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Application of Lattice Boltzmann Method to sensitivity analysis via complex differentiation

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ABSTRACT

Sensitivity analysis of flows computed by Lattice Boltzmann Method via Complex Differentiation is proposed. The theoretical work is illustrated and the proposed method assessed considering the D2Q9 scheme, along with the differentiation of the Lattice Boltzmann Equation. Boundary condition implementation is also detailed. Some examples illustrate the capability of the proposed method.

1. Introduction

The Lattice-Boltzmann Method (LBM) is a powerful tool in Computational Fluid Dynamics (CFD). Its applications range from modelling the incompressible isothermal Navier–Stokes equations to simulating thermal compressible fluids. Unlike most finite elements, finite volumes or finite differences methods, this method does not solve conservation equations for macroscopic quantities (like density or momentum) but operates on a density probability function. It has been shown [1,2] that the LBM is a second-order accurate (in both time and space) discretisation of the BGK Boltzmann equation on a finite set of discrete velocities. Its main advantages are its simple algorithm and its suitability for massive parallel computing. It has become a good alternative to other CFD solvers like finite elements, finite volumes or spectral methods [3–5]. The LBM is an active area of research on stability properties [6], grid refinement [7], fluid–structure interaction [8] or algorithm efficiency [9].

The LBM has also been used in a topology optimisation context by [10]. This study was conducted using a varying porosity model, and an adjoint problem. The adjoint problem technique has very recently been used for LBM in [11]. The classical drawback of adjoint problems is their cost in terms of solution storage when dealing with transient problems. The key point in shape design and optimisation problems (see, for e.g. [12]), as in flow control problems (see, for e.g. [13]) or stability analysis is to compute the derivatives of some flow quantity with respect to a given parameter α. This is called sensitivity analysis, and consists in finding how sensitive a flow is to changes in the value of its parameters or geometry. In this paper, we focus on parameter sensitivity.

Parameter sensitivity analysis can be performed as a series of tests in which the modeler sets different parameter values to see how a change in the parameter causes a change in the flow. This is the general scheme for probabilistic methods [14]. Sensitivity analysis can also be performed by linear stability theory [15,16] or by a differentiation method [e.g. [17]]. The

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gradients of the solution are in general neither readily accessible nor cheap to compute. The complex differentiation method, which was first proposed in [18], offers a straightforward access to the derivative of the solution with respect to any parameter. It has been renewed in [19] and recently gained popularity in the computational fluid dynamics community [13,20–22]. However, it was only used in combination with a Navier–Stokes solver, and, to the knowledge of the authors, never with the LBM.

This paper exposes the combination of a complex differentiation with the Lattice-Boltzmann Method for the computation of sensitivity derivatives. With the proposed method, one is able to compute in a single code run both the solution and its derivative with respect to some parameter. As it is based on a trivial modification of the variables type, it can be easily implemented in a Lattice-Boltzmann solver. The major advantage of the method is the instantaneous availability of the solution and its sensitivity at all time in the simulation. To the knowledge of the authors, it is the first time complex differentiation is used in combination with the Lattice-Boltzmann Method.

The paper is organised as follows: Section 2 exposes the theoretical background for the LBM, Section 3 the differentiation of the Lattice Boltzmann Equation. Section 4 presents the complex differentiation method for the LB equation. Section 5 provides some numerical examples to illustrate the abilities of the proposed method. Some results are compared to analytical solutions and finite difference gradients. Eventually, Section 6 provides some conclusions about the exposed work.

2. The D2Q9 Lattice-Boltzmann Model

The Lattice-Boltzmann Equation method is first recalled, together with the D2Q9 lattice velocity model and the equilibrium function. The link between the distribution function and the macroscopic variables is recalled. The interested reader should report to theoretical analysis of the LBM for more details, like [23,24,2] or the book by Succi [25].

The governing equations for the sensitivity variables are introduced in a second step, following a procedure similar to [2].

2.1. The Lattice Boltzmann Equation

In the absence of external body forces, the evolution of the density probability function is given by the Boltzmann Equation:

$$\frac{\partial f}{\partial t} + \underline{\xi} \cdot \underline{\nabla} f = \mathscr{C}, \tag{1}$$

where $\mathscr{C}$ is the collision operator. We will use the simplified model proposed by [26] [26], arguing that the collisions relax the flow to an equilibrium state, with a characteristic time τ:

$$\mathscr{C} = -\frac{1}{\tau}(f - f^{eq}), \tag{2}$$

where f^{eq} is the Maxwell–Boltzmann equilibrium function that we will detail later.

After Grad's idea [27], the density probability function f can be projected on a Hermite basis. The moments of the density probability function are computed by a Gauss–Hermite quadrature [28],[2, Appendix]). Then, the unknowns reduce to a finite set of values of the density probability function at the discrete velocity integration points. The evolution equations (referred to as the Discrete Velocity Boltzmann Equation, DVBE) for these new unknowns are achieved by evaluating the BGK-Boltzmann equation at the discrete velocities $\underline{\xi}_a$:

$$\frac{\partial f_a}{\partial t} + \underline{\xi}_a \underline{\nabla} f_a = -\frac{1}{\tau}(f_a - f_a^{eq}), \tag{3}$$

where f_a and f_a^{eq} are the distribution function and the equilibrium distribution function expanded, truncated, evaluated at $\underline{\xi}_a$ and correctly scaled. If any, the body force term is generally absorbed in f_a^{eq}.

With a second order time-integration scheme, one eventually obtains the Lattice Boltzmann Equation (LBE), which is of second order in time:

$$g_a(x + \delta x, t + \delta t) = g_a(x, t) - \frac{\delta t}{\tau_g}\left(g_a(x, t) - g_a^{eq}(x, t)\right) \tag{4}$$

with:

$$\tau_g = \delta t/2 + \tau, \tag{5}$$

$$g_a(x, t) = \left(1 + \frac{\delta t}{2\tau}\right) f_a(x, t) - \frac{\delta t}{2\tau} f_a^{eq}(x, t). \tag{6}$$

In fact, the LBM does not compute the density distribution function f, but an equivalent function g that has the same moments. The macroscopic behaviour of the flow is indifferently computed from the functions f or g. In the following, we will continue the discussions calling the unknown function f instead of g.