

Level Set-based Topology Optimization Method for Viscous Flow Using Lattice Boltzmann Method

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1. Abstract

This paper presents a topology optimization method for viscous fluid problems based on the lattice Boltzmann method (LBM). In the field of computational fluid dynamics, the LBM is a new approach for calculating viscous flow behavior that replaces the classical formulation based on the Navier-Stokes (NS) equation. Since the LBM is formulated with a linear equation rather than the nonlinear NS equation, numerical solutions can be stably obtained. Moreover, the explicit scheme of the LBM makes it suitable for implementing large-scale parallel computations. In previous research, the adjoint equation has typically included a large-scale asymmetric matrix in the sensitivity analysis, since the optimization formula is constructed using the discrete lattice Boltzmann equation (LBE). To overcome the problem of extreme computational cost with this approach, we construct an optimization formula governed by the continuous Boltzmann equation, so that an adjoint equation that uses the same framework as that of the Boltzmann equation can be derived. The framework characteristics then allow the adjoint equation to be calculated explicitly, as with the LBE. Here, the optimization formulation is based on the LBE and the adjoint LBE, and we use level set boundary expressions in order to obtain optimal configurations with clear boundaries.

2. Keywords: Topology Optimization, Level Set Method, Lattice Boltzmann Method, Adjoint Method

3. Introduction

In 1973, Pironneau [1] pioneered the structural optimization of fluid problems by constructing a methodology based on shape optimization, and obtained an optimal shape for an obstacle placed in laminar fluid flow, a shape resembling that of a rugby ball. Considerable research has been carried out since then and a number of shape optimization methods applicable to viscous fluid problems have been proposed.

On the other hand, topology optimization [2], in which a structural optimization problem is replaced by a material distribution problem, enables topological changes such as the generation of new holes in the design domain during the optimization process, in addition to changes in the boundaries of a structure. To apply topology optimization to fluid problems, Borrvall and Petersson [3] first proposed a topology optimization method for minimal friction problems in external and internal flow, and constructed a methodology in which both the material and fluid domains are governed by fluid equations by assuming that the material domain is a porous medium. This allows global control of the material distributions, by affecting a fictitious force operating in the material domain. In research based on this methodology, for instance, Hansen et al. [4] proposed a design for flow channels with two outlets and a single inlet, with the aim of controlling the ratio of the flow in the outlets by altering the inlet flow velocity. Such control techniques applied to flow properties are of particular interest in the field of micro-electromechanical systems (MEMS), since they may be especially suitable for novel flow channel devices such as micro flow channels or micro pumps.

Flow in high Reynolds number regimes, however, has seldom been treated in previous research on topology optimization for fluid problems, due to the nonlinearity of the convection term in the Navier-Stokes (NS) equation. This is especially problematic in cases of high Reynolds number flows such as turbulent flow, when numerical calculation incurs enormous computational cost. Furthermore, a traditional approach based on the finite element method (FEM) is difficult to implement in two-phase flow problems because the finite elements are poorly suited to expressing both the interfaces between the different phases and the intricacies of fluid mixing during flow.

To overcome these problems, the lattice Boltzmann method (LBM) has attracted attention as a new methodology for fluid flow analysis [5], replacing approaches based on the NS equation in the field of computational fluid dynamics. The LBM, based on the Boltzmann kinetic equation, is constructed using the lattice Boltzmann equation (LBE), a time evolution of the velocity distribution function applied to fictitious particles, so that the LBE can be treated as a linear and explicit scheme. Consequently, the LBM can be constructed using simple algorithms and by its nature is thus suitable for large-scale parallel computation. Lin et al. [6] applied the LBM to turbulent flow problems and, using parallel computation, obtained numerical results for complex flow regimes. In addition, the LBM preserves the accuracy of particle mass and momentum, enabling it to be applied to two-phase [7]. The LBM is therefore extremely useful when working with complex flows and can be successfully applied to structural optimization problems that include complex fluid flow regimes. In a pioneering study by Pingen et al. [8], a topology optimization methodology using the LBM was constructed and optimal solutions similar to those of previous research based on the NS equation were obtained. However, their approach required dealing with a large-scale asymmetric matrix during the adjoint analysis, since the formulation of the optimization problem was constructed using the LBE as a discrete equation, and the numerical cost of the optimization process was therefore enormous.

