Immersed Boundary-Finite Difference Lattice Boltzmann Method for Predicting Particulate Flows

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(Degree)
博士（工学）
(Date of Degree)
2013-09-25
(Date of Publication)
2014-09-01
(Resource Type)
doctoral thesis
(Report Number)
甲第5941号
(URL)
https://hdl.handle.net/20.500.14094/D1005941

(Attachment: Form 3)

Dissertation Abstract

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Dissertation Title (If written in a foreign language, provide a Japanese translation as well.)

Immersed Boundary-Finite Difference Lattice Boltzmann Method for Predicting Particulate Flows

埋め込み境界法を用いた差分格子ボルツマン法に基づく粒子流数値予測手法に関する研究

Academic Supervisor: Akio Tomiyama

Particulate flows are encountered in a wide variety of engineering applications such as fluid flow in chemical reactors, waste streams with suspended solids, aerosols, and so on. Owing to their diversity, the particle size and the particle shape in these systems vary in an extensive range. The particle Reynolds numbers in particulate flows which are based on the particle size and its velocity vary broadly. Due to these features, the solution of particulate systems is one of the most challenging problems in engineering.

Several numerical methods are available to predict particulate flows. One of them is the immersed boundary method (IBM). IBM allows one to avoid complicated or time-consuming algorithms related to the grid generation or adaptation at each time step which are intrinsic to conventional methods such as the finite element or finite volume methods. In addition, a relatively new approach called the lattice Boltzmann method (LBM) has been proposed as an alternative to predict fluid flows. Some of the features that give LBM advantages in computational efficiency over the conventional methods are: the computation in LBM is much simpler than those in the conventional Navier-Stokes solvers since the time marching procedure in LBM is fully explicit and there is no need to solve Poisson equations; the local nature of the discrete particle collision operator in the lattice Boltzmann equation (LBE) and the fully explicit time integration of LBE makes this method suitable for parallel computing; and easy implementation of the method starting from scratch.

Due to the aforementioned advantages of LBM, various methods combining LBM and IBM (Immersed Boundary LBM: IB-LBM) have been developed for reasonably predicting liquid-solid two-phase flows. Numerical calculations of particulate flows such as flows past a circular cylinder, drafting-kissing-tumbling (DTK) motion of two particles or sedimentation of thousands particles have demonstrated that IB-LBM reasonably predicts the fluid-particle interaction of stationary or moving particles at moderate particle Reynolds numbers.

However, IB-LBM has still some drawbacks. Most of IB-LBMs utilize the single-relaxation time (SRT) model for the particle collision term in the lattice Boltzmann equation due to its simple implementation. Since the relaxation time, τ, is a monotonically increasing function of the kinematic viscosity ν, τ increases with ν, i.e. with decreasing the Reynolds number. The validity of IB-LBMs strongly depends on τ, i.e., numerical errors in velocity near the immersed boundary remarkably increase with decreasing the Reynolds number, i.e. increasing τ. In addition, IB-LBM is not free from restrictions of LBM, e.g., (1) simulation of high Reynolds number flows with a low relaxation time is apt to be unstable so that the spatial resolution must be high to perform stable calculations at

these conditions, and (2) the Lagrangian nature of LBE requires that a discrete particle moves from a lattice point to its neighbor during one time step, and therefore, the lattice spacing and the time step size cannot be altered independently. These drawbacks restrict the use of IB-LBM for predicting flows for a wide range of Reynolds numbers.

In this dissertation, a new numerical method was therefore proposed to overcome the above-mentioned restrictions and predict liquid-solid two-phase flows for a wide range of the particulate Reynolds number. The method is a combination of an immersed boundary method (IBM) and a finite difference lattice Boltzmann method (FDLBM). The use of the finite difference method allows us to set the lattice spacing and the time step size independently. Furthermore, an additional collision term, which works as a negative viscosity at the macroscopic level, is added to the discrete Boltzmann equation for numerical stability. IBM is based on a direct-forcing method, in which an external forcing term to impose the no-slip boundary condition at immersed boundaries is added to the discrete Boltzmann equation. The performance of the proposed method was demonstrated through several two- and three-dimensional calculations.

This dissertation consists of six chapters.

Chapter 1 is the introduction. The above-mentioned problems in available IB-LBM were extracted and a guideline for development of a new IB-LBM applicable to a wide range of particulate flows was determined.

