Local-in-time adjoint-based topology optimization of unsteady fluid flows using the lattice Boltzmann method

Cong CHEN∗, Kentaro YAJI∗∗, Takayuki YAMADA∗, Kazuhiro IZUI∗ and Shinji NISHIWAKI∗

∗ Department of Mechanical Engineering and Science, Graduate School of Engineering, Kyoto University
Kyotodaigaku-katsura, Nishikyo-ku, Kyoto, 615-8540, Japan
E-mail: chen.cong.42x@st.kyoto-u.ac.jp

∗∗ Department of Mechanical Engineering, Graduate School of Engineering, Osaka University
Yamadaoka 2-1, Suita, Osaka, 565-0871, Japan

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Abstract

This paper presents a local-in-time (LT) discrete adjoint-based topology optimization method for unsteady incompressible viscous flows incorporating the lattice Boltzmann method (LBM). For the optimization of unsteady flows, straightforward global implementations of the time-dependent optimization are usually adopted. However, such global implementations require that the entire flow solution history be available to calculate the solution of the adjoint equation reversed in time. For 3-D design optimization problems, the storage requirements can become prohibitively large. In this paper, the LT discrete adjoint-based method is applied to a LBM-based topology optimization to reduce the storage requirement. The basic idea of the LT method is to divide the entire time interval into several subintervals and to approximate the global sensitivity derivative as a combination of local sensitivity derivatives computed for each time subinterval. In this approach, flow solutions for only a single subinterval need to be stored. Since each time subinterval includes only a few (possibly one) time steps, the data storage requirements can be tremendously reduced. This method is applied in a pressure drop minimization problem considering unsteady viscous fluid. Two- and three-dimensional numerical examples are provided to confirm the validity and utility of the presented method.

Key words : Lattice Boltzmann method, Topology optimization, Unsteady flow, Local-in-time, Storage cost

1. Introduction

Structural optimization is a methodology to obtain an optimal structure based on mathematical and physical foundations, and is usually categorized into size, shape, and topology optimization approaches. Since topology optimization allows both shape and topology to be optimized simultaneously, it provides the highest degree of design freedom. The basic idea of topology optimization is the introduction of a fixed design domain that consists of material and void domains (Bendsøe and Kikuchi, 1988). By using the characteristic function, the optimization problem is replaced with a material distribution problem. Topology optimization was originally proposed as the so-called homogenization design method, and the density approach (Bendsøe and Sigmund, 1999), also called the isotropic material with penalization (SIMP) method, is currently the most popular topology optimization approach. Recent developments in topology optimization have been categorized in review papers (Deaton and Grandhi, 2014; Sigmund and Maute, 2013).

Topology optimization of fluid dynamics problems was first pioneered by Borravall and Petersson (2003) for minimization of viscous dissipation in Stokes flows and was later extended to Navier-Stokes flows (Gersborg-Hansen et al., 2005) and non-Newtonian flows (Pingen and Maute, 2010), and has been applied to the design of fluidic devices (Kubo et al., 2016). The topology optimization of fluid flows has focused primarily on steady flows, but unsteady flows are widespread in reality, hence the desirability of extending topology optimization to the realm of unsteady Navier-Stokes flows. Based on the standard approach proposed by Borravall and Petersson (2003), Kreissl et al. (2011) proposed a topology optimization method for unsteady flow channel design problems in which the optimization problem is formulated as
a mean pressure drop minimization problem. Similarly, Deng et al. (2011) investigated the dependency of optimized channel configurations with respect to inlet velocity profiles. Furthermore, Deng et al. (2013) applied their approach to unsteady flow channel design problems in which the body forces that drive fluid flows in the channels are considered. For the optimization of unsteady flows, straightforward global implementation requires that the entire flow solution history be available during the reversed time calculation of the solutions to the adjoint equations. Hence, three-dimensional optimization problems are extremely difficult due to their massive computational cost, and are a challenging topic of research.

On the other hand, several strategies aimed at avoiding massive storage requirements have been developed and reported (Choi et al., 2008; Hou et al., 1997; Nadarajah and Jameson, 2002; Nielsen et al., 2010) in the research fields of inverse problems and optimum shape design problems. These methods can be divided into two groups. The first group of methods, based on the idea of ‘exact,’ requires that the obtained primal and adjoint solutions exactly satisfy the corresponding equations of the original adjoint formulation. The most straightforward approach when using these methods is to store the entire flow solution history on a hard disk (Nadarajah and Jameson, 2002; Nielsen et al., 2010) and then use it when performing the inverse time integration of the adjoint equations. For large-scale problems that are not periodic in time and require a very large number of time steps to integrate the governing equations, the storage and input/output costs may become prohibitive.

The second group of these methods reduces storage cost by constructing sufficiently accurate approximations of either the original optimization problem or the corresponding governing equations, but this yields suboptimal results. Techniques such as receding horizon control (Hou et al., 1997) and non-linear frequency domain methods (Choi et al., 2008; Nadarajah et al., 2006) have been proposed. Receding horizon control techniques replace the original time-dependent optimization problem dealing with the entire time interval with a sequence of local optimal control problems defined for a number of equal subintervals. The optimization problems are solved sequentially, with each subinterval consisting of only a few (possibly one) time steps, which dramatically reduces storage requirements. Hou et al. proved that this technique with distributed controls is stable for problems that have a tracking-type functional governed by the two-dimensional incompressible Navier-Stokes equations. These methods compute only the local sensitivity, leaving the required global sensitivity unsolved, so solutions to optimal design problems are unavailable. Nadarajah et al. (2006) proposed a gradient-based method for the discrete adjoint sensitivity analysis, and Choi et al. (2008) developed an adjoint-based optimization procedure based on the time-spectral formulation, but both of these methods provide suboptimal results and are only applicable to time-periodic problems.

