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De-aliasing and stabilization formalism of the cascaded lattice Boltzmann automaton for under-resolved high Reynolds number flow

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SUMMARY

The central moments formalism of the cascaded lattice Boltzmann automaton is a natural approach to stabilize under-resolved unsteady high Reynolds number flow simulations. On the basis of the two absolute length scales of shear flow simulations which are the physical scale η (Kolmogorov scale) and the numerical scale h (grid spacing), it is argued that higher central moments of the local momentum distribution should go much faster to zero than the explicitly traced hydrodynamic moments. The lattice Boltzmann formalism allows one to adjust these higher moments without affecting the velocity field and its gradients in the same time step. It is shown that setting the higher central moments to zero in each time step stabilizes the model. As an example vortex shedding behind an obstacle which is only one grid spacing wide is shown. Copyright © 2007 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The simulation of turbulent flow is one of the most outstanding challenges of numerical modeling. There seems to be no transformation to the governing equations which would result in a significant reduction in the required number of degrees of freedom to trace the time evolution of a turbulent flow field. The source of this difficulty is to be seen in the concurrence of a (self)-convection and a diffusion term in the Navier–Stokes equation. This combination leads to a coupling of the flow fields on all length and time scales and is known as the closure problem of turbulence. A set of equations describing the evolution of a turbulent flow field is unclosed as long as the molecular processes are

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not resolved. The latter would be intractable for nearly all problems of practical interest. Owing to our inability to resolve turbulence it is natural to ask whether it is possible to ignore the small scales of turbulence and still obtain useful information from under-resolved simulations. The two currently investigated possibilities are to solve a spatially filtered Navier–Stokes equation (this is called LES: large eddy simulations) or to solve a temporal or spatial-averaged Navier–Stokes equation (RANS: Reynolds-averaged Navier–Stokes) [1]. Both methods start from the Navier–Stokes equations. However, the Navier–Stokes equations are by themselves only simplified average descriptions of large quantities of particles. A different starting point would be the Boltzmann transport equation which describes the time evolution of a single particle distribution function. Nominally, the Boltzmann transport equation holds only for dilute gases and not for liquids unless a dilute gas is a sufficient approximation to a liquid. The Boltzmann transport equation can be solved by the lattice Boltzmann method [2, 3]. However, the lattice Boltzmann method was developed for solving the Navier–Stokes equation and the involved moment expansion was therefore truncated at 'Navier–Stokes order'. Here it is shown that the cascaded lattice Boltzmann automaton (LBA), which uses a higher order expansion, can be used to discard high-frequency components of the flow field without the usage of spatial filtering.

2. LATTICE BOLTZMANN METHOD

LBA are cellular automata for the modeling of fluid flow. The automaton is a regular spatial distribution of nodes on a lattice. Each node is connected to a finite set of neighbors *via* links. Links are occupied by particles. The particles occupying a link move in the direction of this link in a streaming step. After the streaming step they occupy the same link on a neighboring node. It follows a scattering step in which the particles on each node get redistributed over the local links in a mass and momentum conserving fashion.

Links between nodes are momentum states. The most prominent difference between the Boltzmann transport equation and the Navier–Stokes equation is seen in the dimensionality of the two models. The Boltzmann transport equation as well as the LBA considers a seven-dimensional problem (time + three spatial + three momentum dimensions). The Navier–Stokes equation, on the other hand, is only four dimensional (time + three spatial dimensions). As a result, the velocity at a given point must have a sharp value in the Navier–Stokes picture. It is necessary to stress that this is an unphysical condition. A gas is not a continuum but an ensemble of many fluctuating particles. In the Navier–Stokes picture only the mean of the velocity distribution is considered a relevant state variable. The Boltzmann transport equation allows for an arbitrary distribution of momentum at a given point in spatial space and time. The LBA reduces the momentum distribution to a small set of discrete speeds. In addition to the mean of the momentum distribution, the variance or second moment is considered a relevant state variable by the standard LBA. However, even this is insufficient for the modeling of turbulent flow because the flux of the momentum variance is typically not accounted for. Again we encounter a closure problem since we would need to consider third-order moments for the fluxes of second-order moments and fourth-order moments for the fluxes of third-order moments and so on to infinity.

The question is whether it is possible to establish a finite truncation of the LBA with a sufficiently wide range of applicability to high Reynolds number flow conditions. The subject of under-resolved simulation of unsteady or even turbulent flow has two aspects. One is that all information contained in the small scales of the flow is lost. That is to say, there is no convincing concept on how a

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turbulence model should account for the backscatter of kinetic energy that has gone below the resolution of the simulation. This problem is probably unsolvable and we will not discuss this here. The other aspect is that a naive truncation at some finite resolution is in general not even numerically stable. This is due to an unphysical backscatter of kinetic energy caused by aliasing. In order to obtain a stable solution we need methods that allow to close the cascade of kinetic energy at the grid resolution. Promising candidates are the nine velocity states cascaded LBA in two dimensions (the so-called D2Q9 lattice) and the 27 velocity states cascaded LBA in three dimensions (D3Q27 lattice).