First, calculations of cavity flows at different Reynolds numbers were carried out using FDLBM with the additional term in Chapter 2 to prove that FDLBM can deal with high Reynolds number flows. Then, IBM was combined with FDLBM to deal with moving particles. The Chapman-Enskog expansion was applied to the discrete Boltzmann equation with the additional collision term and the external forcing term of IBM to prove that the present Boltzmann equation recovers the macroscopic equations for incompressible Newtonian fluids. Two- and three-dimensional simulations of single particles falling in liquids and interaction between two particles were carried out to validate the proposed method. As a result, the following conclusions were obtained:

(1) The velocity distribution of cavity flows at moderate and high Reynolds numbers is stably and accurately predicted using FDLBM.

(2) The continuity and Navier-Stokes equations are recovered by applying the Chapman-Enskog expansion to the discrete Boltzmann equation with the external forcing term.

(3) The motions of particles falling through liquids at intermediate particle Reynolds numbers predicted using IB-FDLBM quantitatively agree with those obtained using IB-LBMs.

(4) The proposed method well predicts the interaction between two intermediate Reynolds number particles, e.g., the drafting-kissing-tumbling (DKT) motion.

In Chapter 3, the applicability of IB-FDLBM to flows at high Reynolds numbers was examined. It is known that when the relaxation time is decreased while keeping the relevant dimensionless numbers constant, the spatial resolution of IB-LBM needs to be increased to stably calculate flows at high Reynolds numbers. On the other hand, in the proposed IB-FDLBM, the additional collision term allows us to alter the fluid viscosity without changing the relaxation time and the spatial resolution, so that the proposed method is expected to be able to deal with flows at high particle Reynolds numbers without increasing the spatial resolution. Simulations of flows past two-dimensional stationary circular and square cylinders and flows past a sphere were carried out for a wide range of particle Reynolds numbers for validation. Free-falling cylinders at intermediate and high Reynolds numbers were also simulated. As a result, the followings were confirmed:

(5) The drag coefficient, the Strouhal number and the flow structure of flows past a stationary cylinder are well predicted for a wide range of *Re*, i.e. $1 \le Re \le 1\times10^5$.

(6) IB-FDLBM can stably simulate flows at high particle Reynolds numbers without increasing the spatial resolution.

(7) IB-FDLBM gives reasonable predictions of the drag coefficients of a sphere in uniform flows for a wide range of Reynolds number, i.e. $1 \le Re \le 1\times10^4$ provided that the ratio of the cylinder diameter to the lattice spacing is high enough.

(8) IB-FDLBM accurately predicts the reduction in the Strouhal number of vortex shedding behind a moving cylinder due to the falling-motion of the cylinder at intermediate Reynolds numbers.

(9) IB-FDLBM also reasonably predicts the motion of the moving cylinder at high Reynolds numbers.

IB-LBM has problems not only at high Reynolds numbers but also at low Reynolds numbers (high relaxation times), that is, errors in velocity near the immersed boundary remarkably increase with decreasing the Reynolds number, i.e. increasing the relaxation time. It is known that the numerical stability and accuracy of LBM mainly depend on the number of discrete velocities and the numerical treatment of the collision term. Therefore a remedy for the above-mentioned problem in IB-LBM at low Reynolds number might be to improve the discrete velocity model and/or the collision model. The increase in the number of discrete velocities however makes the computational cost high. It was therefore decided to use D2Q9 and D3Q19 models, which are the most common models for the discrete velocity. For the collision model, the single relaxation time collision model (SRT) has been often used due to its simplicity and efficiency. It is however well known that numerical errors increase with the relaxation time and non-physical velocity distortion appears at high relaxation times. Therefore the improvement of the collision model was attempted in this study. The multiple-relaxation time (MRT) collision model has been often used instead of SRT to improve the numerical stability and accuracy of LBM. However MRT is much more complicated than SRT: for instance, the number of relaxation times for D3Q19 model is 19 and several relaxation times are arbitrary (no definite principle are present for these arbitrary relaxation times). The simplest multi-relaxation-time model, i.e. the two-relaxation time (TRT) collision model, was therefore utilized. The formulation of TRT is as simple as that of SRT. TRT uses one relaxation time for determining the viscosity and the other for improving the numerical stability and accuracy. In Chapter 4, TRT was implemented into IB-LBM. It is expected that the implementation of TRT helps to remove or reduce the errors appearing at low Reynolds numbers (at high relaxation times). To validate the method, numerical simulations of circular Couette flows, sedimentation of single particles and DTK motion were carried out. The effect of TRT on numerical errors in velocity of symmetric shear flows was analytically and numerically studied. The conclusions obtained are as follows:

(10) IB-LBM with TRT does not cause a non-physical anti-symmetric velocity distribution in a circular Couette flow even at low Reynolds numbers, i.e. at high relaxation times.

