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Continuous and Discrete Adjoint Approach Based on Lattice Boltzmann Method in Aerodynamic Optimization Part I: Mathematical Derivation of Adjoint Lattice Boltzmann Equations

Mohamad Hamed Hekmat* and Masoud Mirzaei

Center of Excellence for Design & Simulation of Space Systems, K. N. Toosi University of Technology, Tehran, 891567, Iran

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Abstract. The significance of flow optimization utilizing the lattice Boltzmann (LB) method becomes obvious regarding its advantages as a novel flow field solution method compared to the other conventional computational fluid dynamics techniques. These unique characteristics of the LB method form the main idea of its application to optimization problems. In this research, for the first time, both continuous and discrete adjoint equations were extracted based on the LB method using a general procedure with low implementation cost. The proposed approach could be performed similarly for any optimization problem with the corresponding cost function and design variables vector. Moreover, this approach was not limited to flow fields and could be employed for steady as well as unsteady flows. Initially, the continuous and discrete adjoint LB equations and the cost function gradient vector were derived mathematically in detail using the continuous and discrete LB equations in space and time, respectively. Meanwhile, new adjoint concepts in lattice space were introduced. Finally, the analytical evaluation of the adjoint distribution functions and the cost function gradients was carried out.

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1 Introduction

Adjoint method is one of the gradient-based techniques in which cost function gradient vector with respect to design variables is calculated indirectly by solving an adjoint equ-

*Corresponding author.
Email: mhekmat@dena.kntu.ac.ir (M. H. Hekmat), mirzaei@kntu.ac.ir (M. Mirzaei)

ation. Although, there is an additional cost arising from solving the adjoint equation, the gradients of cost function can be altogether achieved with respect to each design variable. Consequently, the total cost to obtain these gradients is independent of the number of design variables and amounts to the cost of two flow solution roughly [1]. There are two approaches to develop the adjoint equation: continuous and discrete. Continuous adjoint approach utilizes the differential forms of flow field governing equations and cost function. Variations of the cost function and the flow field equations with respect to the flow field variables and the design variables are combined through the use of Lagrange multipliers, also called adjoint variables. Via gathering the terms associated with the variation of the flow field variables, the adjoint equation and its boundary conditions are reached. The terms associated with the variation of the design variables produce the cost function gradient vector. The flow field equations and the adjoint equation with its boundary conditions must finally be discretized using suitable numerical methods. In this approach, physical significance of the adjoint variables is very clear, since we are dealing with a continuous differential equation that can be solved even analytically in some special cases. But, in the discrete adjoint approach, the adjoint equation is directly extracted from a set of discrete flow field equations and cost function gained from numerical approximation of the equations. Discrete adjoint equation is derived by collecting together all the terms multiplied by the variation of the discrete flow variables. Major disadvantage of this approach is the complexity of the adjoint equation derived from the discrete flow field (Navier-Stokes) equations; so that the complete extraction of all the discrete terms in the adjoint equation and the gradient vector requires a lot of algebraic manipulations. In addition, the viscous flux in the Navier-Stokes (NS) equations further increases the complexity of deriving them in viscous flows. The discrete adjoint equation becomes very complicated when the flow field (NS) equations are discretized with higher order schemes and using flux limiters. Therefore cost of discrete equation derivation from the NS equations is more while the implementation of the continuous adjoint method is very simple. The discrete adjoint method requires more computational efforts in comparison with the continuous one. Another critical issue of interest is the relative accuracy of the calculated gradients by the two approaches. The continuous adjoint approach provides the inexact gradient to the exact cost function. On the other hand, the discrete adjoint approach provides the exact gradient to the inexact cost function [2]. Here, the exact cost function is defined as the continuous form of the cost function, and the inexact cost function as the value computed from the discrete field equations and the boundary conditions. In other words, the continuous gradient is calculated from the discretized continuous adjoint equation, derived from the continuous flow field equations and cost function. Therefore, the continuous gradient is not exactly consistent with the cost function which is evaluated numerically. The advantage of the discrete adjoint method is that the resulting discrete gradient is exactly consistent with the discrete cost function and the method does not suffer from this inconsistency. Therefore resulting gradients from discrete method have more consistency with resulting gradients from finite difference method. In this case, however, the difference between discrete and continuous methods is often negligible.

In numerical optimization problems, there are factors that affect the efficiency of an optimization method in real and practical issues, thereby restricting or extending the applicability of the method. The most important of these factors are implementation and computational costs. Regardless of the inherent limitations of various optimization techniques, methods which have lower implementation and computational costs have higher efficiencies and would be more useful in practice. In comparison with the conventional flow field (NS) equations, the LB method uses the Boltzmann transport equation to solve the flow field that is less complicated. Therefore, the implementation of this method would be considerably easier. Importance of this benefit will become more conspicuous when a gradient technique is exploited in optimization problems involving the flow field equations (irrespective of the flow field solution) in optimization process. Simplicity of the Boltzmann equation, as an alternative to the conventional flow field equations, can be very helpful in facilitating the process of extracting the continuous adjoint equation (and particularly the discrete adjoint equation). The conventional numerical solution methods for flow equations such as finite volume and finite element approaches usually use body-fitted grid systems i.e., regular structured and unstructured grids to discretize the solution domain. Application of these types of grids to the complex three-dimensional problems is very difficult. This issue becomes more intricate when analyzing the flow fields with moving boundaries or in some optimization problems. Besides, accuracy and numerical robustness strongly depend on the grid quality. These challenges can be overcome utilizing immersed boundary techniques [3]. Nevertheless, the LB method uses inherently immersed boundary grid system. This unique feature of the LB method enables the modeling of complicated geometries and the analysis of flows around them, straightforwardly and without the need for conventional body-fitted grid generation. So, through exploiting the LB method, the optimization of special geometries is done with lower cost. Furthermore, it can remove the drawbacks of non-gradient techniques, which necessitate a lot of flow solutions (due to the selective random design variables) and consequently the application of grid generation. Additionally, in gradient methods, there is no need to consider some grid modification techniques. The inherent parallel processing nature of the LB method owing to data transfer from the nearest neighbor in terms of streaming and fully localized calculations of collision phase, distinguishes it from the conventional methods of computational fluid dynamics. This capability of the LB method seems to be very effective in the analysis of complex unsteady flows and in some cases like optimization with a lot of design variables or constraints that demand long computational times. As a result, it is possible that some optimization techniques are employed which are not efficient for computational fluid dynamics due to the high computational cost (e.g., adjoint method in problems with high number of constraints or non- gradient methods in problems with high number of design variables). Hence, the significance of flow optimization utilizing the LB method becomes obvious regarding its advantages as a novel flow field solution method compared to the other conventional techniques.