3. CASCADED LBA

The derivation of the cascaded LBA is lengthy. Here we provide only an overview. For a detailed derivation we have to point to the original work [4, 5].

The cascaded LBA differs from the original LBA mainly in the choice of the scattering operator which acts on a single-node momentum distribution function. The cascaded LBA considers the same number of central moments κ_n of the momentum distribution function f as the distribution vector has components. A central moment is defined as an integral observable quantity of a distribution displaced by the mean of the distribution x_0:

$$\kappa_n = \int (x - x_0)^n f \, \mathrm{d}x \tag{1}$$

The mean of the momentum distribution is the velocity at the given point. In the original moment formulation of the LBA [6] raw moments were used, which were obtained for a resting velocity reference frame. This led to a breakdown of Galilean invariance since a resting reference frame had to be defined. The result is a loss of stability whenever the velocity of the fluid is more than very slightly larger than zero with respect to the static frame of reference. The cascaded LBA overcomes this flaw at the cost of more complicated equations. The utilization of central moments requires a re-orthogonalization of the moments in each scattering event. Algorithmically this is done by scattering the lowest order moments first and proceeding with higher orders while introducing compensations for errors introduced at the lower order (moments are processed in a scattering cascade, hence 'cascaded' LBA). Equilibria for all considered moments can be obtained from symmetry considerations. Each moment can then be relaxed with a different relaxation rate corresponding to different transport coefficients. The viscosity of the fluid is easily linked to the relaxation rates of second-order moments. The cascaded LBA can be used to simulate high Reynolds number unsteady flows with nominally arbitrarily under-resolved meshes without causing instabilities. In this respect, it is similar to a conceptually different approach of entropic stabilization of LBA [7, 8].

4. DE-ALIASING FORMALISM

The lattice Boltzmann formalism traces momentum distributions of which density, velocity, spatial gradients of velocity, and second gradients of velocity (curvature) are distinctive central moments. That is to say, velocity gradients and velocity curvature are accessible locally without the need for numerical differentiation. Moreover, it is possible to manipulate the gradient and curvature fields

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without affecting the velocity field in the same time step. From the differential equation point of view (Navier–Stokes picture) this would be contradictory. But there is no such contradiction in the Boltzmann picture. The moment method leads us naturally to a de-aliasing formalism for under-resolved simulations. Owing to Shannon's theorem any discretely sampled field that contains information up to the sampling frequency must be contaminated by aliasing. In the lattice Boltzmann algorithm aliasing shows up in the curvature moment first. Since the velocity field, the gradient field, and the curvature field are independent entities, aliasing results in an inconsistency of these fields, which can easily be removed.

An under-resolved high Reynolds number simulation might be characterized by two absolute length scales: the absolute physical length scale η (Kolmogorov length) which is the length below which there is no turbulent energy, and the absolute numerical length scale h, which is the grid spacing. It is appropriate to analyze the velocity field using the spatial variable ηx, where x is dimensionless. In order to exist on the lattice any velocity wave must have a wavelength which is an integer multiple of h: $w = nh$. Such a wave and its derivatives might be written as

$$u = u_0 \sin\left(\frac{\eta}{nh} x\right) \tag{2}$$

$$u' = u_0 \frac{\eta}{nh} \cos\left(\frac{\eta}{nh} x\right) \tag{3}$$

$$u'' = -u_0 \left(\frac{\eta}{nh}\right)^2 \sin\left(\frac{\eta}{nh} x\right) \tag{4}$$

The curvature moment is typically not taken into account because it has no direct influence on the Navier–Stokes equation. However, we can make a clear statement for the ratio of the curvature moment to the velocity moment:

$$\Upsilon = \frac{u''}{u} = -\left(\frac{\eta}{nh}\right)^2 \tag{5}$$

The important point here is that u and u'' are absolute (dimensionless) quantities. When the grid Reynolds number is large ($h \gg \eta$) Υ should go to zero. However, since u has a finite value which is independent from h and η, Υ can go to zero only if u'' is zero. In praxis one observes large amplitudes in the curvature moments which must, according to the above argument, emerge nearly entirely from aliasing. But it is straightforward to discard the unresolved length scales: we can adjust the curvature moment independently from the velocity field and the gradient field. Hence, we can simply set it to zero in each time step. Doing this results in a hyper-viscosity of the fluid which is empirically found to be [5] $v_x \sim 5k_x^2 v_x^4$, where k_x is a wave number of a shear wave measured in inverse grid spacings and v_x is a superimposed velocity field in x direction measured in grid spacings per time step. This hyper-viscosity is not a Galilean invariant as it depends on the flow velocity v_x. However, the dependence is of fourth order and the hyper-viscosity can be made small by choosing small non-dimensional velocities which is anyway necessary due to the inherent compressibility of lattice Boltzmann models. The cascaded LBA with removal of curvature moments can now be applied to arbitrarily under-resolved flow conditions.