Yamaleev et al. (2010) proposed a LT discrete adjoint-based optimization methodology that combines the best features of both groups of methods described above. This methodology reduces storage cost by approximating the original adjoint equations for a set of local time subintervals so that each subinterval involves only a few (possibly one) time steps. This enables the original unsteady optimization problem to converge to a local minimum with no additional computational overhead, compared with global-in-time (GT) methods. Furthermore, since the global sensitivity derivative can be calculated, this method can be directly used for solving optimization problems. The low storage cost offered by LT methods makes them useful for solving large-scale topology optimization problems dealing with unsteady fluid flows and may also open new avenues for solving realistic design optimization problems. An additional advantage is that large-scale topology optimization problems can be handled using currently available computer technology.

Little research concerning three-dimensional topology optimization problems dealing with unsteady fluid flow has been reported. In this paper, based on the LT method, we propose a new topology optimization method for two- and three-dimensional flow channel design problems considering unsteady viscous flows. The fluid flow is calculated using the lattice Boltzmann method (LBM), which enables efficient calculation of the flow field simply by solving time evolution equations, without integrating Poisson’s equation for the pressure field. As a perfect explicit method, the LBM is highly compatible with the above-mentioned LT method. Additionally, since the LBM method is simple, computationally efficient, as well as highly scalable for parallel processing, it is extremely useful when working with complex and large-scale flow problems and can be successfully applied to topology optimization problems. Pingen et al. (2007) pioneered a topology optimization method using the LBM for steady-state viscous flows and clarified that optimized configurations can be obtained for the standard pressure drop minimization problems. Yaji et al. (2014) proposed a topology optimization method applying the adjoint lattice Boltzmann method (Krause et al., 2013), based on a continuous adjoint sensitivity analysis that enables explicit calculation of the adjoint equation, to solve two- and three-dimensional pressure drop minimization problems. On the other hand, Liu et al. (2014) applied a discrete sensitivity analysis to topology optimization problems dealing with steady-state viscous flows. Yonekura and Kanno (2015) proposed a radical way of
Fig. 1 A sketch of the algorithm using the local-in-time methodology.

solving optimization problems in which the adjoint calculation is completely free under low Reynolds number conditions. Nørgaard et al. (2016) recently proposed a topology optimization method using the LBM for unsteady flow problems and treated two-dimensional optimization problems. Their study indicated that a massive amount of memory storage is necessary even when solving two-dimensional topology optimization problems when dealing with unsteady flows. In this paper, we investigate the effectiveness of the LT method for overcoming the issue of memory storage when dealing with unsteady fluid topology optimization problems, and construct an efficient approach for large-scale topology optimization problems.

The rest of the paper is organized as follows. In Section 2, we present the general idea of the discrete time-dependent optimization problem using the LT methodology. In Section 3, the core concepts of the LBM are discussed. Section 4 presents the formulation of the optimization problem for a pressure drop minimization problem. The numerical implementation and optimization algorithm based on global- and local-in-time methodologies are then described in Section 5. In Section 6, two- and three-dimensional numerical examples are introduced to validate the utility of the LT-based topology optimization method. We draw conclusions in Section 7.

2. Local-in-time method

In this section, we discuss the basic concept of the LT method (Yamaleev et al., 2010) for solving a transient optimization problem, which is formulated as follows:

$$\min_d J(f^0, ..., f^N, d) = J\left(\sum_{n=0}^{N} J^n(f^n, d)\right),$$  \hspace{1cm} (1)$$

where \(d\) is the design variables vector and \(f^n\) is the state variables vector that satisfies the discrete governing equation, \(R^n = 0\), at time steps \(n = 0, ..., N\). The objective function, \(J\), is a differentiable function \(J\) that depends on the sum of \(J^n\) from all time steps. For simplicity, the equality and inequality constraints are neglected here.

It is widely known that the adjoint variable method is useful when considering a large number of design variables, since the computational cost for obtaining the design sensitivities is independent of the number of design variables. In transient optimization problems, however, the adjoint variable method requires the storage of the governing equation solutions for all time steps, in order to obtain the design sensitivities. For large-scale optimization problems such as three-dimensional time-dependent topology optimization problems, the storage requirements can become prohibitive.

The LT method is a promising approach to overcome this storage problem. Figure 1 shows a sketch of the algorithm using the local-in-time methodology. As shown in Fig. 1, the entire time interval with time step \(n \in [0, N]\) into \(K\) subintervals, and each time subinterval contains \(N/K\) time steps. At the end of the \(k\)th subinterval, the number of time step would be \(kN/K\). The optimization problem (1) is then reformulated as

$$\min_d J(f^0, ..., f^N, d) = \sum_{k=1}^{K} J^k = \sum_{k=1}^{K} J\left(\sum_{n=N_{k-1}+1}^{N_k} J^n(f^n, d)\right),$$  \hspace{1cm} (2)$$

where \(J^k\) represent the derivatives of the local objective functions at each time subinterval \([N_{k-1}, N_k]\) \((k = 1, ..., K)\). Within each time subinterval, the flow equations are solved forwardly while the sensitivity derivatives are calculated backward in time. The design sensitivities are now given by the sum of the local design sensitivities as follows:

$$\frac{dJ}{dd} = \sum_{k=1}^{K} \frac{dJ^k}{dd}. \hspace{1cm} (3)$$
The LT algorithm sequentially solves the local equations for each time subinterval to obtain the global sensitivity, while each subinterval consists of only a few (possibly one) time steps. Therefore, the storage requirement can be greatly reduced, compared with that when the standard formulation (1) is used. In this paper, we apply the LT method to a topology optimization problem considering unsteady fluid flows, the details of which will be discussed in Section 5.

