the shape perturbation on the objective function. On the other hand, the increasing width of the autocorrelation function reflected a relatively uniform shape perturbation, resulting in uniformly thicker structures, which are similar to the deterministic solution. Consequently, it is important to consider the geometrical uncertainty in a topology optimization procedure particularly when the magnitude of the variations is large and the correlation length of the variations is small.

In conclusion, this thesis developed a structural design methodology based on multi-objective and manufacturing-oriented topology optimization techniques. The integration of techniques proposed in each chapter will make the conventional topology optimization techniques more useful and practicable. I believe that this thesis improve the applicability of topology optimization and accelerate its industrial application, which results in the new design framework of a variety of devices.

Appendix A

Sensitivity analysis

A.1 Sensitivity analysis for the structural mechanics problem

Here, sensitivities are derived for the following problem, based on the concept of topological derivative:

$$\inf_{\Omega} F = \int_{\Omega} f_d(\mathbf{u}) d\Omega + \int_{\partial\Omega} f_b(\mathbf{u}) d\Gamma. \quad (\text{A.1})$$

Here, the displacement field $\mathbf{u}$ satisfies the following equations:

$$\begin{cases} -\operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u})) = \mathbf{f} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_D & \text{on } \Gamma_D \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u})) \mathbf{n} = \mathbf{t} & \text{on } \Gamma_N \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u})) \mathbf{n} + k\mathbf{u} = \mathbf{g} & \text{on } \Gamma_R, \end{cases} \quad (\text{A.2})$$

with $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$. The elastic tensor $\mathbf{C}$ is assumed to be isotropic, which leads

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (\text{A.3})$$

where λ and μ are Lamé constants, and δ_{ij} is the Kronecker delta.

Now, let B_ε denote a ball of radius ε , centered in a point $\mathbf{x}_0 \in \Omega$. Then a domain with a hole can be expressed as $\Omega_\varepsilon = \Omega - \bar{B}_\varepsilon$. The topological derivative in (1.28) can be calculated

via the shape sensitivity [39], as follows:

$$D_{\mathbf{T}}F = \lim_{\varepsilon \rightarrow 0} \frac{1}{b'(\varepsilon)|\mathbf{V} \cdot \mathbf{n}|} F'(\Omega_\varepsilon)(\mathbf{V}), \quad (\text{A.4})$$

where the velocity $\mathbf{V}$ is chosen as

$$\mathbf{V} = \begin{cases} V_n \mathbf{n} & \text{on } \partial B_\varepsilon \\ 0 & \text{on } \partial \Omega, \end{cases} \quad (\text{A.5})$$

with V_n being a negative constant.

Therefore, the shape sensitivity for the following problem is firstly derived, based on the adjoint variable method:

$$\inf_{\Omega_\varepsilon} F = \int_{\Omega_\varepsilon} f_d(\mathbf{u}_\varepsilon) d\Omega + \int_{\partial \Omega} f_b(\mathbf{u}_\varepsilon) d\Gamma, \quad (\text{A.6})$$

where $\mathbf{u}_\varepsilon$ is the solution of

$$\begin{cases} -\operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) = \mathbf{f} & \text{in } \Omega_\varepsilon \\ \mathbf{u}_\varepsilon = \mathbf{u}_D & \text{on } \Gamma_D \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) \mathbf{n} = \mathbf{t} & \text{on } \Gamma_N \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) \mathbf{n} + k\mathbf{u}_\varepsilon = \mathbf{g} & \text{on } \Gamma_R \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) \mathbf{n} = 0 & \text{on } \partial B_\varepsilon. \end{cases} \quad (\text{A.7})$$

Note that the shape sensitivity analysis is based on a problem in which the hole B_ε already exists.

By considering the governing equation and the boundary conditions as equality constraints, the Lagrangian $\mathcal{L}$ is defined as

$$\begin{aligned} \mathcal{L}(\mathbf{v}, \mathbf{q}, \boldsymbol{\mu}_D, \boldsymbol{\mu}_N, \boldsymbol{\mu}_R, \boldsymbol{\mu}_B) = & \int_{\Omega} f_d(\mathbf{v}) d\Omega + \int_{\partial \Omega} f_b(\mathbf{v}) d\Gamma + \int_{\Omega} \mathbf{q} \cdot (\mathbf{f} + \operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v}))) d\Omega \\ & + \int_{\Gamma_D} \boldsymbol{\mu}_D \cdot (\mathbf{v} - \mathbf{u}_D) d\Gamma + \int_{\Gamma_N} \boldsymbol{\mu}_N \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} - \mathbf{t}) d\Gamma \\ & + \int_{\Gamma_R} \boldsymbol{\mu}_R \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} + k\mathbf{v} - \mathbf{g}) d\Gamma + \int_{\partial B_\varepsilon} \boldsymbol{\mu}_B \cdot (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} d\Gamma, \end{aligned} \quad (\text{A.8})$$

where $\mathbf{v}$ is a variable that is independent from the domain Ω_ε , and $\mathbf{q}$, μ_D , μ_N , μ_R , and μ_B are Lagrange multipliers. The necessary conditions for optimality are given as the stationary conditions of the Lagrangian with respect to the state variable and the Lagrange multipliers.

