LATTICE BOLTZMANN METHODS: APPLICATIONS IN COMPUTATIONAL FLUID MECHANICS

by

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The development of novel numerical methods for applications in computational fluid dynamics has made rapid progress in recent years. These new techniques include the lattice gas and lattice Boltzmann methods. Compared to the traditional CFD methods, the lattice Boltzmann methods are based on a more rigorous physical modelling, the Boltzmann equation. This allows to circumvent many deficiencies inherent in existing Navier Stokes based approaches. Thus, the lattice Boltzmann methods have attracted a lot of attention in the fluid dynamics community and emerged as an attractive alternative in many application areas. In the present paper, we discuss some perspectives of the lattice Boltzmann methods, in particular for industrial applications and present some successful examples from projects related to aerodynamics, chemical and process engineering.

INTRODUCTION

In the past years, the methods of *lattice gas cellular automata* (LGCA) and the *lattice Boltzmann Methods* (LBM) have attained a certain maturity and subsequently challenged the *traditional* methods of computational fluids mechanics (CFD) in many areas. In that context, traditional methods of CFD are understood to include all numerical schemes, that aim to solve the Navier-Stokes equations by some direct discretisation. In contrast to that, the LBM is based on a more rigorous description of the transport phenomena, the Boltzmann equation. Compared to other attempts, that have been made to solve this equation in the past, the LBM makes use of several significant, physically motivated simplifications that allow to construct efficient and competitive or even superior computational codes as compared to the classical approaches.

Lattice gas cellular automata and even more lattice Boltzmann methods are relatively new. Just about 15 years ago, the field of LGCA started almost out of the blue with the now famous paper of Frisch, Hasslacher and Pomeau [9], who showed that some simplified kind of "billiard game" representing the propagation and collision of fluid particles leads to the Navier Stokes equations in a suitable macroscopic limit. In particular, the authors showed how the propagation and collisions of particles have to be abstracted in order to conserve mass and momentum and how the underlaying lattice has to be designed in order to provide sufficient symmetries to the discretised Boltzmann equation. Each month, several papers appear to present new models or to investigate existing models, to demonstrate and assess the use of LBM in application fields or to evaluate high performance computing (HPC) aspects. Summerschools, special conferences and LBM sessions in existing conferences have been organised to satisfy also the growing interest of developers and potential users in this technique. Besides that, commercial products are available with remarkable success (see *e. g.* [6]).

The goal of the present paper is to show the potential of the lattice Boltzmann method in CFD and in related areas. Besides the classical application fields, such as aerodynamics, these are in particular problems related to chemical and process engineering. Due to the complexity of the relevant transport and chemical conversion mechanisms, that have to be modelled, these areas open new challenges also for the LBM.

In the present paper, after a short summary of the basic principles of the LBM, examples related to turbulent flows, reacting flows and the respective application fields are discussed.

THE LATTICE BOLTZMANN METHOD

From a gaskinetical, i.e. microscopic, point of view, the movement of a fluid may be considered as the propagation and collision of molecular particles governed by fundamental laws of physics. The modelling of this motion may be carried out on several levels, starting with the Hamilton equation of a set of discrete particles. Since this approach prohibits itself because of the large number of molecules to be considered, several attempts have been made to simplify this picture by extracting only the essential criteria required to model *e. g.* the motion of a Newtonian fluid. In that context, the lattice gas automata may be seen as an abstraction of the fluid making use of the fact, that the statistics of the gas may be correctly described by a significantly reduced number of molecules and by applying simplyfied dynamics of the particles. This can be explained by the fact, that the conservation principles as well as associated symmetries are the basic building blocks for the continuum equations of fluids. Thus, in oder to simulate a continuum flow, the approximation of the *computer gas* has to recover only these principles to a certain extend. The FHP automata, named after [9], was a first successful attempt to construct a discrete

model to compute the motion of a Newtonain fluid. The arithmetic description of the microdynamics can be formally expressed by the following evolution equation

$$n_i(t + \Delta t, \vec{x} + \vec{c}_i \Delta t) = n_i(t, \vec{x}) + \Delta_i \tag{1}$$