Execution of the adjoint optimization approach by means of conventional NS-based computational methods has been extensively studied in recent decades, for instance, through the works of Jameson [4–6], Elliot and Peraire [7], Nadarajah [8], Hekmat et al. [9, 10], Tonomura et al. [11], Peter and Dwight [12], Hicken and Zingg [13] and Freund [14]. Nonetheless, there are few researches in combination of the adjoint method and the LB method. Tekitek et al. [15], for the first time, performed the discrete adjoint approach via the LB method. They extracted the discrete adjoint equation based on the LB equation to identify the unknown parameters of the LB method without representing a general framework or new concepts, or evaluating the details of the adjoint variables and gradients. In addition, Pingen et al. [16, 17] explored the ability of the incompressible LB method in topology optimization problems. Their major work was focused on the extraction of steady discrete adjoint equation and gradient of cost function using the steady LB equation and its implicit solution. Moreover, they examined the performance of mathematical algorithms (e.g., iterative and direct algorithms) to solve these equations implicitly. Their research was restricted to optimization in steady flows and did not offer an overall framework for implementation and computation. Krause et al. [18] derived the continuous adjoint equation by means of the continuous Boltzmann equation for optimization in incompressible flows. The negative aspect of their suggested approach was the intricacy of the extraction process and consequently, high implementation cost. The study only included the continuous adjoint method and did not discuss the discrete adjoint method.

In the present research, for the first time, both continuous and discrete adjoint approaches were scrutinized via the LB method. This study introduced a general framework with low complexity to apply the continuous and discrete adjoint approaches based on the LB method. The proposed procedure was not restricted to flow fields and could be exploited for both steady and unsteady flows. Firstly, the continuous and discrete adjoint LB equations and the cost function gradient vector were derived mathematically in detail using the continuous and discrete LB equations in space and time, respectively. Also, new adjoint concepts in lattice space were established. Introduction of these concepts can be useful in applying the LB equation solution strategies to the adjoint equations. Eventually, the analytical evaluation of the adjoint distribution functions and the cost function gradients was accomplished.

2 Lattice Boltzmann method

Unlike the conventional numerical methods of the flow field solution based on the discretization continuous macroscopic equations, the LB method is based on the mesoscopic kinetic equations. The basic idea of this method is to construct simple kinetic models which consider the microscopic processes so that the macroscopic averaged properties follow the considered macroscopic equations. Because of molecular and kinetic nature of the LB method, it has properties that distinguish it from other conventional computational fluid dynamics methods.

2.1 Lattice Boltzmann equation

There are two ways to extract LB equation. The first way is using the lattice gas automata (LGA) and substitution of the average of the Boolean occupation number with the particle distribution function [19]. The second way is derivation of LB equation using the Boltzmann transport equation. The Boltzmann transport equation is based on the kinetic theory of gases and it describes the statistical interaction of particles at the molecular level. For a system without an external force, the Boltzmann equation can be written as

$$\frac{\partial f}{\partial t}+c\cdot\nabla f=\Omega, \tag{2.1}$$

where $f=f(x,c,t)$ is the density distribution function, c is the particle velocity vector, x is location vector in physical space, t is time and $\Omega=\Omega(f)$ is the collision operator. The solution of the Boltzmann equation is very difficult due to the presence of the collision term. But in 1954, the simple model of BGK for the collision operator was presented [20]:

$$\Omega=\omega(f^{eq}-f)=\frac{1}{\lambda}(f^{eq}-f). \tag{2.2}$$

The coefficient ω is called the collision frequency and λ is called the relaxation time. The local equilibrium distribution function is denoted by f^{eq}. After introducing BGK approximation, the Boltzmann equation (2.1) can be approximated as

$$\frac{\partial f}{\partial t}+c\cdot\nabla f=\frac{1}{\lambda}(f^{eq}-f). \tag{2.3}$$

In the LB method, the above equation is discretized in velocity or phase space and assumed it is valid along specific directions, linkages. Hence, the discrete Boltzmann equation can be written along i direction as

$$\frac{\partial f_i}{\partial t}+c_i\cdot\nabla f_i=\frac{1}{\lambda}(f_i^{eq}-f_i), \tag{2.4}$$

where f_i is the distribution function along i direction and f_i^{eq} is the corresponding local equilibrium distribution function. The left-hand side of the above equation represents the streaming or propagation process, where the distribution function streams along the lattice link i with velocity $c_i=\Delta x/\Delta t$ (Δx and Δt are displacement and time steps, respectively) and the right-hand side represents the rate of change of the distribution function in the collision process. Eq. (2.4) is now discretized with respect to space and time, using a first order upwind finite difference approximation in time and space, resulting in the discretized LB equation:

$$\frac{f_i(x,t+\Delta t)-f_i(x,t)}{\Delta t}+c_i\cdot\frac{f_i(x+\Delta x,t+\Delta t)-f_i(x,t+\Delta t)}{\Delta x}=\frac{1}{\lambda}[f_i^{eq}(x,t)-f_i(x,t)]. \tag{2.5}$$

Since $c_i = \Delta x/\Delta t$, Eq. (2.5) can be simplified as

$$f_i(x+c_i\Delta t, t+\Delta t) = (1-\beta)f_i(x,t) + \beta f_i^{eq}(x,t), \tag{2.6}$$

where $\beta = \Delta t/\lambda$ is inverse of dimensionless relaxation time. Relation (2.6) is fully discretized LB equation in time, location space and velocity space.