Stationary conditions with respect to the Lagrange multipliers $\mathbf{q}$, μ_D , μ_N , μ_R , and μ_B yield

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{q}}, \delta \mathbf{q} \right\rangle = \int_D \delta \mathbf{q} \cdot (\mathbf{f} + \operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v}))) d\Omega = 0 \quad (\text{A.9})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mu_D}, \delta \mu_D \right\rangle = \int_{\Gamma_D} \delta \mu_D \cdot (\mathbf{v} - \mathbf{u}_D) d\Gamma = 0 \quad (\text{A.10})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mu_N}, \delta \mu_N \right\rangle = \int_{\Gamma_N} \delta \mu_N \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} - \mathbf{t}) d\Gamma = 0 \quad (\text{A.11})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mu_R}, \delta \mu_R \right\rangle = \int_{\Gamma_R} \delta \mu_R \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} + k\mathbf{v} - \mathbf{g}) d\Gamma = 0 \quad (\text{A.12})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mu_B}, \delta \mu_B \right\rangle = \int_{\partial B_\varepsilon} \delta \mu_B \cdot (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{v})) \mathbf{n} d\Gamma = 0, \quad (\text{A.13})$$

where the notation $\langle \partial \mathcal{L} / \partial X, \delta X \rangle$ represents the partial derivative of the Lagrangian $\mathcal{L}$ with respect to X in the direction δX . These conditions are satisfied when $\mathbf{v} = \mathbf{u}_\varepsilon$ because the integrand of these conditions become 0.

Next, we consider the stationary condition with respect to the state variable. The stationary condition with respect to the state variable $\mathbf{v}$ is given using an integration by parts twice, as follows:

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}}, \delta \mathbf{v} \right\rangle &= \int_{\Omega_\varepsilon} \delta \mathbf{v} \cdot \frac{\partial f_d}{\partial \mathbf{v}}(\mathbf{v}) d\Omega + \int_{\partial \Omega} \delta \mathbf{v} \cdot \frac{\partial f_b}{\partial \mathbf{v}}(\mathbf{v}) d\Gamma \\ &\quad + \int_{\partial \Omega_\varepsilon} \mathbf{q} \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\delta \mathbf{v})) \mathbf{n}) d\Gamma - \int_{\partial \Omega_\varepsilon} \delta \mathbf{v} \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{q})) \mathbf{n}) d\Gamma \\ &\quad + \int_{\Omega_\varepsilon} \delta \mathbf{v} \cdot \operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{q})) d\Omega + \int_{\Gamma_D} \mu_D \cdot \delta \mathbf{v} d\Gamma \\ &\quad + \int_{\Gamma_N} \mu_N \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\delta \mathbf{v})) \mathbf{n}) d\Gamma + \int_{\Gamma_R} \mu_R \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\delta \mathbf{v})) \mathbf{n} + k\delta \mathbf{v}) d\Gamma \\ &\quad + \int_{\partial B_\varepsilon} \mu_B \cdot ((\mathbf{C} : \boldsymbol{\varepsilon}(\delta \mathbf{v})) \mathbf{n}) d\Gamma \\ &= 0. \end{aligned} \quad (\text{A.14})$$

For the satisfaction of this condition, we introduce the adjoint variable $\mathbf{p}_\varepsilon$, which is the solution of

$$\begin{cases} -\operatorname{div}(\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon)) = \frac{\partial f_d}{\partial \mathbf{u}} & \text{in } \Omega_\varepsilon \\ \mathbf{p}_\varepsilon = 0 & \text{on } \Gamma_D \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon)) \mathbf{n} = \frac{\partial f_b}{\partial \mathbf{u}} & \text{on } \Gamma_N \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon)) \mathbf{n} + k \mathbf{p}_\varepsilon = \frac{\partial f_b}{\partial \mathbf{u}} & \text{on } \Gamma_R \\ (\mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon)) \mathbf{n} = 0 & \text{on } \partial B_\varepsilon. \end{cases} \quad (\text{A.15})$$

The stationary condition in (A.14) is then satisfied when $\mathbf{q} = \mathbf{p}_\varepsilon$ at the optimal point $\mathbf{v} = \mathbf{u}_\varepsilon$.

Now, the shape sensitivity is obtained as the partial derivative of the Lagrangian with respect to Ω_ε in the direction $\mathbf{V}$, as follows:

$$\begin{aligned} F'(\Omega_\varepsilon)(\mathbf{V}) &= \left\langle \frac{\partial \mathcal{L}}{\partial \Omega_\varepsilon}, \mathbf{V} \right\rangle \\ &= \int_{\partial B_\varepsilon} (f_d + \mathbf{f} \cdot \mathbf{p}_\varepsilon - \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon) : \mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) V_n d\Gamma. \end{aligned} \quad (\text{A.16})$$