3. Lattice Boltzmann method

The basic idea of the LBM is that the fluid regime is represented as an aggregation of fictitious particles. The fluid’s macroscopic variables such as velocity and pressure can be calculated sequentially using moments of the velocity distribution functions of the particles. The LBM is a numerical approach based on the kinetic theory of gases. In this section, we discuss the concept of the LBM, and its application to an incompressible viscous fluid in an isothermal field. In the following, as in the previous study of Yaji et al. (2016), we use dimensionless variables. Consider an aggregation of fictitious particles whose velocities are restricted to a finite set \( \{c_i\}_{i=1}^{g} \) of vectors. The velocity distribution function of the particles is governed by the discrete Boltzmann equation, as follows:

\[
Sh \frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = \frac{1}{\epsilon_f} (f_i - f_i^{eq}),
\]

where \( Sh = U/c \) is a non-dimensional parameter (the Strouhal number) and \( t \in [t_0, t_1] \) represents time. \( \epsilon_f \) is the dimensionless relaxation time that expresses the average time from one collision to the next collision. For different lattice gas models, the finite set \( g \) of vectors \( c_i \) \((i = 1, 2, ..., g)\) is defined differently. Here, for the two-dimensional case, we employ the nine-velocity (D2Q9) model, which has the following velocity vectors:

\[
[c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, c_9] = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}.
\]

For the three-dimensional case, we employ the fifteen-velocity (D3Q15) model, with velocity vectors as follows:

\[
[c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, c_9, c_{10}, c_{11}, c_{12}, c_{13}, c_{14}, c_{15}] = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 \end{bmatrix}.
\]

The velocity models are shown in Fig.2. The Maxwell distribution as a local equilibrium solution of the Boltzmann equation, \( f_i^{eq} \), is given by

\[
f_i^{eq} = E_i \rho \left( 1 + 3c_i \cdot u + \frac{9}{2} (c_i \cdot u)^2 - \frac{3}{2} ||u||^2 \right),
\]

The weight \( E_i \) is defined as in Eq. (8) for the D2Q9 model, and as in Eq. (9) for the D3Q15 model.

\[
E_i = \begin{cases} 
4/9 & \text{for } i = 1 \\
1/9 & \text{for } i = 2, 3, 4, 5 \\
1/36 & \text{for } i = 6, 7, 8, 9.
\end{cases}
\]

Fig. 2 Particle velocity vectors \( c_i \): (a) D2Q9 model; (b) D3Q15 model.
4. Formulation of topology optimization problems

By allowing the creation of new holes in the design domain during the optimization process, topology optimization provides enhanced degrees of freedom compared with other optimization methods. Topology optimization was first proposed by Bendsoe and Kikuchi (1988), and has been applied in a variety of fields. In this section, we discuss the basic concept of topology optimization and its application in fluid dynamics problems whose objective is the minimization of pressure drop.

4.1. Topology optimization for fluid flows

The basic idea of topology optimization is the introduction of a fixed design domain, \( D \), and the characteristic function, \( \chi(x) \). The fixed design domain \( D \) is composed of a structural domain \( \Omega \) where material exists, and a void domain \( D \setminus \Omega \) that is free of material, with \( \chi(x) \) defined as

\[
\chi(x) = \begin{cases} 
1 & \text{if } x \in \Omega \\
0 & \text{if } x \in D \setminus \Omega,
\end{cases}
\]

In the LBM, the physical field is divided into a square or cubic lattice with spacing \( \Delta x \) and time step \( \Delta t \). Using \( \Delta x \) and \( \Delta t \), the discrete Boltzmann equation can be discretized as the lattice Boltzmann equation (LBE):

\[
f_i(x + c_i \Delta x, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau_f}(f_i(x, t) - f_i^eq(x, t)),
\]

where \( \tau_f = \epsilon_f/\Delta x \) is the dimensionless relaxation time and \( x \) represents the position of particles. The density \( \rho \) and fluid velocity \( u \) are obtained from the following moments of the velocity distribution functions:

\[
\rho = \sum_i q_i f_i, \quad u = \frac{1}{\rho} \sum_i \{ c_i f_i \}.
\]

The flow pressure is represented as follows:

\[
p = \rho \frac{\partial u}{\partial t} = \frac{\rho}{3}.
\]

By applying the asymptotic theory to Eq. (4), Inamuro et al. (1997) verified that the macroscopic variables obtained from Eq. (4) satisfy the following equations, with relative errors of \( O[(\Delta x)^2] \):

\[
\nabla \cdot u = 0,
\]

\[
\nabla \cdot (Sh \frac{\partial u}{\partial t} + (u \cdot \nabla) u) = -\nabla \rho + \nu \nabla^2 u,
\]

which represent the continuity equation, and the Navier-Stokes equations respectively. The kinematic viscosity \( \nu \) is given by

\[
\nu = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \Delta x.
\]

When an extra body force \( F(x, t) \) is applied, the LBE can be computed in two steps, as follows:

Step 1. Compute \( f_i \) without the body force using the following equation.

\[
f_i^p(x + c_i \Delta x, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau_f}(f_i(x, t) - f_i^eq(x, t))
\]

Step 2. Update \( f_i \) according to the body force, as follows:

\[
f_i(x, t + \Delta t) = f_i^p(x, t + \Delta t) + 3\Delta x E_c \cdot F(x, t + \Delta t).
\]
where \( x \) represents a position in \( D \). The structural optimization problem is thereby replaced with a material distribution problem. Since this characteristic function can be highly discontinuous, some relaxation technique must be introduced for the numerical treatment.