In this paper, to overcome this kind of problem in the adjoint analysis, we construct a structural optimization methodology using the continuous adjoint analysis proposed by Krause et al [9]. This approach enables derivation of a continuous adjoint equation, since the formulation is based on the continuous Boltzmann method. Due to the framework characteristics, the adjoint equation can be calculated explicitly, as with the LBE. Since this methodology has not yet been applied to structural optimization problems, we must confirm that it is appropriate for use in a topology optimization method using the LBM. To directly obtain clear boundaries in the optimal configurations, we use level set boundary expressions, based on the phase field method proposed by Yamada et al [10]. In the following sections, the Boltzmann equation and the LBE are first discussed as core concepts of the LBM. Next, the level set-based topology optimization method is described and the formulation using the LBM. The numerical implementation and optimization algorithm are then described and, finally, we introduce two- and three dimensional numerical examples to validate the utility of the presented topology optimization method.

4. Governing equation

The LBM is a new methodology in computational fluid dynamics that can be used instead of the classical approach based on the Navier-Stokes equation. The LBM is constructed using the LBE as a discrete Boltzmann kinetic equation, following the concepts of kinetic theory. The LBM expresses the fluid regime via an aggregation of fictitious particles, and makes it possible to obtain macroscopic values such as fluid velocity, pressure and temperature from the moments of the velocity distribution function that expresses the distribution state of the particles. In this section, we discuss the concept of the LBM applied to a viscous fluid.

4.1 Boltzmann kinetic equation

Here, we discuss the concept of Boltzmann kinetic equation as a continuous problem. Hence, the velocity distribution function $f = f(t, \mathbf{x}, \boldsymbol{\xi})$ is governed by the following equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = Q(f) \quad \text{in } I \times \Omega \times \Xi, \quad (1)$$

where $t \in I(t_0, t_1) \subseteq \mathbb{R}_{\geq 0}$ represents the time, $\mathbf{x} \in \Omega \subseteq \mathbb{R}^d$ ($d = 2, 3$ is the spatial dimension) and $\boldsymbol{\xi} \in \Xi$ ($= \mathbb{R}^d$) are the particle position and velocity, respectively, Q is called a collision operator that expresses the effect of contact between the fictitious particles. Due to the complexity of the framework, numerous approximate models have been proposed for Q . Here, we use the following Bhatnagar-Gross-Krook (BGK) collision model,

$$Q(f) = -\frac{1}{\omega}(f - f^{\text{eq}}), \quad (2)$$

where ω is the relaxation time that expresses the average time until the next collision. f^{eq} is the Maxwell distribution as a local equilibrium solution of the Boltzmann kinetic equation,

$$f^{\text{eq}} = -\frac{\rho}{(2\pi/3)^{d/2}} \exp\left(-\frac{3}{2}(\boldsymbol{\xi} - \mathbf{u})^2\right), \quad (3)$$

where ρ and \mathbf{u} represent the fluid density and velocity, respectively. Here, $\boldsymbol{\xi}$ and \mathbf{u} are normalized by $\sqrt{3RT}$, where R is the gas constant and T is the temperature. The macroscopic variables can be derived

by the moments of velocity distribution function f :

$$\rho = \int_{\Xi} f d\xi, \quad \rho \mathbf{u} = \int_{\Xi} \xi f d\xi. \quad (4)$$