By substituting the shape sensitivity into (A.4), the topological derivative is now expressed as

$$D_T F = \lim_{\varepsilon \rightarrow 0} \frac{-1}{b'(\varepsilon)} \int_{\partial B_\varepsilon} (f_d + \mathbf{f} \cdot \mathbf{p}_\varepsilon - \boldsymbol{\varepsilon}(\mathbf{p}_\varepsilon) : \mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{u}_\varepsilon)) d\Gamma, \quad (\text{A.17})$$

where $b'(\varepsilon)$ is the first derivative of $b(\varepsilon)$ with respect to ε . The explicit expression of the topological derivative is obtained by evaluating the limit in the above equation. For the calculation of the limit when $\varepsilon \rightarrow 0$, it is necessary to make an asymptotic analysis of the solutions $\mathbf{u}_\varepsilon$ and $\mathbf{p}_\varepsilon$, and their gradients. Here, only the result when f_d is a function of $\mathbf{u}$, not $\nabla \mathbf{u}$ is provided. The topological derivative is given as

$$D_T F = -f_d - \mathbf{f} \cdot \mathbf{p} + \boldsymbol{\varepsilon}(\mathbf{p}) : \mathbf{A} : \boldsymbol{\varepsilon}(\mathbf{u}), \quad (\text{A.18})$$

where $\mathbf{A}$ is a fourth-order tensor whose components are

$$A_{ijkl} = \frac{3(1-\nu)}{2(1+\nu)(7-5\nu)} \left(\frac{-(1-14\nu+15\nu^2)E}{(1-2\nu)^2} \delta_{ij} \delta_{kl} + 5E(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right), \quad (\text{A.19})$$

where E is the Young's modulus and ν is the Poisson ratio.

A.2 Sensitivity analysis for the thermal-fluid problem

Here, sensitivity for the optimization problem formulated in Section 2.5 is derived based on the concept of the density approach. Although several previous studies focused on the topological derivative for fluid flow problems, it is limited to simple problems because the topological derivative calculation needs the fundamental solution of the state problem described in the perturbed domain to calculate the limit of the shape derivative in (A.4). In the present study, the topological derivative is assumed to be approximated by the sensitivity in the density approach, for simplicity. That is, we introduce a continuous variable γ that is the projection of the binary discrete variable, χ_ϕ , into the convexified space and calculate the sensitivity as the Gâteaux of the objective functional with respect to γ in the direction $\delta\gamma$. This assumption is not always valid, but is effective when the two phases (herein, fluid and solid domains) are discriminated only by the source term of the governing equations. Sensitivity for the optimization problem in Section 2.4 can be derived in the same manner as the following derivation by considering the terms only related to the total potential energy Φ and taking the Gâteaux derivative of the objective functional with respect to the normalized density θ in the direction $\delta\theta$.

First, the Lagrangian is defined by considering the governing equations in (2.53) and the boundary conditions in (2.46) as the equality constraints, as follows:

$$\begin{aligned}
& \mathcal{L}(\tilde{\mathbf{v}}, \tilde{q}, \tilde{S}, \tilde{\mathbf{v}}_{\text{in}}, \tilde{\mathbf{v}}_{\text{wall}}, \tilde{\mathbf{v}}_{\text{out}}, \tilde{S}_{\text{in}}, \tilde{S}_{\text{out}}, \lambda_1, \lambda_2, \mathbf{v}, q, S, \gamma) \\
& = -w_1 Q(S, \gamma) + w_2 \Phi(\mathbf{v}, \gamma) \\
& \quad - \int_D \nabla \cdot \mathbf{v} \tilde{q} d\Omega + \int_D (\mathbf{v} \cdot \nabla) \mathbf{v} \cdot \tilde{\mathbf{v}} d\Omega + \int_D \nabla q \cdot \tilde{\mathbf{v}} d\Omega - \int_D \nabla \sigma(\mathbf{v}) \cdot \tilde{\mathbf{v}} d\Omega \\
& \quad + \int_D \alpha(\gamma) \mathbf{v} \cdot \tilde{\mathbf{v}} - \int_D \nabla^2 S \tilde{S} d\Omega + \int_D \text{RePr}(\mathbf{v} \cdot \nabla) S \tilde{S} d\Omega - \int_D \beta(\gamma) (1 - S) \tilde{S} d\Omega \\
& \quad + \int_{\Gamma_{\text{in}}} (\mathbf{v} - \mathbf{u}_{\text{in}}) \cdot \tilde{\mathbf{v}}_{\text{in}} d\Gamma + \int_{\Gamma_{\text{wall}}} \mathbf{v} \cdot \tilde{\mathbf{v}}_{\text{wall}} d\Gamma + \int_{\Gamma_{\text{out}}} [\mathbf{n}(-qI + \sigma(\mathbf{v}))] \cdot \tilde{\mathbf{v}}_{\text{out}} d\Gamma \\
& \quad + \int_{\Gamma_{\text{in}}} (S - T_{\text{in}}) \tilde{S}_{\text{in}} d\Gamma + \int_{\Gamma_{\text{out}} \cup \Gamma_{\text{wall}}} \mathbf{n} \cdot \nabla S \tilde{S}_{\text{out}} d\Gamma + \lambda_1 G_1(\gamma) + \lambda_2 G_2(\mathbf{v}, \gamma), \quad (\text{A.20})
\end{aligned}$$

with $\sigma(\mathbf{v}) = (\nabla \mathbf{v} + \nabla \mathbf{v}^T) / \text{Re}$, where $\mathbf{v}$, q and S are state variables, and $\tilde{\mathbf{v}}, \tilde{q}, \tilde{S}, \tilde{\mathbf{v}}_{\text{in}}, \tilde{\mathbf{v}}_{\text{wall}}, \tilde{\mathbf{v}}_{\text{out}}, \tilde{S}_{\text{in}}, \tilde{S}_{\text{out}}, \lambda_1$ and λ_2 are the Lagrange multipliers. The necessary conditions for optimality are given as the stationary conditions of the Lagrangian with respect to the state variables and the Lagrange multipliers.