In an incompressible flow, ideally, so that the divergence of the velocity is zero, the density is assumed equal to initial density, i.e., $\rho = \rho_0$. Therefore, Assuming an order $\mathcal{O}(Ma^2)$ density fluctuation, the equilibrium distribution function in relation (2.6) is obtained using Taylor series expansion of Maxwell-Boltzmann equilibrium distribution and ignoring $\mathcal{O}(Ma^3)$ terms or higher [19, 21]:

$$f_i^{eq} = w_i\rho\left\{1 + \frac{3(c_i\cdot u)}{c^2} + \frac{9(c_i\cdot u)^2}{2c^4} - \frac{3u^2}{2c^2}\right\} \equiv w_i\rho\Theta_i, \tag{2.7}$$

where $u \equiv u(x,t)$ and $\rho \equiv \rho(x,t)$ are the macroscopic velocity vector and density, respectively. Also, w_i is the lattice weight parameter in i direction that depends on the lattice arrangement.

2.2 D2Q9 model

In LB method, the solution domain needs to be divided into lattices. At each lattice node, the factitious particles (distribution function) reside. Some of these particles stream along specified directions to the neighboring nodes. The number of directions of particle movements depends on the lattice arrangement. In this study, the two-dimensional, nine velocity D2Q9 lattice model is used. In this model, the number of velocity vectors in each lattice node is equal to 8 and one stationary particle also is considered in each node with zero velocity (see Fig. 1).

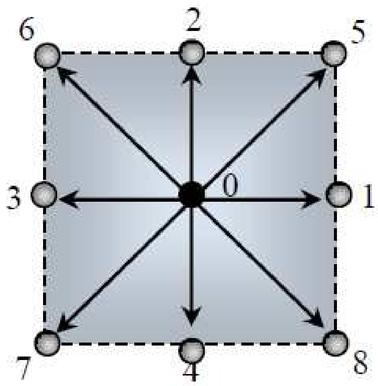

Figure 1: Lattice Arrangement of the D2Q9 Model.

These velocity vectors, $c_i=(c_{ix},c_{iy})$, can be written as

$$c_i=\begin{cases}(0,0), & i=0,\\ (\cos[(i-1)\pi/2],\sin[(i-1)\pi/2])c, & i=1,2,3,4,\\ \sqrt{2}(\cos[(i-5)\pi/2+\pi/4],\cos[(i-5)\pi/2+\pi/4])c, & i=5,6,7,8.\end{cases} \tag{2.8}$$

For the D2Q9 model, the lattice weight parameters w_i are as [19],

$$w_i=\begin{cases}4/9, & i=0,\\ 1/9, & i=1,2,3,4,\\ 1/36, & i=5,6,7,8.\end{cases} \tag{2.9}$$

For low Mach number $(Ma\ll1)$ or low density fluctuation $(\Delta\rho/\rho\ll1)$ flows, it is possible to recover the macroscopic incompressible NS equations from the LB equation using the Chapman-Enskog expansion and choosing kinematic viscosity ν as [16]

$$\nu=\frac{1}{6\beta}(2-\beta)\frac{\Delta x^2}{\Delta t}. \tag{2.10}$$

Also, the macroscopic properties such as density ρ and velocity vector $u=[u^x,u^y]^T$ in lattice units can be evaluated by taking statistical moments of the distribution function, leading to the following equations:

$$\rho=\sum_{i=0}^{8}f_i(x,t),\quad u=\frac{1}{\rho}\sum_{i=0}^{8}c_if_i(x,t). \tag{2.11}$$

There are three notable points about LB method. First, although the standard LB method is used for simulation of incompressible flows, in this method, density is not constant $(\Delta\rho\approx\mathcal{O}(Ma^2))$. Second, in the standard LB method, pressure $p\equiv p(x,t)$ is related to density using the ideal gas equation of state:

$$p=c_s^2\rho, \tag{2.12}$$

where the lattice speed of sound c_s is $c/\sqrt{3}$ for the D2Q9 model [21]. And finally, to facilitate the implementation of LB method, it is common to chose time step Δt and lattice spacing Δx equal to 1 $(c=1)$.

3 Optimization problem statement

On the whole, an aerodynamic optimization problem in an unsteady flow based on the LB method can be expressed in the following general form:

$$\underset{F\in R^9,\kappa\in R^n}{Min I}(F,\kappa)\quad s.t.\ H_t(F,\kappa)=0,\quad t\in[0,t_f]. \tag{3.1}$$

Where $F=[f_i(x,t)]^T_{i=0,\cdots,8}$ is the distribution functions vector, κ is the n-dimensional design variables vector and H_t is the LB equation as a flow field governing equation. I is the value of cost function at the time interval of $[0,t_f]$ that can be written in the general form as

$$I(F,\kappa)=\int_0^{t_f} I_t(F,\kappa)dt=\int_0^{t_f}\int_D I_{tx}(F,\kappa)dDdt, \tag{3.2}$$

where I_t is the cost function at time t and D is the flow field domain on which the cost function is integrated. By utilizing numerical integration rule and supposing that $\Delta x=\Delta t=1$, the cost function (3.2) can be evaluated as

$$I(F,\kappa)=\sum_{t=0}^{t_f} I_t(F,\kappa)=\sum_{t=0}^{t_f}\sum_x I_{tx}(F,\kappa), \tag{3.3}$$

where $\sum_x$ is performed over all the lattice points of D. The design problem is now treated as a control problem wherein the design variables vector depicts the control function, chosen to minimize I exposed to the constraint of satisfaction of the LB equation at any time, any point of the lattice space and any direction of the lattice lines.

3.1 Cost function

The choice of cost function and design variables is one of the most crucial steps in any optimization problem. In fact, the success of an optimization method strongly depends on both the choice of the design variables and the cost function.

The inverse problem is employed, in this study, to validate the adjoint equation, the gradient vector acquired from the LB method and the applied optimization algorithm. Therefore, the target flow field is selected using the target design variables. Subsequently, assuming unknown values for the target design variables, it is favorable to find the optimal design variables that lead to the target flow field. Hence, the local cost function in flow field D at time t can be described as

$$I_{tx}=\frac{1}{2}|w-w_{desired}|^2, \tag{3.4}$$

where $w\equiv w(x,t)=[\rho,u^x,u^y]^T\in R^3$ is the flow field variables vector and $w_{desired}$ is the target flow field variables vector.