The state of the gas at a node $\vec{x}$, the time t and the microscopic velocity $\vec{c}_i$ is described by the boolean variable n_i. The algorithm describes the propagation of the particles from one node to its nearest neighbour in the direction of the discrete particle velocity $\vec{c}_i$. After this streaming step, collision rules Δ_i are applied locally on all nodes of a regular grid ("lattice"). The n_i may be viewed as a binary particle distribution function and eq. (1) as an approximation of the Boltzmann equation, discrete in time, space and velocity. From the moments of n_i and a space time averaging, the macroscopic velocity, pressure *etc.* may be computed.

Although this approach seems promising, there are problems due to spurious invariants and random noise in the solutions. In particular the problem of noise, which is due to the discrete nature of the method, can be overcome by applying the idea of McNamara and Zanetti [21], who defined continous particle distribution functions to replace the averaging process. Thus, the following evolution equation is obtained for the distribution functions N_i:

$$N_i(t + \Delta t, \vec{x} + \vec{c}_i \Delta t) = N_i(t, \vec{x}) + \Delta_i \tag{2}$$

In fact, this equation may be viewed as an approximation of the Boltzmann equation (neglecting acceleration due to external forces), where the velocity space is discretised with few degrees of freedom. The complicated collision term may be replaced by a simple relaxation term based on the Boltzmann H-theorem, i.e. if a Maxwellian equilibrium velocity distribution f^{eq} exists. In this case, the following discrete form of the BGK (Bhatnagar Gross Kroog) approximation of the Boltzmann equation is obtained

$$N_i(t + \Delta t, \vec{x} + \vec{c}_i \Delta t) = N_i(t, \vec{x}) + \frac{1}{\tau}(N_i^{eq} - N_i) \tag{3}$$

Here, τ is the relaxation time. The computation of the moments of the distribution function reduce to the simple numerical quadrature

$$\rho(\vec{x}, t) = \sum_i N_i(\vec{x}, t) \tag{4}$$

$$\rho u_\alpha(\vec{x}, t) = \sum_i \vec{c}_{i\alpha} N_i(\vec{x}, t) \tag{5}$$

$$\Pi_{\alpha\beta}(\vec{x}, t) = \sum_i \vec{c}_{i\alpha} \vec{c}_{i\beta} N_i(\vec{x}, t) \tag{6}$$

The local equilibrium function, which may be obtained from

$$N_i^{eq} = t_p \rho \left\{ 1 + \frac{c_{i\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta}{2c_s^2} \left(\frac{c_{i\alpha} c_{i\beta}}{c_s^2} - \Delta_{\alpha\beta} \right) \right\} \tag{7}$$

has to be computed at each time step for each node from the components of the local (macroscopic) flow velocity u_α and u_β, the fluid density ρ, the speed of sound c_s and the direction dependent lattice geometry weighting factors t_p which are chosen to recover the incompressible time dependent Navier Stokes equations. The viscosity of the simulated fluid can be controlled by the relaxation time according to

$$\nu = \frac{1}{3}\left(\tau - \frac{1}{2}\right) \tag{8}$$

Further technical details of this method may be found in [25, 32]. From the computational point of view the above approach is interesting as it resembles a simple finite difference scheme applied to a first oder (in time and space) hyerpbolic system of equations in diagonal form. This extremely simplifies the design of a numerical scheme. However, finally the solution of the Navier Stokes equations with second order accuracy in the limit of low Mach numbers ($c_s^2 \gg |\vec{v}|^2$) is recovered, as can be shown rigorously in [12] by applying the Chapman Enskog procedure to eq. (3).