Stationary conditions with respect to the Lagrange multipliers $\tilde{\mathbf{v}}, \tilde{q}$ and $\tilde{S}$ yield

$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{q}}, \delta \tilde{q} \right\rangle = - \int_D \nabla \cdot \mathbf{v} \delta \tilde{q} d\Omega = 0 \quad (\text{A.21})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{v}}}, \delta \tilde{\mathbf{v}} \right\rangle = \int_D \left((\mathbf{v} \cdot \nabla) \mathbf{v} + \nabla q - \frac{1}{\text{Re}} \nabla \cdot (\nabla \mathbf{v} + \nabla \mathbf{v}^T) + \alpha(\gamma) \mathbf{v} \right) \cdot \delta \tilde{\mathbf{v}} d\Omega = 0 \quad (\text{A.22})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{S}}, \delta \tilde{S} \right\rangle = \int_D \left(-\nabla^2 S + \text{RePr}(\mathbf{v} \cdot \nabla) S - \beta(\gamma)(1 - S) \right) \delta \tilde{S} d\Omega = 0, \quad (\text{A.23})$$

where the notation $\langle \partial \mathcal{L} / \partial X, \delta X \rangle$ represents the partial derivative of the Lagrangian $\mathcal{L}$ with respect to X in the direction δX . These conditions are satisfied when $q = p$, $\mathbf{v} = \mathbf{u}$ and $S = T$ because the integrand become 0 due to the governing equations. Similarly, stationary conditions for the Lagrange multipliers $\tilde{\mathbf{v}}_{\text{in}}, \tilde{\mathbf{v}}_{\text{wall}}, \tilde{\mathbf{v}}_{\text{out}}, \tilde{S}_{\text{in}}$ and $\tilde{S}_{\text{out}}$ can be satisfied when $q = p$, $\mathbf{v} = \mathbf{u}$ and $S = T$ due to the boundary conditions. For the Lagrange multipliers λ_i for $i = 1, 2$, the KKT (Karush-Kuhn-Tucker) conditions require the satisfaction of

$$\frac{\partial \mathcal{L}}{\partial \lambda_i} = G_i \leq 0, \quad (\text{A.24})$$

$$\lambda_i G_i = 0. \quad (\text{A.25})$$

Next, we consider the stationary conditions with respect to the state variables. The stationary condition with respect to $\mathbf{v}$ yields

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}}, \delta \mathbf{v} \right\rangle &= \int_{\Gamma_{\text{in}}} [-\tilde{q} \mathbf{n} + (\mathbf{v} \cdot \mathbf{n}) \tilde{\mathbf{v}} + \boldsymbol{\sigma}(\tilde{\mathbf{v}} + W_2 \mathbf{v}) \mathbf{n} + \tilde{\mathbf{v}}_{\text{in}}] \cdot \delta \mathbf{v} d\Gamma \\ &+ \int_{\Gamma_{\text{out}}} [-\tilde{q} \mathbf{n} + (\mathbf{v} \cdot \mathbf{n}) \tilde{\mathbf{v}} + \boldsymbol{\sigma}(\tilde{\mathbf{v}} + W_2 \mathbf{v}) \mathbf{n}] \cdot \delta \mathbf{v} d\Gamma \\ &+ \int_{\Gamma_{\text{wall}}} [-\tilde{q} \mathbf{n} + (\mathbf{v} \cdot \mathbf{n}) \tilde{\mathbf{v}} + \boldsymbol{\sigma}(\tilde{\mathbf{v}} + W_2 \mathbf{v}) \mathbf{n} + \tilde{\mathbf{v}}_{\text{wall}}] \cdot \delta \mathbf{v} d\Gamma \\ &- \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{wall}}} \boldsymbol{\sigma}(\delta \mathbf{v}) \mathbf{n} \cdot \tilde{\mathbf{v}} d\Gamma + \int_{\Gamma_{\text{out}}} \boldsymbol{\sigma}(\delta \mathbf{v}) \mathbf{n} \cdot (\tilde{\mathbf{v}}_{\text{out}} - \tilde{\mathbf{v}}) d\Gamma \\ &+ \int_D [\nabla \mathbf{v}^T \tilde{\mathbf{v}} - (\mathbf{v} \cdot \nabla) \tilde{\mathbf{v}} - (\nabla \cdot \mathbf{v}) \tilde{\mathbf{v}} + \nabla \tilde{q} - \nabla \cdot \boldsymbol{\sigma}(\tilde{\mathbf{v}} + W_2 \mathbf{v})] \cdot \delta \mathbf{v} d\Omega \\ &+ \int_D [\alpha(\gamma)(\tilde{\mathbf{v}} + W_2 \mathbf{v}) + \text{RePr} \nabla S \tilde{S}] \cdot \delta \mathbf{v} d\Omega \\ &= 0, \end{aligned} \quad (\text{A.26})$$

where

$$W_2 = 2 \left(\frac{w_2}{\Phi_{\max} - \Phi_{\min}} + \lambda_2 \right). \quad (\text{A.27})$$