3.2 Design variables

In this investigation, the external body forces vector applied to the fluid is regarded as the design variables vector. Thus, the expression

$$V_i=c_s^2(c_i\cdot\kappa) \tag{3.5}$$

is added to the collision term (2.2). In the above equation, $\kappa=[\kappa^x,\kappa^y]^T\in R^2$ is the 2-D body forces (design variables) vector and the dot $(\cdot)$ denotes the scalar product. It can be shown that the existence of the force term (3.5) in the LB equation results in the recovery of the NS equations in the presence of the body force κ [19].

4 Continuous adjoint approach based on lattice Boltzmann method

Up to now, only Krause et al. [18] have applied the continuous adjoint sensitivities in an LB method framework, focusing on the identification of optimal parameters using an adjoint LB formulation. It is to be noted that, in the adjoint approach, generally, the expression for the extracted adjoint equation depends on the definition of the cost function and the design variables vector and therefore on the details of a considered problem. Consequently, according to the intricacy of the extraction process of the continuous adjoint equation reported in [18], if one wants to solve an optimization problem by applying this adjoint based strategy, he/she needs to derive again an analytical expression for the adjoint equation with high implementation cost. In this section, we derive mathematically the continuous adjoint equation and the cost function gradient vector based on the LB equation using the similar procedure reported by Jameson [4]. The proposed approach can be performed similarly for any optimization problem by the corresponding cost function and design variables vector but with a lower implementation cost.

4.1 Derivation of continuous adjoint equation based on lattice Boltzmann method

As previously stated, in the continuous adjoint method, continuous cost function and continuous governing flow field equations are used to derive the continuous adjoint equation and the gradient vector of the cost function. Consider the general continuous form of the cost function (3.2). Since the distribution function f_i depends on the design variables vector κ implicitly, a variation $\delta\kappa$ in the design variables vector causes a variation δf_i in the distribution function and consequently, accordingly, a variation δI in the cost function

$$\delta I=\int_0^{t_f}\int_D\Big(\sum_{i=0}^{8}\frac{\partial I_{tx}}{\partial f_i}\delta f_i+\frac{\partial I_{tx}}{\partial\kappa}^T\delta\kappa\Big)dDdt. \tag{4.1}$$

Now, consider the continuous LB equation in time and space (2.4) with the inserted force term (3.5),

$$\frac{\partial f_i}{\partial t}+c_i\cdot\nabla f_i=\frac{1}{\lambda}(f_i^{eq}-f_i)+c_s^2(c_i\cdot\kappa). \tag{4.2}$$

This equation is the constraint of the optimization problem (3.1) and must be satisfied at any time, any point of the lattice space, and any direction of the lattice lines. As a consequence, a variation in the distribution function f_i because of a variation in the design variables κ is such that the Eq. (4.2) will be always satisfied. So, we have

$$\frac{\partial}{\partial t}\delta f_i+c_i\cdot\nabla\delta f_i-\frac{1}{\lambda}\Big(\sum_{j=0}^{8}\frac{\partial f_i^{eq}}{\partial f_j}\delta f_j-\delta f_i\Big)-c_s^2(c_i\cdot\delta\kappa)=0. \tag{4.3}$$

Now, multiplying the Lagrange multiplier (adjoint variable) $\psi_i\equiv\psi_i(x,t)$ to Eq. (4.3), then summing the products over the entire lattice line directions and ultimately integrating over time and space, we get

$$\begin{aligned}&\int_0^{t_f}\int_D\sum_{i=0}^{8}\psi_i\frac{\partial}{\partial t}\delta f_i dDdt+\int_0^{t_f}\int_D\sum_{i=0}^{8}\psi_i(c_i\cdot\nabla\delta f_i)dDdt\\ &\quad-\frac{1}{\lambda}\int_0^{t_f}\int_D\sum_{i=0}^{8}\Big[\sum_{j=0}^{8}\psi_i\frac{\partial f_i^{eq}}{\partial f_j}\delta f_j-\psi_i\delta f_i\Big]dDdt-c_s^2\int_0^{t_f}\int_D\sum_{i=0}^{8}\psi_i(c_i\cdot\delta\kappa)dDdt=0.\end{aligned} \tag{4.4}$$

Assuming that ψ_i is differentiable, the first term in the above equation can be rewritten via integration by parts, as follows:

$$\int_0^{t_f}\int_D\sum_{i=0}^{8}\psi_i\frac{\partial}{\partial t}\delta f_i dDdt=\sum_{i=0}^{8}\int_D\Big([\psi_i\delta f_i]_0^{t_f}-\int_0^{t_f}\frac{\partial\psi_i}{\partial t}\delta f_i dt\Big)dD. \tag{4.5}$$

Likewise, for the second term in Eq. (4.4) via integration by parts and utilizing the vector identities, we have

$$\begin{aligned}\int_0^{t_f}\int_D\sum_{i=0}^{8}\psi_i(c_i\cdot\nabla\delta f_i)dDdt&=\sum_{i=0}^{8}\int_0^{t_f}\Big(\int_B\psi_i(c_i\cdot n)\delta f_i dB-\int_D\nabla\cdot(\psi_i c_i)\delta f_i dD\Big)dt\\ &=\sum_{i=0}^{8}\int_0^{t_f}\Big(\int_B\psi_i(c_i\cdot n)\delta f_i dB-\int_D[\psi_i(\nabla\cdot c_i)+c_i\cdot\nabla\psi_i]\delta f_i dD\Big)dt\\ &=\sum_{i=0}^{8}\int_0^{t_f}\Big(\int_B\psi_i(c_i\cdot n)\delta f_i dB-\int_D(c_i\cdot\nabla\psi_i)\delta f_i dD\Big)dt,\end{aligned} \tag{4.6}$$

where n is the unit vector perpendicular to the boundary B of the flow field domain D. It should be noted that according to Eq. (2.8), the velocity vector, c_i is constant at any direction of the lattice lines. Therefore, for any time and any point of the lattice space, $\nabla\cdot c_i$ is equal to zero at any direction of the lattice lines. Now, substituting Eqs. (4.5) and (4.6) into (4.4) and collecting together all the terms associated with the variation of the distribution function δf_i and also gathering all the terms included to the variation of the design variables vector $\delta\kappa$ and rearranging them, we have

