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Adjoint parameter sensitivity analysis for the hydrodynamic lattice Boltzmann method with applications to design optimization

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ABSTRACT

We present an adjoint parameter sensitivity analysis formulation and solution strategy for the lattice Boltzmann method (LBM). The focus is on design optimization applications, in particular topology optimization. The lattice Boltzmann method is briefly described with an in-depth discussion of solid boundary conditions. We show that a porosity model is ideally suited for topology optimization purposes and models no-slip boundary conditions with sufficient accuracy when compared to interpolation bounce-back conditions. Augmenting the porous boundary condition with a shaping factor, we define a generalized geometry optimization formulation and derive the corresponding sensitivity analysis for the single relaxation LBM for both topology and shape optimization applications. Using numerical examples, we verify the accuracy of the analytical sensitivity analysis through a comparison with finite differences. In addition, we show that for fluidic topology optimization a scaled volume constraint should be used to obtain the desired “0-1” optimal solutions.

1. Introduction

Design optimization of flow domains based on the Navier–Stokes equations has found widespread acceptance. We refer, for example, to the body of work by Jameson [1] on shape optimization for external and internal flows, as well as to the recent monographs by Gunzburger [2], and Mohammadi and Pironneau [3]. Topology optimization for fluids was introduced by Borrvall and Petersson [4]. In recent years it has received increased attention due to its general applicability to a wide range of problems in hydrodynamics and beyond [5–12].

The primary difference between shape and topology optimization is illustrated in Fig. 1, showing that shape optimization is limited to varying the location of the boundaries in order to improve the performance of an existing design, while topology optimization can lead to conceptually new design features and layouts without the need for an initial close-to-optimum design. For shape optimization, boundaries are generally parameterized such that a change of parameters leads to a change in the boundary. For material-based topology optimization on the other hand, the geometry of a body is represented via an associated material distribution. In the design domain shown in Fig. 1, each computational node/element is associated with a continuous material description function, which defines if a given node/element contains solid material, fluid, or an intermediate fluid-filled porous material. Here, it is generally the goal to obtain optimal solutions without intermediate material distributions, referred to as “0-1” solutions.

The authors have recently presented a topology optimization approach based on a lattice Boltzmann fluid solver in order to obtain optimal designs for internal and external flows [12–15]. The lattice Boltzmann method (LBM) was chosen to benefit from the inherent use of immersed boundary techniques (IBT), a simple porosity model, and the overall simplicity and versatility of the LBM algorithm. A key component of this LBM-based design optimization solver is the use of an adjoint parameter sensitivity analysis. Parameter sensitivity analysis is not limited to design optimization and is for example also used for reliability analysis, system identification, and reduced order models [16–18]. Up to now, only Teritek et al. [17] have applied adjoint sensitivities in an LBM framework, focusing on the identification of two optimal parameters within the multi-relaxation LBM scheme [19] using an adjoint LBM formulation.

In this work, we present the adjoint sensitivity analysis for the single-relaxation LBM scheme in detail, with a focus on the problem formulation for topology optimization, which requires the identification of large numbers of unknown parameters. In addition, the adjoint sensitivity analysis for shape optimization is discussed.

2. The lattice Boltzmann method

2.1. Lattice Boltzmann method overview

In recent years, the lattice Boltzmann method (LBM) has become a popular alternative to conventional, Navier–Stokes based

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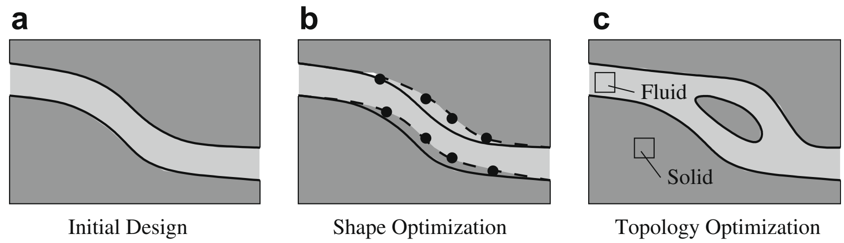

Fig. 1. Comparison of shape and topology optimization.

computational methods for a variety of problems in fluid dynamics. The reader is referred to McNamara and Zanetti [20], Succi [21], and Chen and Doolen [22] for an introduction to LBM schemes and applications. In the following, only those aspects of the lattice Boltzmann method essential for optimization are presented.

The lattice Boltzmann method is based on the discretized Boltzmann equation and constitutes a two-step process:

$$\text{Collision}: \quad \widetilde{f}_\alpha(\mathbf{x}_i, t) = f_\alpha(\mathbf{x}_i, t) - \frac{1}{\tau}\left[f_\alpha(\mathbf{x}_i, t) - f_\alpha^{eq}(\mathbf{x}_i, t)\right], \tag{1}$$

$$\text{Propagation}: \quad f_\alpha(\mathbf{x}_i + \delta t\mathbf{e}_\alpha, t + \delta t) = \widetilde{f}_\alpha(\mathbf{x}_i, t), \tag{2}$$

where $\mathbf{e}_\alpha$ is the velocity vector, f_α is the distribution function associated with the corresponding velocity $\mathbf{e}_\alpha$, $\mathbf{x}_i$ represents the location in physical space, $\mathbf{e}_\alpha\delta t$ is the lattice spacing, δt is the time step, and $\tau = \lambda/\delta t$ is the dimensionless form of the relaxation time λ.