In the same manner, the stationary condition with respect to q is given as

$$\left\langle \frac{\partial \mathcal{L}}{\partial q}, \delta q \right\rangle = \int_{\Gamma_{\text{in}} \cup \Gamma_{\text{wall}}} \tilde{\mathbf{v}} \cdot \mathbf{n} \delta q d\Gamma - \int_D \nabla \cdot \tilde{\mathbf{v}} \delta q d\Omega + \int_{\Gamma_{\text{out}}} (\tilde{\mathbf{v}} - \tilde{\mathbf{v}}_{\text{out}}) \cdot \mathbf{n} \delta q d\Gamma = 0, \quad (\text{A.28})$$

and the stationary condition with respect to S yields

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial S}, \delta S \right\rangle &= \int_{\Gamma_{\text{in}}} (\nabla \tilde{S} \cdot \mathbf{n} + \text{RePr}(\mathbf{v} \cdot \mathbf{n}) \tilde{S} + \tilde{S}_{\text{in}}) \delta S d\Gamma \\ &\quad + \int_{\Gamma_{\text{wall}} \cup \Gamma_{\text{out}}} (\nabla \tilde{S} \cdot \mathbf{n} + \text{RePr}(\mathbf{v} \cdot \mathbf{n}) \tilde{S}) \delta S d\Gamma \\ &\quad - \int_{\Gamma_{\text{in}}} \nabla \delta S \cdot \mathbf{n} \tilde{S} d\Gamma + \int_{\Gamma_{\text{wall}} \cup \Gamma_{\text{out}}} \nabla \delta S \cdot \mathbf{n} (\tilde{S} + \tilde{S}_{\text{out}}) d\Gamma \\ &\quad + \int_D [-\nabla^2 \tilde{S} - \text{RePr} \nabla \cdot (\tilde{S} \mathbf{v}) + \beta(\gamma)(\tilde{S} + W_1)] d\Omega \\ &= 0, \end{aligned} \quad (\text{A.29})$$

where

$$W_1 = \frac{w_1}{Q_{\max} - Q_{\min}}. \quad (\text{A.30})$$

To satisfy these conditions in (A.26), (A.28) and (A.29), we define the following adjoint equations for adjoint variables u_A , p_A and T_A .

$$\begin{cases} -\nabla \cdot \mathbf{u}_A = 0 \\ \nabla \mathbf{u}^T \mathbf{u}_A - (\mathbf{u} \cdot \nabla) \mathbf{u}_A + \nabla p_A - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}_A + W_2 \mathbf{u}) + \alpha(\gamma)(\mathbf{u}_A + W_2 \mathbf{u}) + \text{RePr} \nabla T T_A = 0 \\ -\nabla^2 T_A - \text{RePr}(\mathbf{u} \cdot \nabla) T_A = -\beta(\gamma)(T_A + W_1). \end{cases} \quad (\text{A.31})$$

with the following boundary conditions:

$$\begin{cases} \mathbf{u}_A = 0, T_A = 0 & \text{on } \Gamma_{\text{in}} \\ \mathbf{n}(-p_A \mathbf{I} + \boldsymbol{\sigma}(\mathbf{u}_A + W_2 \mathbf{u})) = -(\mathbf{u} \cdot \mathbf{n}) \mathbf{u}_A, \quad \mathbf{n} \cdot \nabla T_A = -\text{RePr}(\mathbf{u} \cdot \mathbf{n}) T_A & \text{on } \Gamma_{\text{out}} \\ \mathbf{u}_A = 0, \mathbf{n} \cdot \nabla T_A = -\text{RePr}(\mathbf{u} \cdot \mathbf{n}) T_A & \text{on } \Gamma_{\text{wall}}. \end{cases} \quad (\text{A.32})$$

Using the adjoint variables, the stationary conditions with respect to q , $\mathbf{v}$ and S yield the following conditions for the Lagrange multipliers.

$$\tilde{\mathbf{v}} = \mathbf{u}_A, \quad (\text{A.33})$$

$$\tilde{q} = p_A, \quad (\text{A.34})$$

$$\tilde{S} = T_A, \quad (\text{A.35})$$

$$\tilde{\mathbf{v}}_{\text{out}} = \tilde{\mathbf{v}}, \quad (\text{A.36})$$

$$\tilde{\mathbf{v}}_{\text{in}} = -\mathbf{n}(-p_A \mathbf{I} + \boldsymbol{\sigma}(\mathbf{u}_A + W_2 \mathbf{u})) - (\mathbf{u} \cdot \mathbf{n}) \mathbf{u}_A, \quad (\text{A.37})$$

$$\tilde{\mathbf{v}}_{\text{wall}} = -\mathbf{n}(-p_A \mathbf{I} + \boldsymbol{\sigma}(\mathbf{u}_A + W_2 \mathbf{u})) - (\mathbf{u} \cdot \mathbf{n}) \mathbf{u}_A, \quad (\text{A.38})$$

$$\tilde{S}_{\text{in}} = -\nabla T_A \cdot \mathbf{n} - \text{RePr}(\mathbf{u} \cdot \mathbf{n}) T_A, \quad (\text{A.39})$$

$$\tilde{S}_{\text{out}} = -T_A, \quad (\text{A.40})$$

under the condition of $q = p$, $\mathbf{v} = \mathbf{u}$ and $S = T$. Finally, design sensitivity can be obtained by substituting the above stationary conditions into the partial derivative of the Lagrangian with respect to γ as follows:

$$\begin{aligned} \langle F', \delta\gamma \rangle &= \left\langle \frac{\partial \mathcal{L}}{\partial \gamma}, \delta\gamma \right\rangle \\ &= \int_D \left[\beta_{\max}(1-T)(W_1 + T_A) - \alpha_{\max} \mathbf{u} \cdot \left(\frac{W_2}{2} \mathbf{u} + \mathbf{u}_A \right) + \lambda_1 \right] \delta\gamma d\Omega. \end{aligned} \quad (\text{A.41})$$

A.3 Sensitivity analysis for the manufacturing constraints via fictitious physical models

Here, we discuss the sensitivity analysis for manufacturing constraint via fictitious physical models discussed in Chapter 4. In the same manner as Appendix A.2, the topological derivative is assumed to be approximated by the sensitivity in the density approach, for simplicity. That is, a continuous variable γ is introduced to calculate the sensitivity as the Gâteaux of the objective functional with respect to γ in the direction $\delta\gamma$. This assumption is effective because the two phases (herein, solid and void domains) are discriminated only by the source term of the fictitious physical models.