$$\begin{aligned}&\sum_{i=0}^{8}\int_0^{t_f}\int_D\Big(-\frac{\partial\psi_i}{\partial t}-c_i\cdot\nabla\psi_i-\frac{1}{\lambda}\Big(\sum_{j=0}^{8}\psi_j\frac{\partial f_j^{eq}}{\partial f_i}-\psi_i\Big)\Big)\delta f_i dDdt+\sum_{i=0}^{8}\int_0^{t_f}\int_B\psi_i(c_i\cdot n)\delta f_i dBdt\\&\quad+\sum_{i=0}^{8}\int_D[\psi_i\delta f_i]_0^{t_f}dD-c_s^2\sum_{i=0}^{8}\int_0^{t_f}\int_D\psi_i(c_i\cdot\delta\kappa)dDdt=0.\end{aligned}\tag{4.7}$$

As the left hand expression equals zero, it can be subtracted from the variation (4.1) with no change in the result to give

$$\begin{aligned}\delta I=&\int_0^{t_f}\int_D\Big(\sum_{i=0}^{8}\frac{\partial I_{tx}}{\partial f_i}\delta f_i+\frac{\partial I_{tx}}{\partial\kappa}^T\delta\kappa\Big)dDdt\\&+\sum_{i=0}^{8}\int_0^{t_f}\int_D\Big(\frac{\partial\psi_i}{\partial t}+c_i\cdot\nabla\psi_i+\frac{1}{\lambda}\Big(\sum_{j=0}^{8}\psi_j\frac{\partial f_j^{eq}}{\partial f_i}-\psi_i\Big)\Big)\delta f_i dDdt\\&-\sum_{i=0}^{8}\int_0^{t_f}\int_B\psi_i(c_i\cdot n)\delta f_i dBdt-\sum_{i=0}^{8}\int_D[\psi_i\delta f_i]_0^{t_f}dD+c_s^2\sum_{i=0}^{8}\int_0^{t_f}\int_D\psi_i(c_i\cdot\delta\kappa)dDdt.\end{aligned}\tag{4.8}$$

Collecting together all the terms associated with the variation of the distribution function δf_i and also gathering all the terms included to the variation of the design variables vector $\delta\kappa$ and rearranging, we have

$$\begin{aligned}\delta I=&\Big[\sum_{i=0}^{8}\int_0^{t_f}\int_D\Big(\frac{\partial\psi_i}{\partial t}+c_i\cdot\nabla\psi_i+\frac{1}{\lambda}\Big(\sum_{j=0}^{8}\psi_j\frac{\partial f_j^{eq}}{\partial f_i}-\psi_i\Big)+\frac{\partial I_{tx}}{\partial f_i}\Big)\delta f_i dDdt\Big]_{I_1}\\&-\Big[\sum_{i=0}^{8}\int_0^{t_f}\int_B\psi_i(c_i\cdot n)\delta f_i dBdt\Big]_{I_2}-\Big[\sum_{i=0}^{8}\int_D[\psi_i\delta f_i]_0^{t_f}dD\Big]_{I_3}\\&+\Big[\sum_{i=0}^{8}\int_0^{t_f}\int_D\Big(\frac{\partial I_{tx}}{\partial\kappa}^T+c_s^2\psi_i c_i^T\Big)\delta\kappa dDdt\Big]_{II}.\end{aligned}\tag{4.9}$$

Here, subscripts I and II are exploited to indicate the contributions of δf_i from the change associated directly with $\delta\kappa$ in the variation of the cost function δI. Now, the adjoint variable ψ_i is chosen such that changes of the cost function are independent from changes of the flow field variables. As a result, by setting the term I_1 equal to zero in the above equation, the continuous adjoint equation in time and space is attained

$$-\frac{\partial\psi_i}{\partial t}-c_i\cdot\nabla\psi_i=\frac{1}{\lambda}\Big(\sum_{j=0}^{8}\psi_j\frac{\partial f_j^{eq}}{\partial f_i}-\psi_i\Big)+\frac{\partial I_{tx}}{\partial f_i}.\tag{4.10}$$

Furthermore, by setting the term I_2 equal to zero, the adjoint boundary condition

$$\psi_i(c_i\cdot n)=0.\tag{4.11}$$

And, by setting the term I_3 equal to zero and considering constant initial conditions of the flow field solution in the optimization process, the adjoint terminal condition

$$\psi_i(t_f)=0 \tag{4.12}$$

are obtained. The design variable ψ_i is achieved by solving the adjoint equation (4.10) along with the adjoint boundary condition (4.11) and the adjoint terminal condition (4.12); so that the variation of the cost function δI is independent from the variation of the distribution function δf_i. Thus, eliminating the terms I_1 to I_3, we have

$$\delta I=G^T\delta\kappa, \tag{4.13}$$

where

$$G^T=\nabla_\kappa I=\sum_{i=0}^{8}\int_0^{t_f}\int_D\Big(\frac{\partial I_{tx}}{\partial\kappa}^T+c_s^2\psi_i c_i^T\Big)dDdt. \tag{4.14}$$

4.2 Interpretation of the continuous adjoint equation in lattice space

Consider the continuous adjoint equation (4.10). It can be seen that its structure is quite similar to the LB equation. Accordingly, Eq. (4.10) is called the continuous adjoint LB equation. Meanwhile, the adjoint variable ψ_i corresponding to the distribution function f_i can be referred as the adjoint distribution function along i direction. The left hand side term actually displays the adjoint streaming process. In addition, the adjoint collision operator that illustrates the rate of change of the adjoint distribution function in the adjoint collision process can be defined as

$$\sigma_i=\omega(\psi_i^{eq}-\psi_i)=\frac{1}{\lambda}(\psi_i^{eq}-\psi_i), \tag{4.15}$$

where

$$\psi_i^{eq}=\sum_{j=0}^{8}\psi_j\frac{\partial f_j^{eq}}{\partial f_i} \tag{4.16}$$

is called the adjoint equilibrium distribution function. Finally, the adjoint LB equation (4.10) may be rewritten as

$$-\frac{\partial\psi_i}{\partial t}-c_i\cdot\nabla\psi_i=\frac{1}{\lambda}(\psi_i^{eq}-\psi_i)+\hat{V}_i, \tag{4.17}$$

where $\hat{V}_i=\partial I_{tx}/\partial f_i$.