(11) Two- and three-dimensional particulate flows with moving boundaries are reasonably predicted using IB-LBM with TRT.

(12) The analytical solutions obtained for the velocity gradient, the boundary velocity and the boundary slip agree well with the numerical predictions in the same conditions.

(13) The two-relaxation time collision model can remove the boundary slip velocity or accurately impose the boundary velocity at low Reynolds numbers. However it cannot solve both problems at the same time.

In Chapter 5, the two-relaxation time collision model was also implemented into IB-FDLBM to extend the range of applicability of the proposed method to simulations of low Reynolds number flows. First, the Chapman-Enskog expansion was applied to the discrete Boltzmann equation with the two-relaxation time collision term to show the recovery of the macroscopic conservation equations for incompressible Newtonian flows. Simulations of circular Couette flows were carried out to validate the present method. Flows past a circular cylinder and a sphere were calculated to examine the applicability of the method to both low and high particle Reynolds numbers. To accurately deal with the no-slip boundary condition at the immersed boundaries and avoid additional problems appearing in flows at low Reynolds numbers, an implicit direct forcing method was implemented into IB-FDLBM. Finally, sedimentation of multiple particles with various Reynolds numbers was carried out. As a result, the following conclusions were obtained:

(14) The continuity and the Navier-Stokes equations are reasonably recovered, and the kinematic viscosity is determined by one relaxation time.

(15) TRT implemented into IB-FDLBM reduces numerical errors causing non-physical distortion in the fluid velocity at low Reynolds numbers.

(16) Implementation of TRT and the implicit direct forcing method into IB-FDLBM can solve two problems in simulation of low Reynolds number flows, i.e. non-physical velocity distortion and non-physical penetration of flow into a solid body.

(17) IB-FDLBM with TRT gives good predictions of the drag coefficients of a circular cylinder and a sphere in uniform flows for a wide range of the particle Reynolds number.

(18) Particulate flows with various particles are predictable with the proposed method.

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Chapter 6 is the summary of this dissertation.

In summary, an efficient investigation was conducted to extend the applicability of IB-LBM to solve liquid-solid two-phase flows at low and high Reynolds numbers. An IB-FDLBM was developed and its performance was tested in various benchmark problems. Good agreements are found between the present numerical predictions and other numerical and experimental results. Therefore, IB-FDLBM is proved to be an effective method for solving flows including various particles ranging from low to high particle Reynolds numbers.

（別紙１）

論文審査の結果の要旨

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論文題目	Immersed Boundary-Finite Difference Lattice Boltzmann Method for Predicting Particulate Flows （埋め込み境界法を用いた差分格子ボルツマン法に基づく粒子流数値予測手法に関する研究）

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要旨

固体粒子を含む流れは化学反応塔内流動，塗料塗布，廃液流れなど様々な工業工程で利用されている．これら粒子流における粒子の密度や大きさ，形状は様々であり粒子レイノルズ数の値も広範にわたる．このためその数値予測は容易ではなく，高精度・高効率な粒子流数値予測技術の開発が重要課題となっている．埋め込み境界法(Immersed Boundary Method: IBM)は，粒子の移動を計算する手法の一つとして最近注目されている．本手法は固定計算格子上で粒子の移動を表現できるため他の手法に比べ計算効率が高い．一方，複雑な流れ場を単純な計算アルゴリズムで求められる手法として格子ボルツマン法（Lattice Boltzmann Method: LBM)がある．LBM は大規模並列計算の容易さの観点で他の計算手法より格段に優れている．IBM と LBM を組み合わせた粒子流計算手法 IB-LBM により中程度の粒子レイノルズ数の粒子流を良好に予測できることが既に確認されているが，(a)低粒子レイノルズ数において速度分布に非物理的歪みが生じる，(b)高粒子レイノルズ数では数値的不安定性が生じるという未解決問題がある．そこで本論文では，広範囲の粒子レイノルズ数の粒子を含む流れを高精度かつ高効率に計算できる手法の構築を目的としている．