First, the Lagrangian, $\mathcal{L}$ is defined as

$$\begin{aligned} \mathcal{L}(\tilde{\xi}_1, \dots, \tilde{\xi}_m, \xi_1, \dots, \xi_m, \gamma) = & \int_D (1 - \gamma) \prod_{i=1}^m \xi_i dD \\ & + \sum_{i=1}^m \int_D \tilde{\xi}_i \left(L^2 \operatorname{div}(\Lambda_i \cdot \nabla \xi_i) - LV \mathbf{d}_i \cdot \nabla \xi_i + \beta \gamma (1 - \xi_i) \right) dD \\ & + \sum_{i=1}^m \int_{\Gamma_{\text{in}}} \mu_i \xi_i d\Gamma + \sum_{i=1}^m \int_{\partial D \setminus \Gamma_{\text{in}}} \nu_i \mathbf{n} \cdot \Lambda_i \cdot \nabla \xi_i d\Gamma, \end{aligned} \quad (\text{A.42})$$

where ξ_i is the state variable and $\tilde{\xi}_i$ is the Lagrange multiplier for the governing equation of the i th fictitious physical model with $i \in \{1, \dots, m\}$. The stationary condition for the Lagrange multiplier $\tilde{\xi}_j$ requires that the partial derivative of the Lagrangian with respect to the Lagrange multiplier $\tilde{\xi}_j$ is equal to 0, as follows:

$$\left\langle \frac{\partial \mathcal{L}}{\partial \tilde{\xi}_j}, \delta \tilde{\xi}_j \right\rangle = \int_D \delta \tilde{\xi}_j \left(L^2 \operatorname{div}(\Lambda_j \cdot \nabla \xi_j) - LV \mathbf{d}_j \cdot \nabla \xi_j + \beta \gamma (1 - \xi_j) \right) dD = 0, \quad (\text{A.43})$$

for all indices $j \in \{1, \dots, m\}$. The above conditions can be satisfied if the state variable ξ_j for $j \in \{1, \dots, m\}$ respectively corresponds to the solution of the governing equation, ψ_j for $j \in \{1, \dots, m\}$. Similarly, stationary conditions for the Lagrange multiplier μ_j and ν_j leads

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mu_j}, \delta \mu_j \right\rangle = \int_{\Gamma_{\text{in}}} \delta \mu_j \xi_j d\Gamma = 0, \quad (\text{A.44})$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \nu_j}, \delta \nu_j \right\rangle = \int_{\partial D \setminus \Gamma_{\text{in}}} \delta \nu_j \mathbf{n} \cdot \Lambda_j \cdot \nabla \xi_j d\Gamma = 0, \quad (\text{A.45})$$

for all indices $j \in \{1, \dots, m\}$. These conditions are also satisfied when the state variable ξ_j for $j \in \{1, \dots, m\}$ respectively corresponds to ψ_j for $j \in \{1, \dots, m\}$ due to the boundary conditions. The stationary condition requiring that the partial derivative of the Lagrangian with respect to the state variable ξ_j is equal to 0 is given using an integration by parts, as follows:

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial \xi_j}, \delta \xi_j \right\rangle &= \int_D \delta \xi_j (1 - \gamma) \prod_{\substack{i=1 \\ i \neq j}}^m \xi_i dD + \int_{\partial D} \tilde{\xi}_j \mathbf{n} \cdot L^2 \Lambda_j \cdot \nabla \xi_j d\Gamma - \int_{\partial D} \delta \xi_j \mathbf{n} \cdot L^2 \Lambda_j^T \cdot \nabla \tilde{\xi}_j d\Gamma \\ &\quad + \int_D \delta \xi_j L^2 \operatorname{div} (\Lambda_j^T \cdot \nabla \tilde{\xi}_j) dD - \int_{\partial D} \delta \xi_j LV \mathbf{n} \cdot \mathbf{d}_j \tilde{\xi}_j d\Gamma + \int_D \delta \xi_j LV \mathbf{d}_j \cdot \nabla \tilde{\xi}_j dD \\ &\quad - \int_D \delta \xi_j \beta \gamma \tilde{\xi}_j dD + \int_{\Gamma_{\text{in}}} \delta \xi_j \mu_j d\Gamma + \int_{\partial D \setminus \Gamma_{\text{in}}} \nu_j \mathbf{n} \cdot \Lambda_j \cdot \nabla \delta \xi_j d\Gamma \\ &= 0, \end{aligned} \quad (\text{A.46})$$

for all indices $j \in \{1, \dots, m\}$. To satisfy these conditions, the adjoint equation are defined as