4.2 Lattice Boltzmann equation

The LBM is formulated as a discrete Boltzmann kinetic equation with respect to space and time in order to implement as a numerical scheme for analyzing the incompressible viscous fluid flow. In the following configuration, the discrete space Ω_h defined in Ω is divided into an equally-spaced lattice $h \in \mathbb{R}_{>0}$, and the discrete time interval $I_h := \{t \in I : t = t_0 + kh^2, k \in \mathbb{N}\}$. The discrete velocity distribution function f_i is governed by the LBE:

$$\tilde{f}_i(\mathbf{x}, t) = f_i(\mathbf{x}, t) - \frac{1}{\omega} (f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)), \quad (5)$$

$$\tilde{f}_i(\mathbf{x}, t) = f_i(\mathbf{x} + \mathbf{c}_i h^2, t + h^2) \quad \text{in } I_h \times \Omega_h \times \Xi_h. \quad (6)$$

Equation (5) expresses the effect of particle collisions and Eq. (6) represents the propagation process for the particle positions at the next time step. Ξ_h is the discrete velocity space defining the particle velocity \mathbf{c}_i , which has $q \in \mathbb{N}$ directions. The value of q is defined differently in various lattice gas models. In the two-dimensional case, the nine velocity model has the following velocity vectors,

$$\begin{aligned} & [\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3, \mathbf{c}_4, \mathbf{c}_5, \mathbf{c}_6, \mathbf{c}_7, \mathbf{c}_8, \mathbf{c}_9] \\ &= \frac{1}{h} \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}. \end{aligned} \quad (7)$$

In the three-dimensional case, the fifteen velocity model has the following vectors,

$$\begin{aligned} & [\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3, \mathbf{c}_4, \mathbf{c}_5, \mathbf{c}_6, \mathbf{c}_7, \mathbf{c}_8, \mathbf{c}_9, \mathbf{c}_{10}, \mathbf{c}_{11}, \mathbf{c}_{12}, \mathbf{c}_{13}, \mathbf{c}_{14}, \mathbf{c}_{15}] \\ &= \frac{1}{h} \begin{bmatrix} 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{bmatrix}. \end{aligned} \quad (8)$$

The discrete local equilibrium distribution function f_i^{eq} is obtained by the Maxwell distribution (3), approximated using the Taylor expansion as follows:

$$f_i^{\text{eq}} = w_i \rho \left(1 + 3h^2 \mathbf{c}_i \cdot \mathbf{u} + \frac{9}{2} h^2 (\mathbf{c}_i \cdot \mathbf{u})^2 - \frac{3}{2} h^4 \mathbf{u} \cdot \mathbf{u} \right). \quad (9)$$

For the two-dimensional nine-velocity model, weight w_i is defined so that $w_1 = 4/9$, $w_2 = w_3 = w_4 = w_5 = 1/9$, $w_6 = w_7 = w_8 = w_9 = 1/36$, and for the three-dimensional fifteen-velocity model, weight w_i is defined so that $w_1 = 2/9$, $w_2 = w_3 = \dots = w_7 = 1/9$, $w_8 = w_9 = \dots = w_{15} = 1/72$. The density ρ , velocity \mathbf{u} , and pressure p are obtained from the following moments of the velocity distribution function:

$$\rho = \sum_i f_i, \quad \mathbf{u} = \frac{1}{\rho} \sum_i \mathbf{c}_i f_i, \quad p = \frac{\rho}{3}. \quad (10)$$

5. Optimization problem

In this section, using the LBM, we construct the formulation of the level set-based topology optimization method for the pressure drop minimization problem under internal flow. Since the adjoint method used in the sensitivity analysis is based on the adjoint LBE in this research, we use the Boltzmann equation to formulate the optimization problem.

5.1 Level set method boundary expression

Here, the level set method represents fluid and solid domains, and the boundaries between them, $\partial\Omega$, using the iso-surface of the level set function as follows:

$$\begin{cases} 0 < \phi(\mathbf{x}) \leq 1 & \text{if } \mathbf{x} \in \Omega \setminus \partial\Omega, \\ \phi(\mathbf{x}) = 0 & \text{if } \mathbf{x} \in \partial\Omega, \\ -1 \leq \phi(\mathbf{x}) < 0 & \text{if } \mathbf{x} \in D \setminus \Omega, \end{cases} \quad (11)$$