Based on the density approach, Borravall and Petersson (2003) proposed a topology optimization method for minimum energy dissipation in a Stokes flow problem. In this method, the fixed design domain is considered as a porous medium, while the material distribution is expressed either as the presence of fluid or of an impermeable solid domain. In our study, the design variables are defined as \( \gamma (0 \leq \gamma \leq 1) \), with \( \gamma = 0 \) referring to a solid domain \( D \setminus \Omega \), and \( \gamma = 1 \) referring to a fluid domain \( \Omega \). Here, we introduce an artificial body force \( F \) given by:

\[
F = -\alpha \gamma u,
\]

where \( \alpha \gamma \) is defined as

\[
\alpha \gamma = \alpha_{\text{max}} + (\alpha_{\text{min}} - \alpha_{\text{max}}) \frac{\gamma(1 + q)}{\gamma + q},
\]

\( q \) is a tuning parameter to control the convexity of \( \alpha \gamma \). In this study, according to numerical experiments we carried out in advance based on previous studies, we set \( q = 1 \times 10^{-3} \). Since the material distribution of the design domain is represented as a porous medium, \( \alpha \gamma \) is the so-called inverse permeability, as defined in Eq. (20). \( \gamma = 0 \) corresponds to solid domains \( D \setminus \Omega \) with permeability zero, i.e., \( \alpha_{\text{max}} \to \infty \), and \( \gamma = 1 \) corresponds to fluid domains \( \Omega \) with an infinite permeability, i.e., \( \alpha_{\text{min}} = 0 \).

4.2. Pressure drop minimization problem

In this study, we formulate the pressure drop minimization problem for the design of a flow channel that can efficiently transport unsteady fluid between inlets and outlets in an internal flow system. As shown in Fig. 3, the boundaries in this study are divided into three different types: a no-slip boundary \( \Gamma_W \), a prescribed velocity boundary \( \Gamma_V \), and a prescribed pressure boundary \( \Gamma_P \). We apply the boundary conditions for the prescribed velocity and pressure proposed by Zhou and He (1997). The pressure drop minimization problem is formulated as

\[
\begin{align*}
\min_{\gamma} & \quad J = \int_I \int_{\Gamma} -n \cdot (p + |u|^2/2) d\Gamma dt, \\
\text{subject to} & \quad \int_D \gamma d\Omega - V_{\text{max}} \leq 0,
\end{align*}
\]

where \( \Gamma = \Gamma_V \cup \Gamma_W \cup \Gamma_P \), and \( n \) represents the outward normal vector at the boundary. \( J \) is the objective functional that represents the total pressure drop between the inlet and outlet. In this study, we deal with the optimization of unsteady flow, so the time integration of the pressure drop between inlets and outlets must be considered. \( I := [t_0, t_1] \) represents the observation time interval with an arbitrary final time \( t_1 \). \( V_{\text{max}} \) is the volume ratio of fluid with respect to the volume of \( D \).

5. Numerical implementation

In this section, we introduce the numerical implementation of our proposed method. We first describe the optimization algorithm and then explain the sensitivity analysis, based on the GT methodology that is the standard approach for solving optimization problems considering unsteady fluid flows. Next, we discuss the proposed method based on the LT methodology.

5.1. Optimization algorithm

For a general topology optimization based on the GT method, the lattice Boltzmann equations are calculated through the entire time interval and then the adjoint equations are calculated backwards in time using the result of the fluid field.
The procedure for the optimization based on the straightforward GT method includes the following steps (Fig. 4): (a) initial values of the state, adjoint, and design variables are set throughout the fixed design domain $D$; (b) pressure and velocity are calculated by solving the Lattice Boltzmann equation; (c) the objective functional is calculated; (d) if the termination criterion is satisfied, an optimal configuration is obtained and the optimization is finished, otherwise the adjoint equations are calculated and the procedure advances to step (e); (e) the design sensitivities are calculated using the current state and adjoint variables; (f) the design variables $\gamma$ are updated using the Method of Moving Asymptotes (MMA), after which the optimization procedure returns to step (b) of the iterative loop. These procedures are iterated until the following criterion for the value of the objective functional is met:

$$\left| \frac{J_k - J_{k-1}}{J_k} \right| < \epsilon_{opt},$$

where $k$ is the number of optimization steps and $\epsilon_{opt}$ is set as $\epsilon_{opt} = 1.0 \times 10^{-3}$.