$$\begin{cases} -L^2 \operatorname{div} (\Lambda_j \cdot \nabla \tilde{\psi}_j) - LV \mathbf{d}_j \cdot \nabla \tilde{\psi}_j = -\beta \gamma \tilde{\psi}_j + (1 - \gamma) \prod_{\substack{i=1 \\ i \neq j}}^m \psi_i & \text{in } D \\ \tilde{\psi}_j = 0 & \text{on } \Gamma_{\text{in}} \\ L \mathbf{n} \cdot (\Lambda_j \cdot \nabla \tilde{\psi}_j) = -V \mathbf{n} \cdot \mathbf{d}_j \tilde{\psi}_j & \text{on } \partial D \setminus \Gamma_{\text{in}}, \end{cases} \quad (\text{A.47})$$

for all indices $j \in \{1, \dots, m\}$. Substituting the adjoint variable $\tilde{\psi}_j$ for $\tilde{\xi}_j$ in the condition formulation (A.46) satisfies the stationary conditions at the optimal point $\xi_j = \psi_j$ for $j \in \{1, \dots, m\}$ due to the symmetry of the diffusion tensor, i.e. $\Lambda_j^T = \Lambda_j$. Finally, the design sensitivity can be derived by substituting the stationary conditions into the partial derivative of the Lagrangian with respect to γ in the direction $\delta \gamma$, as follows:

$$\langle F'_M, \delta \gamma \rangle = \int_D \delta \gamma \left(- \prod_{i=1}^m \psi_i + \sum_{i=1}^m \tilde{\psi}_i \beta (1 - \psi_i) \right) dD. \quad (\text{A.48})$$

A.4 Sensitivity analysis for a reliability-based design problem

Here, sensitivities for the MPTP search and updating of the design variables in Chapter 5 are derived based on the adjoint variable method for the following problem:

$$\inf_{\hat{\varphi} \in L^\infty(D; [-1,1])} F = c \quad (\text{A.49})$$

with a reliability constraint

$$\min_{\xi \in S} h(\xi, \mathbf{u}, \hat{\varphi}) \geq 0, \quad (\text{A.50})$$

where

$$h(\xi, \mathbf{u}, \hat{\varphi}) = c - \left(\int_D f_d(\mathbf{u}, \theta(\mathbf{x}, T)) d\Omega + \int_{\partial D} f_b(\mathbf{u}) d\Gamma \right). \quad (\text{A.51})$$

This problem is equivalent to the following min-max problem:

$$\inf_{\hat{\varphi} \in L^\infty(D; [-1,1])} F = \max_{\xi \in S} \int_D f_d(\mathbf{u}, \theta(\mathbf{x}, T)) d\Omega + \int_{\partial D} f_b(\mathbf{u}) d\Gamma, \quad (\text{A.52})$$

so the sensitivity analysis is performed to the above formulation. With the equality constraints comprised of the governing equation for linear elasticity, the fictitious advection equation, and the PDE-filter, the Lagrangian is defined as

$$\begin{aligned} \mathcal{L}(\hat{\varphi}, \xi_i^j, \zeta, \bar{\eta}, \eta, \mathbf{v}, \tilde{\zeta}, \tilde{\eta}_H, \tilde{\eta}_0, \tilde{\eta}, \tilde{\mathbf{v}}) = & \int_D f_d(\mathbf{v}, \eta(\mathbf{x}, T)) d\Omega + \int_{\partial D} f_b(\mathbf{v}) d\Gamma \\ & + \int_{\Gamma_t} \mathbf{t} \cdot \tilde{\mathbf{v}} d\Gamma - \int_D \boldsymbol{\varepsilon}(\tilde{\mathbf{v}}) : \mathbf{C} \eta(\mathbf{x}, T)^p : \boldsymbol{\varepsilon}(\mathbf{v}) d\Omega \\ & - A \left[\int_{\Gamma_t} k_{\text{in}} \tilde{\mathbf{v}} \cdot \mathbf{v} d\Gamma + \int_{\Gamma_{\text{out}}} k_{\text{out}} \tilde{\mathbf{v}} \cdot \mathbf{v} d\Gamma \right] \\ & + \int_0^T \int_D \tilde{\eta} \left(\frac{\partial \eta}{\partial t} + \mathbf{V} \cdot \nabla \eta \right) d\Omega dt \\ & + \int_D \tilde{\eta}_0 (\eta(\mathbf{x}, 0) - \bar{\eta}) d\Omega + \int_D \tilde{\eta}_H (\bar{\eta} - H_e(\zeta)) d\Omega \\ & + \int_D (\tilde{\zeta} \varphi - R^2 \nabla \tilde{\zeta} \cdot \nabla \zeta - \tilde{\zeta} \zeta) d\Omega, \end{aligned} \quad (\text{A.53})$$

where $\zeta, \bar{\eta}, \eta, \mathbf{v}, \tilde{\zeta}, \tilde{\eta}_H, \tilde{\eta}_0, \tilde{\eta}$ and $\tilde{\mathbf{v}}$ are variables that are independent of $\hat{\varphi}$ and ξ_i^j . $A = 0$ for the minimum mean compliance problem, and $A = 1$ for the optimum design problem for