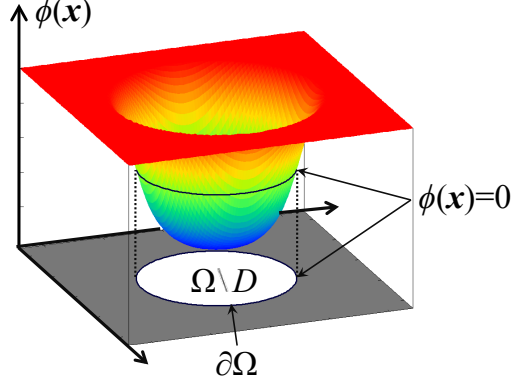


Figure 1: Fixed design domain D and level set function ϕ

where D represents the fixed design domain, $\Omega \subseteq D$ represents the fluid domain governed by the Boltzmann equation, and $D \setminus \Omega$ represents the solid domain. As shown in Fig. 1, the fluid and solid domains are defined as the level set function assumes positive and negative values, respectively. Here, the level set function is constrained to values lying between -1 and 1 , and Tikhonov regularization, as we discuss later, is used in the formulation of the optimization problem.

5.2 Expansion of fluid domain

To expand the fluid domain Ω to the fixed design domain D , the expanded velocity $\tilde{\mathbf{u}}$ is defined as

$$\tilde{\mathbf{u}} := \chi_\phi \mathbf{u}, \quad (12)$$

where χ_ϕ is the characteristic function representing the existence of the fluid domain Ω , defined as follows:

$$\chi_\phi = \begin{cases} 1 & \text{if } \phi(\mathbf{x}) \geq 0, \\ 0 & \text{if } \phi(\mathbf{x}) < 0. \end{cases} \quad (13)$$

By replacing the velocity \mathbf{u} in the Maxwell distribution f^{eq} shown in Eq. (3) with the expanded velocity $\tilde{\mathbf{u}}$ of Eq. (12), the Boltzmann equation is made dependent on the characteristic function χ_ϕ . Consequently, the space of the Boltzmann equation in Eq. (1) can be considered as $I \times \Omega \times \mathbb{R}^d \mapsto I \times D \times \mathbb{R}^d$, which allows the flow regime to be represented using the LBE, obtained by the discrete Boltzmann equation in the fixed design domain D . Therefore, an optimal configuration can be obtained by controlling χ_ϕ , governed by ϕ as a design variable in the optimization problem.

5.3 Optimization problem

Here, the topology optimization method based on the Boltzmann equation is formulated for a general form of objective functional J , constructed by integrating j_Γ and j_D , as follows:

$$\inf_{\phi} J = \int_I \int_{\Gamma} j_\Gamma(\rho[f], \mathbf{u}[f]) d\Gamma dt + \int_I \int_D j_D(\rho[f], \mathbf{u}[f], \phi) d\Omega dt, \quad (14)$$

$$\text{s.t. } V = \int_D \chi_\phi d\Omega - V_{\max} \leq 0, \quad (15)$$

$$E = \int_I \int_D \int_{\Xi} g \left\{ \frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f + \frac{1}{\omega} (f - f^{\text{eq}}) \right\} d\boldsymbol{\xi} d\Omega dt = 0, \quad (16)$$

where V is a volume constraint that prescribes the limit quantity V_{\max} of the fluid domain and E is the weak form of Eq. (6) using test function $g(t, \mathbf{x}, \boldsymbol{\xi})$.

Since the characteristic function χ_ϕ allows discontinuity in infinitesimal intervals throughout the fixed design domain D , the above optimization problem formulation is ill-posed. To regularize the optimization problem, an expanded objective functional J_R is defined as follows, based on the Tikhonov regularization scheme:

$$J_R := J + R_\tau, \quad (17)$$

where the regularization term R_τ is defined as follows, using a regularization coefficient, τ :

$$R_\tau := \frac{1}{2} \tau \int_D |\nabla \phi|^2 d\Omega. \quad (18)$$

Consequently, the regularized optimization problem is formulated as

$$\inf_{\phi} J_R = J + R_\tau, \quad (19)$$

$$\text{s.t. } V \leq 0, \quad (20)$$

$$E = 0. \quad (21)$$

The above optimization problem is now replaced by an unconstrained problem, using Lagrange's method of undetermined multipliers.