5.2. Sensitivity analysis based on global-in-time method

Based on the adjoint lattice Boltzmann method (ALBM) proposed by Krause et al. (2013), we now discuss the sensitivity analysis for the optimization problem discussed in Section 3.2. The basic idea of the ALBM is the utility of the LBM in solving both the state and adjoint fields. Due to the similarity of the locality properties, this approach can make use of highly efficient algorithms, while the design sensitivities can be obtained without using matrix operations. Yaji et al. (2014) first proposed a topology optimization method based on the ALBM, and have recently proposed an improved method (Yaji et al., 2016) that deals with the discrete Boltzmann equation, whereas the original ALBM uses a continuous formulation. In this improved approach, various boundary conditions can be precisely introduced, since the discrete Boltzmann equation incorporates discrete particle velocities that respectively correspond to the boundary conditions in the LBM.

In our study, we implement a sensitivity analysis based on the ALBM incorporating the discrete Boltzmann equation. First, the expanded objective functional is introduced as follows:

$$\bar{J} = J + R,$$

where $R$ is a functional of residual error of the discrete Boltzmann equation, defined as

$$R = \int_D \sum_{i=1}^{\tilde{g}} \tilde{f}_i \left\{ Sh \frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i + \frac{1}{\epsilon_f}(f_i - f_i^{eq}) + 3\alpha_f E_i \epsilon_i \cdot \tilde{u} \right\} d\Omega dt = 0.$$ (24)

According to Yaji et al. (2016), the adjoint equation is defined as

$$-Sh \frac{\partial \tilde{f}_i}{\partial t} - c_i \cdot \nabla \tilde{f}_i = -\frac{1}{\epsilon_f}(\tilde{f}_i - f_i^{eq}) - 3\alpha_f E_i \epsilon_i \cdot \tilde{u},$$ (25)

where $\tilde{u}$ and $f_i^{eq}$ are defined as

$$\tilde{u} = \frac{1}{\rho} \sum_{j=1}^{\tilde{g}} E_j \epsilon_j \tilde{f}_j,$$ (26)
\[ \tilde{j}_i^{\text{eq}} = \tilde{\rho} + 3(c_i - \tilde{u}) \cdot \tilde{j}, \]  
where \( \tilde{\rho} \), and \( \tilde{j} \) are defined as follows (Vergnault and Sagaut, 2014):

\[ \tilde{\rho} = \sum_{j=1}^{e} \tilde{j}_i E_j \left( 1 + 3c_j \cdot \tilde{u} + \frac{9}{2} \mathcal{H}_j^{(2)} : (\tilde{u} \otimes \tilde{u}) \right), \]

\[ \tilde{j} = \sum_{j=1}^{e} \tilde{j}_i E_j (c_j + 3\mathcal{H}_j^{(2)} \tilde{u}), \]

where ‘\( \otimes \)’ and ‘\( : \)’ represent the tensor product and the tensor inner product, respectively. \( \mathcal{H}_j^{(2)} \) represents the second Hermite polynomial in the discrete case and \( \mathcal{H}_j^{(2)} = c_j \otimes c_j - 3\delta \). ‘\( \delta \)’ here is the Kronecker delta. The Gâteaux differential of the expanded objective functional is considered, as follows:

\[ \langle J', \delta\gamma \rangle = \frac{d}{d\theta} J(\gamma + \theta \delta\gamma) \bigg|_{\theta=0} = \int_J \int_D (3\alpha'_f u \cdot \tilde{u}) \delta\gamma d\Omega dt, \]

where \( \alpha'_f \) is defined as

\[ \alpha'_f = (\alpha_{\text{min}} - \alpha_{\text{max}}) \left( \frac{1 + q}{\gamma + q} - \frac{1 + q}{(\gamma + q)^2} \right). \]

Since the adjoint equation (25) has the same construction as that of the discrete Boltzmann equation (4), it can be calculated in the same way as for the lattice Boltzmann equation (10). The adjoint field can be calculated using the following procedure.

**Step 1.**
\[ \tilde{j}_i'(x, c_i \Delta x, t - \Delta t) = \tilde{j}_i(x, t) - \frac{1}{\tau_f} \left( \tilde{j}_i(x, t) - \tilde{j}_i^{\text{eq}}(x, t) \right) \]

**Step 2.**
\[ \tilde{j}_i(x, t - \Delta t) = \tilde{j}_i'(x, t - \Delta t) - 3\Delta \alpha_{\text{f}, f}(x) E \cdot \tilde{c}_i \cdot \tilde{u}(x, t - \Delta t) \]

We note that the directions of convection and time with respect to the adjoint equation are the inverse of those for the LBE. This is a typical feature of adjoint problems in transient optimization problems.

### 5.3. Local-in-time method based optimization using the LBM

With the general implementation of the LT method introduced in Section 2, we now discuss the details of applying the LT method in an optimization using the lattice Boltzmann method.

As mentioned in the foregoing section, at each iteration when using the GT method, the LBE is integrated forward in time whereas the adjoint equation is integrated backwards in time throughout the entire time interval. Since the adjoint variables in Eq. (25) depend on the values of \( f_i \), the solutions of the flow problem must be stored for all time periods over which the optimization problem is solved. As mentioned previously, for three-dimensional time-dependent optimization problems, the storage requirements may become excessive. In this section, the optimization procedure and sensitivity analysis based on the LT method is introduced to reduce the high storage costs of the GT method.