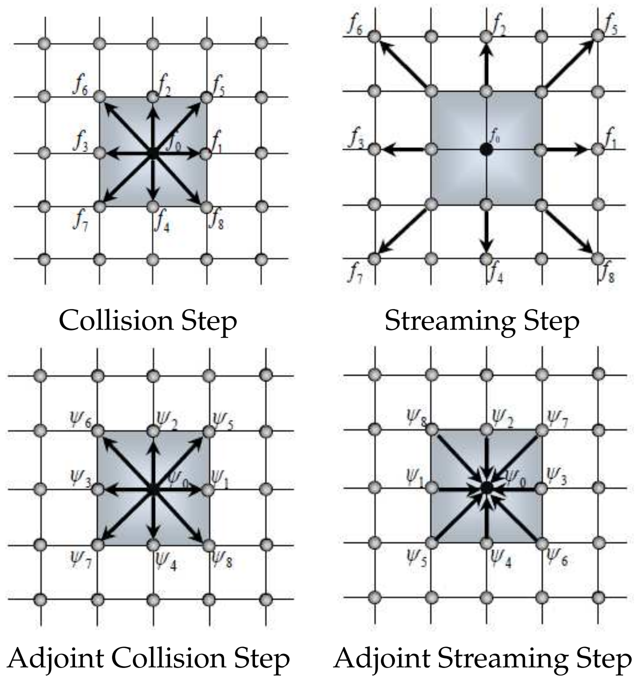

Figure 2: Streaming Steps of the LB and the Adjoint LB Equations.

Unlike the LB equation that needs the initial conditions to be solved, the adjoint LB equation possesses the terminal condition (4.12). Therefore, Eq. (4.17) can be discretized in space and time as follows:

$$-\frac{\psi_i(x,t)-\psi_i(x,t-\Delta t)}{\Delta t}-c_i\cdot\frac{\psi_i(x,t-\Delta t)-\psi_i(x-\Delta x,t-\Delta t)}{\Delta x}$$
$$=\frac{1}{\lambda}[\psi_i^{eq}(x,t)-\psi_i(x,t)]+\hat{V}_i(x,t). \tag{4.18}$$

Since $c_i=\Delta x/\Delta t$, the above equation can be simplified as

$$\psi_i(x-c_i\Delta t,t-\Delta t)=(1-\beta)\psi_i(x,t)+\beta\psi_i^{eq}(x,t)+\hat{V}_i(x,t). \tag{4.19}$$

This equation is almost similar to the discretized LB equation (2.6) with the inserted external body force term (3.5). The main difference of these equations is in their streaming steps. In the LB equation, the distribution function f_i in a lattice node streams to the adjacent node along i lattice line with velocity c_i as forward in time. Conversely, in the adjoint LB equation, the adjoint distribution function ψ_i in a lattice node streams to the adjacent node along i lattice line with velocity $-c_i$ as backward in time. Fig. 2 demonstrates the difference between the streaming steps of the LB and the adjoint LB equations.

Comparing the presented procedure with that reported in [18], it can be found that the proposed model is more straightforward and has lower complexity. In addition, unlike, the previous model, we could achieved to the continuous adjoint LB equation and new adjoint concepts in lattice space (e.g., the adjoint equilibrium distribution function which only depends on the microscopic flow and adjoint properties) without involving in details of the LB method. Other advantage of the present model is that it can also be used similarly to extract the discrete adjoint equation (for more details, see Section 5).

4.3 Analytical evaluation of the adjoint distribution function

To evaluate the adjoint distribution function ψ_i using the adjoint LB equation (4.19), first, the adjoint equilibrium distribution function ψ_i^{eq} and the source term $\hat{V}_i$ should be evaluated. According to Eq. (4.16), to determine the equilibrium distribution function, the derivative of the distribution function is required. For the equilibrium distribution function (2.7), using the chain rule, we have

$$\frac{\partial f_j^{eq}}{\partial f_i}=\frac{\partial f_j^{eq}}{\partial \rho}\frac{\partial \rho}{\partial f_i}+\frac{\partial f_j^{eq}}{\partial u^x}\frac{\partial u^x}{\partial f_i}+\frac{\partial f_j^{eq}}{\partial u^y}\frac{\partial u^y}{\partial f_i}. \tag{4.20}$$

Partial derivatives of the equilibrium distribution function with respect to the macroscopic flow field variables can be obtained as

$$\frac{\partial f_j^{eq}}{\partial \rho}=w_j\Theta_j,\quad \frac{\partial f_j^{eq}}{\partial u^x}=w_j\rho\frac{\partial \Theta_j}{\partial u^x},\quad \frac{\partial f_j^{eq}}{\partial u^y}=w_j\rho\frac{\partial \Theta_j}{\partial u^y}. \tag{4.21}$$

With assuming $c=1$,

$$\frac{\partial \Theta_j}{\partial u^x}=-3u^x+\begin{cases} 0, & j=0,2,4,\\ 3+9u^x, & j=1,\\ (-3)+9u^x, & j=3,\\ 3+9[u^x-(-1)^j u^y], & j=5,8,\\ (-3)+9[u^x-(-1)^j u^y], & j=6,7, \end{cases} \tag{4.22a}$$

$$\frac{\partial \Theta_j}{\partial u^y}=-3u^y+\begin{cases} 0, & j=0,1,3,\\ 3+9u^y, & j=2,\\ (-3)+9u^y, & j=4,\\ 3+9[u^y-(-1)^j u^x], & j=5,6,\\ (-3)+9[u^y-(-1)^j u^x], & j=7,8. \end{cases} \tag{4.22b}$$