$$\inf_{\phi} \bar{J}_R = J_R + E + \lambda G + R_\tau, \quad (22)$$

where \bar{J}_R is the Lagrangian, and $\lambda \in \mathbb{R}$ are the Lagrange multipliers. This optimization problem is then replaced by the following time evolution equation of the level set function $\phi = \phi(\varsigma, \mathbf{x})$ by introducing a fictitious time, $\varsigma \in \Psi[\varsigma_0, \varsigma_1] \subseteq \mathbb{R}_{\geq 0}$, as follows:

$$\frac{\partial \phi}{\partial \varsigma} = -K \bar{J}'_R = -K(\bar{J}' - \tau \nabla^2 \phi), \quad (23)$$

where $K > 0$ is a constant of proportionality. The results of the time evolution formulation are assumed to be proportional to the gradient of Lagrangian \bar{J}_R with respect to the level set function ϕ . Here, the sensitivity \bar{J}' of $\bar{J} := J + \mu E + \lambda G$ is considered as the topological derivative. Due to this assumption, topological changes such as the generation of new fluid domains in the solid domain and new solid domains in the fluid domain are allowed during the optimization process.

5.4 Sensitivity analysis

The design sensitivity that is required to update the level set function during the optimization process is derived using the adjoint method.

$$\bar{J}' = J(f', \phi) + J(f, \phi) + E(f', g, \phi) + E(f, g', \phi) + E(f, g, \phi') + \lambda G(\phi'). \quad (24)$$

In the above equation, the gradient of E with respect to the test function g is equal to the equilibrium equation E , and can be eliminated. Since calculating the gradient of E with respect to f is enormously costly when using numerical schemes such as the finite difference method, an adjoint equation is defined using g , as follows,

$$J(f', \phi) + E(f', g, \phi) = 0. \quad (25)$$

In previous research, a methodology to calculate the above equation in a discrete form was proposed, using a matrix scheme, but even for a two-dimensional case, an $(N \times 9)^2$ asymmetric matrix for the number of lattice nodes N then had to be dealt with. Hence, the calculating the discrete adjoint equation was extremely costly.

On the other hand, since we construct the adjoint equation in a continuous form, it can be formulated in the same manner as the Boltzmann kinetic equation, and represented as follows:

$$\frac{\partial g}{\partial t} + \boldsymbol{\xi} \cdot \nabla g = \frac{1}{\omega} (g - g^{\text{eq}}) - j'_D \quad \text{in } I \times \Omega \times \Xi, \quad (26)$$

where g^{eq} is defined as

$$g^{\text{eq}} := \int_{\Xi} g(\hat{\boldsymbol{\xi}}) \frac{((\mathbf{u} - \boldsymbol{\xi})(\mathbf{u} - \hat{\boldsymbol{\xi}}) + RT)}{\rho RT} f^{\text{eq}}(\hat{\boldsymbol{\xi}}) d\hat{\boldsymbol{\xi}}. \quad (27)$$

Due to the similar configuration of equations X and Y, equation (26) can be discretized with respect to space and time as with the LBE, so that the adjoint lattice Boltzmann equation (ALBE) is derived as follows:

$$\tilde{g}_i(\mathbf{x}, t) = g_i(\mathbf{x}, t) - \frac{1}{\omega} (g_i(\mathbf{x}, t) - g_i^{\text{eq}}(\mathbf{x}, t)) - j'_D, \quad (28)$$

$$\tilde{g}_i(\mathbf{x}, t) = g_i(\mathbf{x} - \mathbf{c}_i h^2, t - h^2) \quad \text{in } I_h \times \Omega_h \times \Xi_h. \quad (29)$$