第１章では，粒子流数値予測技術の現状を整理し，埋め込み境界法を用いた格子ボルツマン法が有する課題を抽出し，本研究の目的を記述している．

第２章では，差分格子ボルツマン法(Finite Difference Lattice Boltzmann Method: FDLBM)と埋め込み境界法を組み合わせた粒子流数値予測手法，IB-FDLBM を提案している．高粒子レイノルズ数における数値的安定性を確保するため離散ボルツマン方程式に人工粘性項を付与し，埋め込み境界法には陽的外力法を採用している．まず，種々のキャビティ流れの計算を実施し，本手法により中・高レイノルズ数の流れを安定かつ高精度に計算できることを確認している．また，使用する離散ボルツマン方程式が巨視的流体方程式と無矛盾であることを基礎式のマルチスケール展開により確認している．さらに，中程度の粒子レイノルズ数における二次元及び三次元の粒子運動シミュレーションを実施し，中程度の粒子レイノルズ数の単一粒子の運動及び粒子間相互干渉を伴う運動を精度良く予測できることを確認している．

第３章では，高粒子レイノルズ数流れへの適用性を検討している．まず，円柱及び球まわりの流れを対象とした計算により，1 から 10^5 にわたる広範囲のレイノルズ数において円柱の抗力係数とストローハル数を精度よく予測できること，及び 1 から 10^4 の球の抗力係数を精度よく予測できることを確認している．つぎに，移動境界問題への適用性を検証するために自由落下円柱の計算を実施し，自由落下円柱の渦放出ストローハル数が静止円柱の場合に比べて低下する現象を定量的に良好に予測できること，及び高レイノルズ数の自由落下円柱の運動も安定に計算できることを確認している．

第４章では，低レイノルズ数における速度分布の非物理的歪みの解決を図っている．誤差低減の方法として格子ボルツマン方程式における分子間衝突項のモデルに着目し，単一緩和時間モデルから二緩和時間モデルへの変更を試みている．本モデルを IB-LBM に組み込み，速度分布の非物理的歪みが顕著となる回転クエット流れを計算した結果，二緩和時間モデルにより速度歪みの大幅な低減を得ている．また，中程

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度のレイノルズ数の粒子運動が良好に計算できることも確認されている．さらに，二緩和時間モデルに含まれる各種のパラメータが速度の非物理的歪みに及ぼす影響を調べるため格子ボルツマン方程式から理論解を求めている．理論解と数値解の比較により理論解の妥当性を確認するとともに，各種パラメータが数値誤差に及ぼす影響を明確にし，二緩和時間モデルによれば埋め込み境界における速度の誤差あるいは速度勾配の誤差を除去できるが，これらを同時には除去できないことを示している．

第５章では，まず，二緩和時間モデルを第２章で構築した IB-FDLBM に組み込み，低粒子レイノルズ数問題への適用性を検討している．まず，二緩和時間モデルを組み込んだ差分格子ボルツマン方程式をマルチスケール展開し巨視的流体方程式が正しく再現されること，及び回転クエット流れの数値計算により低レイノルズ数でも非物理的速度歪みが生じないことを確認している．次に，円柱まわりの流れと球まわりの流れの計算により低粒子レイノルズ数問題への適用性を調べた結果，低レイノルズ数における新たな問題として固体表面で流体の非物理的浸透が認められた．この非物理的浸透を防止するため埋め込み境界法を陽的外力法から陰的外力法に変更している．その結果，陰的外力法と二緩和時間モデルの併用により低粒子レイノルズ数における非物理的速度歪みと固体表面での非物理的浸透の両者を解決できることを確認している．最終的に，陰的外力法に基づく埋め込み境界法と二緩和時間衝突項モデルに基づく差分格子ボルツマン法を組み合わせた粒子流計算手法を構築し，本手法により広範囲のレイノルズ数における円柱及び球の抗力係数を精度良く予測できること，及び広範囲の粒子レイノルズ数の粒子を同時に含む粒子流の計算を効率良く行なえることを確認している．

第６章では，得られた成果が総括されている．

以上，本研究は，既存の数値計算手法では取扱い困難であった様々な粒子レイノルズ数の固体粒子を含む固液二相流や複雑構造物を含む流れを精度良くかつ効率的に計算できる簡便な数値計算手法を構築したものであり，流体工学及び計算工学における価値ある集積であると認める．よって，学位申請者の Rojas Molina Roberto Carlos は，博士（工学）の学位を得る資格があると認める．