The entire time interval is divided into \( K \) subintervals such that \( t_0 = T_0 < \cdots < T_k = N\Delta t = t_1 \), where \( T_k = \Delta t N_t \). In this paper, \( K = \sqrt{N} \) which is an optimal number according to Yamaleev et al. (2010). \( \Delta t \) is a constant time step, the same interval that is used in the LBE. When calculating the fluid flow, the solution of the LBE obtained at the end of a subinterval \( f_i(x, N_t) \) is used as the initial condition for the calculations of the following interval. Therefore, the partitioning in this method does not alter the solution obtained by the lattice Boltzmann equation. The extended objective functional for time subinterval \( (T_{k-1}, T_k) \) for \( 1 \leq k \leq K \) is given by

\[ J^k = \sum_{k=N_t+1}^{N_t} \left\{ \int_T -n \cdot u(p + |u|^2/2) dt + \int_D \sum_{j=1}^{e} f_i \left( \left( \frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i + \frac{1}{\epsilon_f} (f_i - f_i^{\text{eq}}) + 3\alpha_{\text{f}, f} E \cdot \tilde{c}_i \cdot \tilde{u} \right) d\Omega \right) \right\} \Delta t, \]

so the global objective functional can now be represented as

\[ J = \sum_{k=1}^{K} J^k. \]

The global sensitivity for the entire time interval is calculated as the sum of the local sensitivity derivatives calculated for each subinterval \( (T_{k-1}, T_k) \), as follows:

\[ \langle J', \delta\gamma \rangle = \sum_{k=1}^{K} \langle J^k, \delta\gamma \rangle. \]
For the GT method, the adjoint equations, Eq. (25), are calculated as Eqs. (32) and (33) in two steps, while for the LT method, the local adjoint equation for subinterval \((T_{k-1}, T_k)\) for \(1 \leq k \leq K\) (Eq. (32)) can be derived as follows:

\[
\begin{align*}
\hat{f}_i(x - c_i \Delta x, N_k) - \hat{f}_i(x, N_k + 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, N_k + 1) - \hat{f}_i^{eq}(x, N_k + 1)) \quad \text{(for } n = N_k) \\
\hat{f}_i(x - c_i \Delta x, n) - \hat{f}_i(x, n + 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, n + 1) - \hat{f}_i^{eq}(x, n + 1)) \quad \text{(for } N_{k-1} + 1 \leq n \leq N_k - 1) \\
\hat{f}_i(x - c_i \Delta x, 0) - \hat{f}_i(x, 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, 1) - \hat{f}_i^{eq}(x, 1)) \quad \text{(for } n = 0),
\end{align*}
\]

where \(\hat{f}_i(x, n)\) is the solution of the adjoint equations defined for \(N_{k-1} < n \leq N_k\). In Eq. (37), \(\hat{f}_i(x, N_k + 1)\) requires that the adjoint problem for subinterval \((T_{k-1}, T_k)\) be coupled with the adjoint problem for \((T_k, T_{k+1})\). Hence, the storage cost for the computation of Eq. (37) is equivalent to solving the adjoint problem for the entire time interval \((T_0, T_K)\). To reduce the storage cost, the set of equations in Eq. (37) for \(1 \leq k \leq K\) is decoupled by approximating \(\hat{f}_i(x, N_k + 1)\) as \(\tilde{f}_i\):

\[
\begin{align*}
\left( \tilde{f}_i \right)_m &= \left( \hat{f}_i(x, N_k + 1) \right)_{m-1} \\
\left( \tilde{f}_i \right)_1 &= 0,
\end{align*}
\]

where \(m\) is the iteration number of the optimization procedure. The LT adjoint equations defined for \((T_{k-1}, T_k)\) can be rewritten as follows:

\[
\begin{align*}
\hat{f}_i(x - c_i \Delta x, N_k) - \hat{f}_i(x, N_k + 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, N_k + 1) - \hat{f}_i^{eq}(x, N_k + 1)) \quad \text{(for } n = N_k) \\
\hat{f}_i(x - c_i \Delta x, n) - \hat{f}_i(x, n + 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, n + 1) - \hat{f}_i^{eq}(x, n + 1)) \quad \text{(for } N_{k-1} + 1 \leq n \leq N_k - 1) \\
\hat{f}_i(x - c_i \Delta x, 0) - \hat{f}_i(x, 1) &= -\frac{1}{\tau_i} (\hat{f}_i(x, 1) - \hat{f}_i^{eq}(x, 1)) \quad \text{(for } n = 0),
\end{align*}
\]

where \(\hat{f}_i(x, n)\) represent the local adjoint variables, which are approximations of the corresponding adjoint solutions, \(\tilde{f}_i(x, n)\). Note that the approximated adjoint problem (39) only incurs a storage cost for \((T_{k-1}, T_k)\). Step 2 as in Eq. (33) for the GT approach remains the same as in the LT method.

6. Numerical examples for pressure drop minimization problems

In this section, two- and three-dimensional numerical examples are presented to demonstrate the capability and utility of the proposed topology optimization method using the LBM for unsteady Navier-Stokes flows. The Reynolds number is given by

\[
Re = \frac{LU_{in}}{\nu},
\]

where \(L\) is the characteristic length, the reference speed \(U_{in}\) is defined as the mean speed at the inlet, and \(\nu\) represents the kinematic viscosity of the fluid. In this study, we set \(Re = 1\) for all numerical examples.
GT and LT methods. The fixed design domain is discretized using 100
\[\Delta\] lattices, the value of \(L_{in1}, L_{in2}, L_{in3}\) and \(L_{in4}\) was set as \(L_{in1} = 84, L_{in2} = 67, L_{in3} = 33, L_{in4} = 16\). The optimized result based on the GT method is shown in Fig. 6(a). Snapshots of the optimization procedure are provided in Fig. 7. This result agrees with the result of a topology optimization of unsteady flow using the FEM proposed by Deng et al. (2011). Snapshots of the velocity vector of the unsteady flow at specific points in time are shown in Fig. 8.