The exact form of the velocity vector $\mathbf{e}_\alpha$ in the lattice Boltzmann scheme (1,2) depends on the lattice configuration. In this study, we use the two-dimensional, nine velocity D2Q9 lattice model with nine velocity vectors at each lattice site. In addition, the one-dimensional, three velocity D1Q3 model is used to illustrate the details of the LBM sensitivity analysis. For low Mach number flow conditions, the equilibrium distribution function f^{eq} in Eq. (1) can be derived by a Taylor series expansion of the Maxwell–Boltzmann equilibrium distribution, as shown by He and Lou [23]:

$$f_\alpha^{eq} = w_\alpha\rho\left[1 + 3(\mathbf{e}_\alpha \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\right], \tag{3}$$

where ρ represents the macroscopic density, the vector $\mathbf{u}$ is the macroscopic velocity, and w_α are lattice weights that depend on the lattice geometry. The macroscopic parameters, such as density, velocity, pressure, and viscosity are evaluated by taking statistical moments of the distribution function f.

2.2. LBM boundary conditions

A variety of LBM schemes for open and closed boundaries exist [24,25]. For the purpose of optimization, we are particularly interested in "no-slip" boundaries modeled with immersed boundary conditions such as the standard LBM bounce-back (BB) boundary conditions or represented via a porosity model [12,15]. We revisit these boundary conditions with a specific focus on their suitability for gradient-based optimization schemes. One can distinguish between local and global immersed boundary techniques (IBT) [26]; local immersed boundaries require a modification of the equations at distinct grid points in the mesh along the obstacle boundaries, whereas global IBT have the same equations everywhere in the domain, using a forcing term to represent boundaries. In the lattice Boltzmann method, the treatment of traditional "no-slip" boundaries can be considered as local and the porosity model as global immersed boundary techniques. For shape optimization (Fig. 1b), local boundary definitions are sufficient, as the contours of the designs are explicitly parameterized in the optimization process. In contrast, for topology optimization (Fig. 1c) it is advantageous to have a generalized, global boundary definition, such that the material distribution can evolve over the full design domain at minimal computational cost and complexity. Thus, we first introduce traditional, local LBM boundary conditions to show their accuracy and discuss their applicability to gradient-based methods. Second, we present the porosity model by Spaid and Phelan [27] as a globally defined boundary condition and show that it is well suited and sufficiently accurate for generalized shape and topology optimization. It should be noted at this point, that we are not concerned with the accurate modeling of porous flow but instead use porosity as a vehicle to smoothly transition between fluid and solid.

2.2.1. Local IBT: bounce-back boundary conditions

The standard bounce-back (BB) boundary condition is the simplest of the LBM "no-slip" boundary conditions. Three main variants exist: the widely used "half-way" BB boundary condition [28,29] and two variations of the "node" BB boundary condition referred to as "node" [30–33] and "node^b" [34] in the following discussion. Fig. 2 illustrates the differences between these basic BB boundary conditions.

The "half-way" BB boundary is the most elegant representation as it eliminates the boundary node 'B' from the LBM scheme. However, as the particle distribution 'f_{F1}' propagates from the first fluid node 'F' towards the boundary and returns to the first fluid node 'F', this scheme requires a modification of the propagation step (2) and complicates the computational implementation. Using the "node" BB condition the propagation step remains untouched. The boundary node 'B' is used as a storage location for the particle distribution 'f_{F1}' after the first propagation. The following standard collision step (1) is replaced by the bounce-back operation (5), followed by a second propagation. Thus, while the "node" BB condition creates an effective boundary half-way between the fluid node 'F' and the boundary node 'B', it effectively leads to a one time-step delay at the boundary [32]. This delay, however, does not affect the solution of steady-state problems as considered for the topology optimization applications in this work. Finally, the "node^b" BB condition avoids the time-step delay by moving the boundary onto the boundary node 'B' by adding an additional collision operation at the boundary.

Concluding this discussion, the three standard BB conditions are generally first order accurate in velocity and zeroth order accurate in pressure. However, when the modeled boundary location is half-way between the nodes for the "half-way" and "node" BB conditions or on the node for the "node^b" BB condition, the accuracy is improved to second-order accuracy in velocity and first order accuracy in pressure [35].

Due to its simplicity and sufficiency for steady-state LBM computations, the "node" bounce-back boundary condition is used in the current work. At the boundary node, the collision step (1) is replaced with a reversal of the distribution function f_α across the lattice symmetries:

$$f_\alpha = f_{\bar{\alpha}}, \tag{4}$$

where $\alpha = [0, 1, 2, 3, 4, 5, 6, 7, 8]$ and $\bar{\alpha} = [0, 3, 4, 1, 2, 7, 8, 5, 6]$ for the D2Q9 lattice, leading to the following operation