a compliant mechanism. Note that we herein use the Heaviside projection method with a smoothed Heaviside function in (1.8). The design sensitivity can be derived by taking the necessary conditions for optimality of the Lagrangian with respect to these variables. First, setting the partial derivative of the Lagrangian equal to zero with respect to variables $\tilde{\zeta}$, $\tilde{\eta}_H$, $\tilde{\eta}_0$, $\tilde{\eta}$ and $\tilde{\mathbf{v}}$ yields the stationary conditions for $\zeta = \varphi$, $\bar{\eta} = \bar{\theta}$, $\eta = \theta$ and $\mathbf{v} = \mathbf{u}$, respectively. Next, setting the partial derivative of the Lagrangian equal to zero with respect to variables ζ , $\bar{\eta}$, η and $\mathbf{v}$ at the optimal point for $\tilde{\zeta}$, $\tilde{\eta}_H$, $\tilde{\eta}_0$, $\tilde{\eta}$ and $\tilde{\mathbf{v}}$ yields the stationary conditions for $\tilde{\zeta} = \varphi_A$, $\tilde{\eta} = \theta_A$, $\tilde{\eta}_H = \tilde{\eta}_0 = \theta_A(\mathbf{x}, 0)$ and $\tilde{\mathbf{v}} = \mathbf{u}_A$, where $\mathbf{u}_A$, θ_A and φ_A are the solutions of the following adjoint equations.

Adjoint equation for linear elasticity:

$$\begin{aligned} & \int_D \frac{\partial f_d(\mathbf{u}, \theta)}{\partial \mathbf{u}} \cdot \tilde{\mathbf{u}}_A d\Omega + \int_{\partial D} \frac{\partial f_b(\mathbf{u})}{\partial \mathbf{u}} \cdot \tilde{\mathbf{u}}_A d\Gamma - A \left[\int_{\Gamma_i} k_{in} \tilde{\mathbf{u}}_A \cdot \mathbf{u}_A d\Gamma + \int_{\Gamma_{out}} k_{out} \tilde{\mathbf{u}}_A \cdot \mathbf{u}_A d\Gamma \right] \\ & - \int_D \boldsymbol{\varepsilon}(\tilde{\mathbf{u}}_A) : \mathbf{C} \theta(\mathbf{x}, T)^p : \boldsymbol{\varepsilon}(\mathbf{u}_A) d\Omega = 0, \end{aligned} \quad (\text{A.54})$$

for all variables $\tilde{\mathbf{u}}_A \in \mathcal{U}$. This adjoint equation is conventional except that the advected normalized density $\theta(\mathbf{x}, T)$ is used.

Adjoint equation for fictitious advection equation:

$$\begin{cases} -\frac{\partial \theta_A}{\partial t} - \nabla \cdot (\mathbf{V} \theta_A) = 0 & \text{for } (\mathbf{x}, t) \in D \times [0, T] \\ \theta_A(\mathbf{x}, t) = 0 & \text{for } (\mathbf{x}, t) \in \Gamma_+ \times [0, T] \\ \theta_A(\mathbf{x}, T) = p \boldsymbol{\varepsilon}(\mathbf{u}_A) : \mathbf{C} \theta^{(p-1)} : \boldsymbol{\varepsilon}(\mathbf{u}) - \frac{\partial f_d(\mathbf{u}, \theta)}{\partial \theta} & \text{for } \mathbf{x} \in D, \end{cases} \quad (\text{A.55})$$

where $\Gamma_+ = \partial D|_{\mathbf{V} \cdot \mathbf{n} > 0}$. This is a retrograde advection equation with respect to time and velocity, starting from final time T , and the initial condition given at time T is a conventional sensitivity for density approaches in topology optimization. Therefore, this adjoint equation represents the sensitivity mapping from a perturbed (advected) shape to an unperturbed shape.

Adjoint equation for Helmholtz-type of PDE filter:

$$-R^2 \nabla^2 \varphi_A + \varphi_A = -\theta_A(\mathbf{x}, 0) \frac{dH_e}{d\varphi}. \quad (\text{A.56})$$

This adjoint equation implies that the PDE filter will also be applied to the sensitivity, $-\theta_A(\mathbf{x},0)dH_e/d\varphi$. The gradient of performance function h then corresponds to the gradient of the Lagrangian with respect to ξ_i^j at the optimal point for $\zeta, \bar{\eta}, \eta, \mathbf{v}, \tilde{\zeta}, \tilde{\eta}_H, \tilde{\eta}_0, \tilde{\eta}$ and $\tilde{\mathbf{v}}$, calculated as

$$\frac{\partial h}{\partial \xi_i^j} = \frac{\partial L}{\partial \xi_i^j} = \int_0^T \int_D \theta_A \lambda_i \psi_i \mathbf{e}_j \cdot \nabla \theta \, d\Omega dt. \quad (\text{A.57})$$

This gradient is used to obtain the MPTP. Finally, the design sensitivity, i.e., the gradient of the objective functional with respect to $\hat{\varphi}$, is equal to the partial derivative of the Lagrangian with respect to $\hat{\varphi}$ at the optimal point for $\zeta, \bar{\eta}, \eta, \mathbf{v}, \tilde{\zeta}, \tilde{\eta}_H, \tilde{\eta}_0, \tilde{\eta}, \tilde{\mathbf{v}}$ and ξ , preceded by a minus sign, as follows:

$$\langle F', \delta \hat{\varphi} \rangle = - \left\langle \frac{\partial \mathcal{L}}{\partial \hat{\varphi}}, \delta \hat{\varphi} \right\rangle = - \int_D \varphi_A \delta \hat{\varphi} \, d\Omega. \quad (\text{A.58})$$

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