To confirm that the optimal result shown in Fig. 6(a) corresponds to a double pipe problem for unsteady flow, we compare this result with that of the same double pipe optimization problem under steady flow. To solve the double pipe problem under steady flow, we impose the velocities obtained through Eq. (42) and Eq. (43) on the inlets, and obtain the optimal designs shown in Fig. 6(b) and (c), respectively. The objective function values of the optimal results shown in Fig. 6(a) and (b) are listed in Table 1.

\[
\begin{align*}
\vec{u}_{in1} &= \vec{u}_i(y - L_{in2})(L_{in1} - y) \\
\vec{u}_{in2} &= \vec{u}_i(y - L_{in3})(L_{in3} - y) \\
\vec{u}_{in3} &= \vec{u}_i(y - L_{in2})(L_{in1} - y) \\
\vec{u}_{in4} &= -\vec{u}_i(y - L_{in3})(L_{in3} - y)
\end{align*}
\]

The optimal result for unsteady flow shown in Fig. 6(a) is different than the results shown in Fig. 6(b) and (c). According to Eq. (41), as \(t \in ([\pi/2, \pi) \cup (3\pi/2, 2\pi])\), fluid flows in from \(\Gamma_{i1}\) (or \(\Gamma_{i2}\)) and flows out from \(\Gamma_{i2}\) (or \(\Gamma_{i1}\)). As shown in Fig. 8(d) and (h), the presence of the vertical channel allows the fluid to flow in from one entrance and flow out from the other one. A cross comparison of the objective function values in Table 1 supports the reasonable conclusion that the vertical channel suppresses the dissipation of pressure.

6.1. Two-dimensional double pipe problem

A double pipe is used to investigate the feasibility of the proposed optimization method (Fig. 5) based on both the GT and LT methods. The fixed design domain is discretized using 100\(\Delta\) lattices. The entire time interval \([t_0, t_1]\) is discretized into \(N = 3600\) time steps. \(\alpha_{min}\) and \(\alpha_{max}\) are set as 0 and \(4 \times 10^2\), respectively, and the volume constraint is set as \(V_{max} = 0.33\).

In this study, the transient velocities at inlets \(\Gamma_{i1}\) and \(\Gamma_{i2}\) are imposed based on Eq. (41), as follows:

\[
\begin{align*}
\vec{u}_{in1} &= \vec{u}_i(y - L_{in2})(L_{in1} - y) \\
\vec{u}_{in2} &= \vec{u}_i(y - L_{in3})(L_{in3} - y) \\
\end{align*}
\]

As shown in Fig. 5, \(L_{in1}\) and \(L_{in2}\) represent the \(y\)-coordinates at both ends of inlet \(\Gamma_{i1}\), while \(L_{in3}\) and \(L_{in4}\) represent that of inlet \(\Gamma_{i2}\). Since the design domain was discretized using 100\(\Delta\) lattices, the value of \(L_{in1}, L_{in2}, L_{in3}\) and \(L_{in4}\) was set as \(L_{in1} = 84, L_{in2} = 67, L_{in3} = 33, L_{in4} = 16\). The optimized result based on the GT method is shown in Fig. 6(a). Snapshots of the optimization procedure are provided in Fig. 7. This result agrees with the result of a topology optimization of unsteady flow using the FEM proposed by Deng et al. (2011). Snapshots of the velocity vector of the unsteady flow at specific points in time are shown in Fig. 8.

Fig. 6 Optimal results: (a) unsteady viscous flow; (b) steady flow with inlet velocity based on Eq. (42); and (c) steady flow with inlet velocity based on Eq. (43).

Fig. 7 Snapshots of optimization procedure for double pipe in Fig.6(a)

![Optimal result for unsteady flow with inlet velocities based on Eq. (41)](image1)

![Optimal result for steady flow with inlet velocities based on Eq. (42)](image2)

![Optimal result for steady flow with inlet velocities based on Eq. (43)](image3)
Fig. 8  Velocity vector snapshots of unsteady double pipe flow corresponding to the optimal design in Fig.6(a).

Fig. 9  Convergence histories of objective functional based on the GT and LT methods.
The same problem is now solved using the LT method. The entire time interval is set as 3600 time steps, with the number of time subintervals $K$ set as $\sqrt{N} = 60$, an optimal number as previously mentioned. For a volume constraint of $V_{\text{max}} = 0.33$, a comparison of the convergence history of the objective functional for the GT and LT methods is provided in Fig. 9. A comparison of the optimal results for different volume constraints based on the LT and GT methods is shown in Fig. 10.

These two figures, (Fig. 9 and Fig. 10), indicate that although the flow path shape and the convergence history of the objective function of LT method are somewhat different in details as GT method, it is understood that the same result as GT method can be obtained by LT method in general. It is therefore reasonable to conclude that the LT method can be applied to topology optimization for unsteady flows using the lattice Boltzmann method.