4.1. Vortex shedding at minimal resolution

To demonstrate the ability of the cascaded LBA to resolve the flow field down to the grid resolution we investigate a problem which is slightly under-resolved. The flow field behind a cylinder

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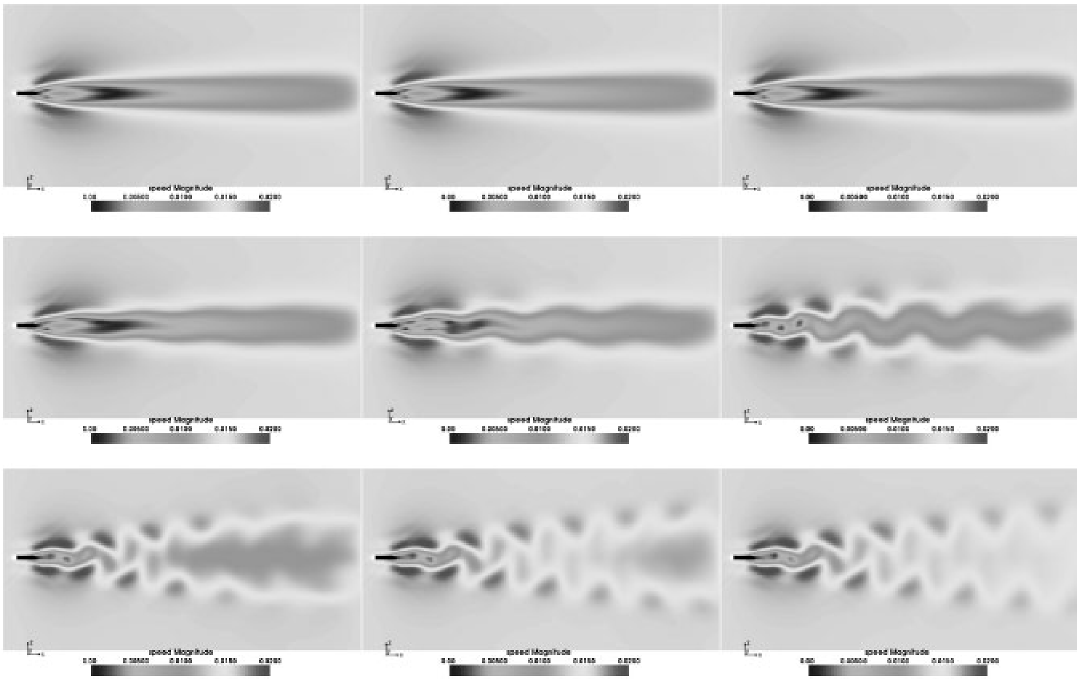

Figure 1. Successive time steps of the onset of vortex shedding behind a minimal cylinder of size $1\times 1\times 30$ grid nodes at Reynolds number 79. Note that the grid Reynolds number is also 79. The cascaded LBA shows the qualitative correct behavior down to a single grid spacing.

of dimension $1\times 1\times 30$ lattice spacings on the cartesian grid is simulated at Reynolds number 79. Laminar vortex shedding behind the obstacle is supposed to start at Reynolds number 40. A representation of the obstacle by just one grid point in two directions is enough to capture the complicated process of vortex shedding (see Figure 1). The simulation is not very accurate since the flow field is so coarse. The Strouhal number measured from Figure 1 is slightly below 0.11. Empirical Strouhal numbers for this Reynolds number are close to 0.15 [9]. The vortices are slightly too large compared with literature values. This can be explained by the fact that the minimal size of the vortices is constrained by the grid spacing and that the physically correct vortices would be smaller than one grid spacing. The point here is that vortex shedding starts at the right Reynolds number irrespective of the lack of resolution. A simulation with a higher viscosity at Reynolds number 20 yields no vortex shedding (in line with physics). In this case two stationary vortices of minimal size are present, again in line with our expectations.

5. CONCLUSIONS

In this paper the cascaded lattice Boltzmann de-aliasing formalism was derived from the ratio of the two relevant absolute length scales, the physical Kolmogorov scale and the numerical grid spacing. It was argued that the curvature moments go to zero when the grid Reynolds number becomes

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large. Since the curvature moments are contaminated by numerical aliasing this condition has to be enforced explicitly by equilibration of the corresponding degrees of freedom. This does not introduce any additional cost to the method. In fact, the equilibration of the curvature moments was used in the cascaded LBA from the beginning. The small scales of turbulence are removed from the simulation. It is a disputable question whether the stabilizing hyper-viscosity can be interpreted as a turbulence closure model. Even the best turbulence model can obviously not account for length scales which are not represented in the simulation. Allowing for arbitrary coarse resolutions by keeping the details of the flow at grid resolution, as was shown here, is the first step toward turbulence modeling.

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