Also, the partial derivatives of the macroscopic flow field variables with respect to the distribution function using the conservative equations (2.11) can be evaluated as

$$\frac{\partial \rho}{\partial f_i}=1,\quad \frac{\partial u^x}{\partial f_i}=\begin{cases} 0, & i=0,2,4,\\ 1, & i=1,5,8,\\ -1, & i=3,6,7, \end{cases}\quad \frac{\partial u^y}{\partial f_i}=\begin{cases} 0, & i=0,1,3,\\ 1, & i=2,5,6,\\ -1, & i=4,7,8. \end{cases} \tag{4.23}$$

Finally, the partial derivatives of the cost function with respect to the distribution function with considering the cost function (3.4) and using the chain rule can be obtained as,

$$\begin{aligned}\frac{\partial I_{tx}}{\partial f_i} &= \frac{\partial I_{tx}}{\partial \rho}\frac{\partial \rho}{\partial f_i} + \frac{\partial I_{tx}}{\partial u^x}\frac{\partial u^x}{\partial f_i} + \frac{\partial I_{tx}}{\partial u^y}\frac{\partial u^y}{\partial f_i} \\ &= (\rho - \rho_{desired})\frac{\partial \rho}{\partial f_i} + (u^x - u^x_{desired})\frac{\partial u^x}{\partial f_i} + (u^y - u^y_{desired})\frac{\partial u^y}{\partial f_i}. \end{aligned} \tag{4.24}$$

5 Discrete adjoint approach based on lattice Boltzmann method

In this section, we derive mathematically the discrete adjoint equation and the cost function gradient vector based on the LB equation using the similar procedure reported by Nadarajah [8].

As previously stated, in the discrete adjoint method, discrete cost function and discrete governing flow field equations are used to derive the discrete adjoint equation and the gradient vector of the cost function. Consider the general discrete form of the cost function (3.3) and the discrete LB equation (2.6) with the inserted force term (3.5):

$$f_{i,t} = \Phi_{i,t}(f_{i,t-1}, \kappa), \quad t = 1, \cdots, t_f, \tag{5.1}$$

where

$$\Phi_{i,t} = (1-\beta) f_{i,t-1} + \beta f^{eq}_{i,t-1} + c_s^2 (c_i \cdot \kappa), \tag{5.2}$$

and $f_{i,t} \equiv f_i(x,t)$. Since the distribution function $f_{i,t}$ depends on the design variables vector κ implicitly $(f_{i,t} = f_{i,t}(\kappa))$, a variation $\delta\kappa$ in the design variables vector causes a variation $f_{i,t}$ in the distribution function and consequently, these variations lead to a variation δI in the cost function (3.3):

$$\delta I = \sum_{t=0}^{t_f}\sum_x \delta I_{tx} = \sum_{t=1}^{t_f}\sum_x \Big[\sum_{i=0}^{8}\frac{\partial I_{tx}}{\partial f_{i,t}}\delta f_{i,t} + \frac{\partial I_{tx}}{\partial \kappa}^T \delta\kappa\Big]. \tag{5.3}$$

It should be noted that with considering constant value for initial condition of the LB equation, in the optimization process, variation of the distribution function and the design variables at $t=0$ are zero.

Also, the variation in the distribution functions due to the variation in the design variables is such that the LB equation (5.1) will be always satisfied. Hence, we have

$$\delta f_{i,t} - \delta\Phi_{i,t}(f_{i,t-1}, \kappa) = \delta f_{i,t} - \sum_{j=0}^{8}\frac{\partial \Phi_{i,t}}{\partial f_{j,t-1}}\delta f_{j,t-1} - \frac{\partial \Phi_{i,t}}{\partial \kappa}^T \delta\kappa = 0, \quad t = 1, \cdots, t_f. \tag{5.4}$$

Now, multiplying the adjoint variable $\psi_{i,t} \equiv \psi_i(x,t)$ to (5.4) and summing the product over all of the lattice line directions and finally summing over time and space and considering $\delta f_{i,t}=0$ and $\delta\kappa=0$ at $t=0$, we get

$$\sum_{t=1}^{t_f}\sum_x\sum_{i=0}^{8}\psi_{i,t}\Big(\delta f_{i,t}-\frac{\partial\Phi_{i,t}}{\partial\kappa}^T\delta\kappa\Big)-\sum_{t=2}^{t_f}\sum_x\sum_{i=0}^{8}\sum_{j=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial f_{j,t-1}}\delta f_{j,t-1}=0. \tag{5.5}$$

Since the left hand side term is equal to zero, it can be subtracted from the variation (5.3) with no change in the result to give

$$\begin{aligned}\delta I=&\sum_{t=1}^{t_f}\sum_x\Big[\sum_{i=0}^{8}\frac{\partial I_{tx}}{\partial f_{i,t}}\delta f_{i,t}+\frac{\partial I_{tx}}{\partial\kappa}^T\delta\kappa\Big]-\sum_{t=1}^{t_f}\sum_x\sum_{i=0}^{8}\psi_{i,t}\Big(\delta f_{i,t}-\frac{\partial\Phi_{i,t}}{\partial\kappa}^T\delta\kappa\Big)\\&+\sum_{t=2}^{t_f}\sum_x\sum_{i=0}^{8}\sum_{j=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial f_{j,t-1}}\delta f_{j,t-1}\\=&\sum_x\Big[\sum_{i=0}^{8}\Big\{\sum_{t=1}^{t_f}\Big(\frac{\partial I_{tx}}{\partial f_{i,t}}-\psi_{i,t}\Big)\delta f_{i,t}+\sum_{t=2}^{t_f}\sum_{j=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial f_{j,t-1}}\delta f_{j,t-1}\Big\}\\&+\sum_{t=1}^{t_f}\Big(\frac{\partial I_{tx}}{\partial\kappa}^T+\sum_{i=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial\kappa}^T\Big)\delta\kappa\Big].\end{aligned} \tag{5.6}$$