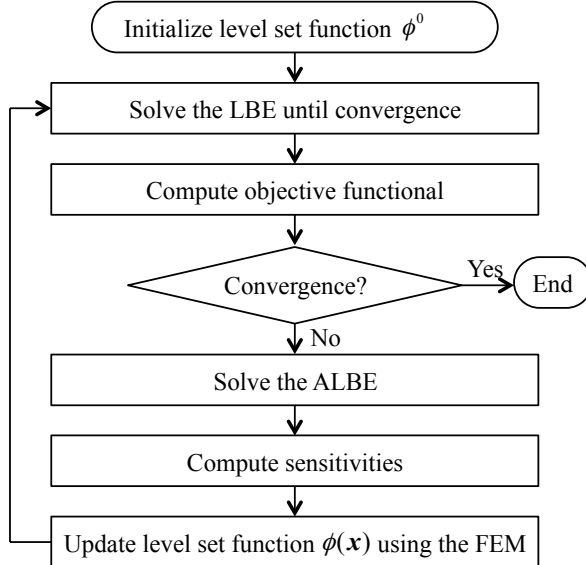


Figure 2: Optimization procedure flowchart

The ALBE is explicitly calculated, and suitable for parallel computation owing to the simplicity of its algorithm. Here, we note that the gradient of integrand j_Γ is included in the boundary condition of the ALBE. The details of the derivation method for the boundary conditions can be found in previous work [9].

Consequently, using the adjoint variable g_i , the design sensitivity of Eq. (24) is obtained as

$$\begin{aligned} \bar{J}' &= E(f_i, g_i, \phi') + \lambda G(\phi') \\ &= g_i w_i \rho (3h^2 \mathbf{c}_i \cdot \mathbf{u} + 9h^4 \chi_\phi (\mathbf{c}_i \cdot \mathbf{u})^2 - 3h^2 \chi_\phi \mathbf{u} \cdot \mathbf{u}) + \lambda. \end{aligned} \quad (30)$$

6. Optimization algorithm

The optimization flowchart is represented in Fig. 2. First, the initial level set function $\phi^0 = 1$ is set in the fixed design domain D . Next, the LBE is calculated until a steady-state condition is realized. If the objective functional is converged, the optimized structure is obtained and the optimization is finished, otherwise the ALBE is calculated and the level set function is then updated based on Eq. (23), using the design sensitivity in Eq. (30), and the procedure returns to the first step of the iterative loop. These procedures are repeated until the objective functional is converged. Here, we use the FEM to update the level set function, based on the method used in previous research [10].

7. Numerical examples

In this section, two- and three-dimensional numerical examples are provided. All numerical examples use the same parameters for the optimization: $\tau = 5.0 \times 10^{-3}$, $K = 1$, and $\phi^0 = 1$, which sets the initial configuration as being filled with fluid in the fixed design domain D .

7.1 Two-dimensional channel flow problem

First, we confirm the applicability of our methodology by comparing it with a previous FEM-based approach. The design requirements for the two-dimensional channel flow problem are shown in Fig. 3(a). The left and right inlets velocities are respectively defined as $\mathbf{u}_l = (U, 0)^T$ and $(-U, 0)^T$ using the characteristic velocity $U = 5.0 \times 10^{-2}$. The volume constraint $V_{\max} = 0.4$, grid size $h = 1.0 \times 10^{-2}$, and the relaxation time $\omega = 0.8$, which is a physically proper value in order to represent the fluid properties as a continuum. The kinematic viscosity of the fluid is then obtained as $\nu = 1/3(\omega - 1/2)h = 10^3$. Hence, the Reynolds number is represented as $\text{Re} = UL/\nu = 10$, where we define the characteristic length L as the width of the inlet.