The optimal results for a volume constraint of $V_{\text{max}} = 0.5$ for different numbers of time subintervals $K$ are shown in Fig. 11, and the convergence histories of the objective functional are shown in Fig. 12. Figure 11 shows that the configurations have similar appearances, and the smaller $K$ is, the more optimal result obtained by LT and GT method resembles because of the possible error caused in the process of approximating. Figure 12 shows that their convergence histories are identical, which means that although the flow path shape are slightly different, LT method was able to provide the same result in minimizing the pressure loss with different $K$. Based on these results, we conclude that the optimization is basically unaffected by the particular number of time subintervals $K$. For the purpose of reducing memory cost, on the other hand, the optimal number of time subintervals is $K = \sqrt{N}$.

We now compare the storage costs for the GT and LT methods. In this study, the computer code was developed in Fortran and run on a PC with a 3.60 GHz CPU (Intel core i7-4790) and 16 GB of RAM. Most of the storage cost due to the parallel computation of velocity distribution functions, which were written in a double-precision floating-point format that occupies 8 bytes of computer memory per function. For the D2Q9 100 $\times$ 100 lattice with 3600 time steps, a memory requirement of $8 \times 100 \times 100 \times 3600 \times 9 = 2592$MB would be required when using the GT method, while only $8 \times 100 \times 100 \times (3600/60 + 60) \times 9 = 86.4$MB are required for the LT method. Therefore, we can confirm that the LT method efficiently reduces the storage cost.

### 6.2. Three-dimensional problem

Here, we discuss a three-dimensional problem for pressure drop minimization. We consider the problem shown in Fig. 13, with the volume constraint set as $V_{\text{max}} = 0.2$. The inlets and outlets are circles of identical radius. As shown in Fig. 13, $R_1, R_2, R_3$ and $R_4$ refer to four points at the centers of the inlet and outlet circles, with their coordinates listed in Table 6.2. The analysis domain is discretized using $80\Delta x \times 80\Delta x \times 80\Delta x$ lattices. The velocities set at the inlets are
formulated as follows:

\[ \begin{align*}
    u_{in1} &= u_{in}(1 - \frac{(y-y_1)^2 + (z-z_1)^2}{R_1^2}) \cos(t) \quad t \in [0, 2\pi] \\
    u_{in2} &= u_{in}(1 - \frac{(y-y_2)^2 + (z-z_2)^2}{R_2^2}) \sin(t) \quad t \in [0, 2\pi],
\end{align*} \tag{44} \]

where \( u_{in1} \) and \( u_{in2} \) are the velocities at the inlets with centers \( R_1 \) and \( R_2 \), respectively. \( R \) represents the radius of inlet circles, while \( y_1, y_2, z_1 \) and \( z_2 \) represent the \( y \)- and \( z \)-coordinates of these circles’ centers respectively.

Figure 14 shows the optimal configuration for this problem, in different orientations. The result validates that the proposed method can be successfully applied to a three-dimensional case. For this problem, we also considered optimizations using different numbers of time subintervals \( K \). The obtained configurations are shown in Fig. 15, and the convergence histories of the objective functional are displayed in Fig. 16. Since the configurations closely resemble each other, and the convergence histories are identical, we conclude that the optimization results are essentially independent of the numbers of time subintervals \( K \) for 3-D problems.

7. Conclusion

This paper presented a topology optimization method for unsteady incompressible viscous flows based on the LBM and the local-in-time discrete adjoint-based method. The method was applied to two- and three-dimensional pressure drop minimization problems. We achieved the following:

1. A topology optimization problem was formulated for a pressure drop minimization problem under unsteady incompressible viscous flows based on the LBM. The unsteady fluid flow was governed by the Navier-Stokes equations and calculations were based on the lattice Boltzmann equation. The design sensitivity was derived based on the ALBM.

2. An algorithm was formulated based on the local-in-time discrete adjoint-based methodology for the topology optimization problem, using the LBM. The local design sensitivities were calculated for time subintervals using the ALBM and the global design sensitivity was derived as the sum of all local sensitivities.

3. Two- and three-dimensional numerical examples were provided to validate the utility of the LT-based topology optimization method. Optimal designs obtained by the GT and LT methods were compared. Identical objective functional

Fig. 11  Optimal results for different numbers of time subintervals: (a) \( K = 10 \); (b) \( K = 60 \); and (c) \( K = 200 \).

Fig. 12  Objective functional convergence histories for different numbers of time subintervals \( K \).
Fig. 13  Design setting for the three-dimensional problem.

Table 2  Optimization parameter values

|          | \( R_1 \) coordinates | \( R_2 \) coordinates | \( R_3 \) coordinates | \( R_4 \) coordinates | Radius | \( V_{max} \) |
|----------|-------------------------|------------------------|------------------------|------------------------|--------|--------------|
|          | (1,60,20)               | (1,60,20)              | (80,20,20)             | (80,60,60)             | 10     | 0.2          |

Fig. 14  Optimal configuration of the three-dimensional problem. The iso-surface of \( \gamma = 0.5 \) is shown as the optimal configuration.
Fig. 15  Optimal results for different numbers of time subintervals: (a) $K = 40$; (b) $K = 60$; and (c) $K = 200$.

Fig. 16  Convergence histories of objective functional for different numbers of time subintervals $K$ in 3-D problem.
convergence rates were observed and the obtained optimal configurations based on the proposed method were similar to those obtained by FEM-based and GT-based methods used in previous studies.

(4) Optimal designs for different numbers of time subintervals $K$ were compared, with only minor differences observed in the obtained optimal configurations. The dramatic reduction in the cost of data storage provided by the presented LT method validates its effectiveness for topology optimization problems where memory storage is an issue. These properties of the LT method enable it to solve realistic large-scale time-dependent design optimization problems.

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