The terms inside { } can be rewritten as

$$\begin{aligned}&\sum_{t=1}^{t_f}\Big(\frac{\partial I_{tx}}{\partial f_{i,t}}-\psi_{i,t}\Big)\delta f_{i,t}+\sum_{t=2}^{t_f}\sum_{j=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial f_{j,t-1}}\delta f_{j,t-1}\\=&\sum_{t=1}^{t_f}\Big(\frac{\partial I_{tx}}{\partial f_{i,t}}-\psi_{i,t}\Big)\delta f_{i,t}+\sum_{t=1}^{t_f-1}\sum_{j=0}^{8}\psi_{i,t+1}\frac{\partial\Phi_{i,t+1}}{\partial f_{j,t}}\delta f_{j,t}\\=&\Big(\frac{\partial I_{t_f x}}{\partial f_{i,t_f}}-\psi_{i,t_f}\Big)\delta f_{i,t_f}+\sum_{t=1}^{t_f-1}\Big[\Big(\frac{\partial I_{tx}}{\partial f_{i,t}}-\psi_{i,t}\Big)\delta f_{i,t}+\sum_{j=0}^{8}\psi_{i,t+1}\frac{\partial\Phi_{i,t+1}}{\partial f_{j,t}}\delta f_{j,t}\Big].\end{aligned} \tag{5.7}$$

Substituting Eq. (5.7) into (5.6), we have

$$\begin{aligned}\delta I=&\sum_x\Big[\sum_{i=0}^{8}\Big\{\Big(\frac{\partial I_{t_f x}}{\partial f_{i,t_f}}-\psi_{i,t_f}\Big)\delta f_{i,t_f}+\sum_{t=1}^{t_f-1}\Big[\Big(\frac{\partial I_{tx}}{\partial f_{i,t}}-\psi_{i,t}\Big)\delta f_{i,t}+\sum_{j=0}^{8}\psi_{i,t+1}\frac{\partial\Phi_{i,t+1}}{\partial f_{j,t}}\delta f_{j,t}\Big]\Big\}\\&+\sum_{t=1}^{t_f}\Big(\frac{\partial I_{tx}}{\partial\kappa}^T+\sum_{i=0}^{8}\psi_{i,t}\frac{\partial\Phi_{i,t}}{\partial\kappa}^T\Big)\delta\kappa\Big].\end{aligned} \tag{5.8}$$

The adjoint variable $\psi_{i,t}$ is chosen such that the changes of the cost function are independent from the changes of the distribution function $f_{i,t}$. Therefore, by setting the terms in the first line of the above equation equal to zero, the terminal adjoint condition and the discrete adjoint equation are obtained

$$\psi_{i,t_f}=\frac{\partial I_{t_f x}}{\partial f_{i,t_f}}, \quad \psi_{i,t}=\frac{\partial I_{tx}}{\partial f_{i,t}}+\sum_{j=0}^{8}\psi_{j,t+1}\frac{\partial \Phi_{j,t+1}}{\partial f_{i,t}}, \quad t=t_f-1,\cdots,1. \tag{5.9}$$

Thus, eliminating the terms including $\delta f_{i,t}$ in Eq. (5.8), we have

$$\delta I=\sum_x\sum_{t=1}^{t_f}\Big[\frac{\partial I_{tx}}{\partial \kappa}^T+\sum_{i=0}^{8}\psi_{i,t}\frac{\partial \Phi_{i,t}}{\partial \kappa}^T\Big]\delta\kappa. \tag{5.10}$$

Finally, the gradient vector G will be achieved by

$$G=\nabla_\kappa I=\sum_x\sum_{t=1}^{t_f}\Big[\frac{\partial I_{tx}}{\partial \kappa}+\sum_{i=0}^{8}\psi_{i,t}\frac{\partial \Phi_{i,t}}{\partial \kappa}\Big]. \tag{5.11}$$

Similarly, the adjoint distribution functions as stated for the continuous adjoint method can be evaluated.

It is noted that, according to Eq. (5.9), the proposed discrete procedure is not restricted to flow fields and can be implemented for both steady and unsteady flows in contrary to the provided model in [16, 17].

6 Conclusions and future works

In this research, for the first time, both continuous and discrete adjoint equations were derived based on the LB method for unsteady aerodynamic optimization problems. Firstly, the continuous adjoint equation was derived with complete details by means of the continuous LB equation in time and in space. As it was expected, the continuous adjoint LB equation was rather similar to the continuous LB equation. Therefore, the equation possesses all inherent aspects of the original LB equation (e.g., simplicity, parallelizability, etc.) and it is anticipated that the computational cost for solving the equation will be nearly equal to that of the LB equation. The discrete adjoint LB equation was also derived from the discrete LB equation in space and time. Comparison of the derivation trend of this equation with the derivation of the discrete adjoint equation from the NS equations shows that the present equation includes less complexity and so its implementation cost is lower. Finally, it can be said that the simplicity of the LB equation as an alternative for the conventional flow field equations can facilitate the derivation process of the continuous adjoint equation and specifically the discrete adjoint equation. Besides, all the advantages of the LB equation over the NS equations are expected for the adjoint LB equation compared to the adjoint equation extracted from the NS equations. These benefits can be useful in optimization problems.

In part II of this investigation, the results of the implementation of the method for inverse problem of a fluid flow will be reported and the accuracy of cost function gradients will be evaluated relative to the results of the finite difference approach. Moreover, since different representations of the forcing term have also been proposed (e.g., in [22]), the effect of various forcing term selections on the efficiency and computational cost of the presented optimization approach will be discussed, in more details.

Nomenclature

c	Particle velocity vector
D	Flow field domain
f	Density distribution function
F	Density distribution function vector
G	Gradient vector of cost function with respect to design variables
H	Flow field governing equations
I	Cost function in optimization problem
n	Dimension of design variables vector
P	Pressure
t	Time
u	Velocity vector or component in physical space
w	Flow field variables vector in physical space/Lattice weight parameters
x	Location vector in physical space
Ma	Mach number
ρ	Density
β	Inverse of dimensionless relaxation time
λ	Relaxation time
ψ	Adjoint distribution function
∂	Partial derivative operator
δ	Exact differential operator
∇	Napla vector operator
ω	Collision frequency
κ	Design variables vector
Ω	Collision operator
σ	Adjoint collision operator
ν	Kinematic viscosity
f	Terminal time index
i	Direction in LB method
T	Transpose
t	Time index
s	Sound speed index
x	Variable of horizontal direction in physical space/Location index

y Variable of vertical direction in physical space/Location index
I Contribution due to variation of the flow field variables
II Contribution due to variation of the design variables
eq Equilibrium sate index

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