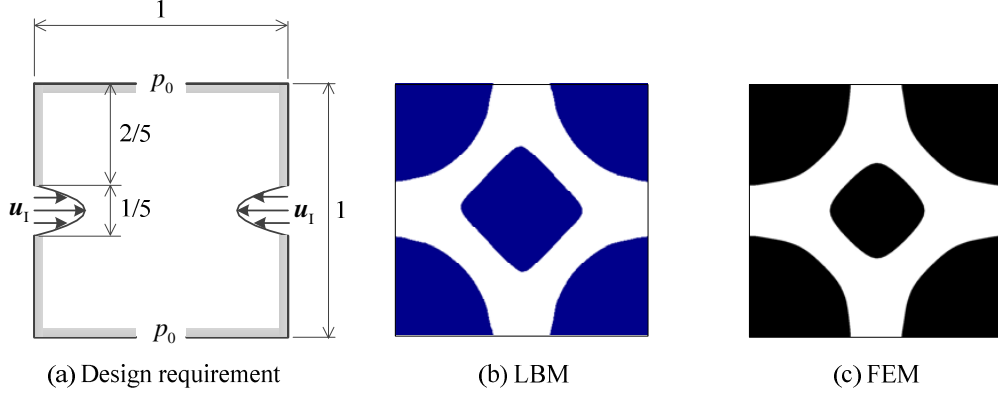


Figure 3: Optimal configuration in two-dimensional flow channel problem

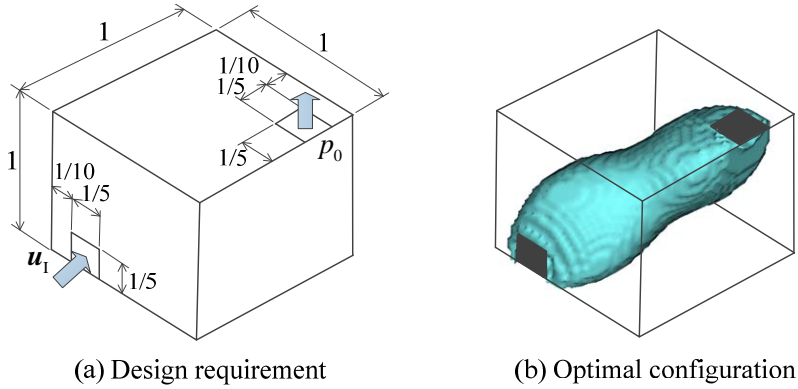


Figure 4: Optimal configuration in three-dimensional flow channel problem

Figure 3(b) shows the optimal configurations based on the FEM (a) and LBM (b) approaches for the flow channel problem. The general similarity of the configurations confirms that the proposed LBM can obtain appropriate results.

7.1 Three-dimensional channel flow problem

Next, the previous two-dimensional case is extended to a three-dimensional channel flow problem. The design model is shown in Fig. 4(a). In this figure, the inlet velocity is defined as $\mathbf{u}_I = (U, 0, 0)$ using $U = 5.0 \times 10^{-2}$, and the outlet pressure is $p_0 = 0.33$. The volume constraint, relaxation parameter, and cubic grid size are respectively set as $V_{\max} = 0.3$, $\omega = 0.8$, and $h = 3.0 \times 10^{-2}$. The kinematic viscosity of the fluid is then obtained as $\nu = 1/3(\omega - 1/2)h = 111$, and the Reynolds number is represented as $Re = UL/\nu = 0.01$

As shown in Fig. 4(b), the proposed method can derive a valid optimal structure in the three-dimensional case.

8. Conclusion

In this study, we constructed a level set-based topology optimization method for a pressure drop minimization problem using the LBM. We obtained the following results

- (1) A pressure drop minimization problem was formulated to represent solid/fluid domain boundaries, using the level set function.
- (2) The adjoint lattice Boltzmann equation was derived by basing the formulation of the optimization problem on the continuous Boltzmann kinetic equation, and was applied to obtain the design sensitivity.

- (3) The optimization algorithm was constructed for the steady state flow problem using the lattice Boltzmann method.
- (4) Clear optimal configurations for two- and three-dimensional flow channel problems were obtained. Furthermore, we demonstrated that a topology optimization method using the LBM can derive optimal configurations that are similar to those obtained via the FEM.

In future research, the proposed method will be extended to multiphase flow problems that may be particularly relevant to cutting edge engineering applications such as microfluidic systems in MEMS devices.

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