The approach presented above is just the basic version of the LBM. Many improvements have been designed in order to broaden the methods range of applicability, see *e. g.* the review articel of Chen and Doolen [3]. Current issues are the multi time relaxations methods to enhance the stability of the method [5, 17], implicit methods [15] or the application of nonuniform and locally refined meshes [7, 30] and of improved boundary conditions for Cartesian meshes [22]. For various applications, particularly in chemical and process engineering, the convective and diffusive transport of energy and species are of key importance. Examples of a few among many interesting contributions made in this field by varios authors can be found *e. g.* in [8, 27]. Thermal models have been proposed in [4, 10], reaction diffusion problems have been investigated *e. g.* in [2, 11, 31]. The simulation of multiphase flows and immiscible fluids were the subject of several investigations where the LBM provided interesting alternatives to model particle interaction, surface tension, *etc.* In modelling suspensions of particles for example, the interactions of the fluid and particles may be treated in different ways, either by dicretising and mapping moving particles in a Lagrangian sense [16] or by a combination of an integer lattice gas model for the disperse phase and the BGK for the fluid phase [19].

Models for turbulent flows have been adapted from classical LES approaches, as applied to the Navier Stokes equations, by changing the relaxation parameter in eq. (8) in order to scale the viscosity according to a subgrid model, such as published in [13]. Alternatively, two equation models have been propsed by *e. g.* [24, 28, 29].

The following sections present some practical results related to chemical engineering and aerodynamics, that show the applicability of LBM in various technical fields.

APPLICATION OF LBM IN CHEMICAL ENGINEERING

In chemical industries, packed beds and porous media are frequently used as reaction, separation or purification units. The design of these devices is usually based on pseudo homogeneous equations with averaged semi empirical models such as dispersion and mass transfer correlations. The design concepts based on these models fail if local flow phenomena such as channeling effects become dominant. Therefore, several attempts have been made in oder to improve these models. However, new design methodologies are required if no or insufficent empirical data are available. Lattice Boltzmann methods can been used to directly simulate the flow field in these configurations together with chemical reactions and diffusion effects. This allows to analyse in detail the hydrodynamic effects, *e. g.* the channeling due to inhomogeneous void space distributions and other flow anomalies and to quantify their influence on the prediction of the bulk conversion and selectivity of the reactor. The lattice Boltzmann method has been chosen mainly because of its ability to model highly complex geometries and fluids.

The "direct" numerical simulation of flows through packed beds uses a digitized image of the structure under considerations. This may be obtained from computer tomographic data [1] of a real probe of the material or as synthetically generated geometriy. A Monte Carlo (MC) approach [18] is used to generate randomly distributed packed beds of spherical pellets. Following the marker and cell approach, this geometry can easily be transferred to the uniform, Cartesian mesh, which is typically used in lattice Boltzmann methods. Due to the low memory requirements of these methods, meshes with several million elements may easily be used to capture the geometric details. The fluid is modelled assuming that a species A is transported by a carrier gas through the structure shown in Fig. 1. This species may be adsorbed by the solid particles and convert to species B. This reaction and adsorption is assumed

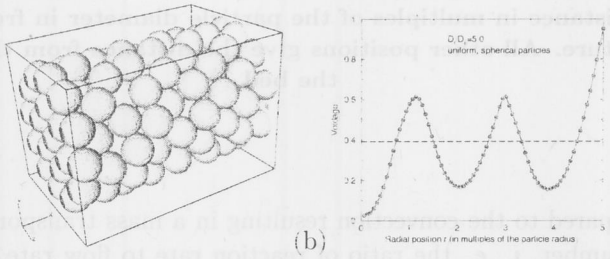

Figure 1. Image of the packed bed structure generated by an MC simulation (a) and the radial voidage profile extracted from the structure (b). The tube to particle diameter ratio is 5, leading to a severe wall effect (channeling), namely very high porosities in the region close to the wall of the tube

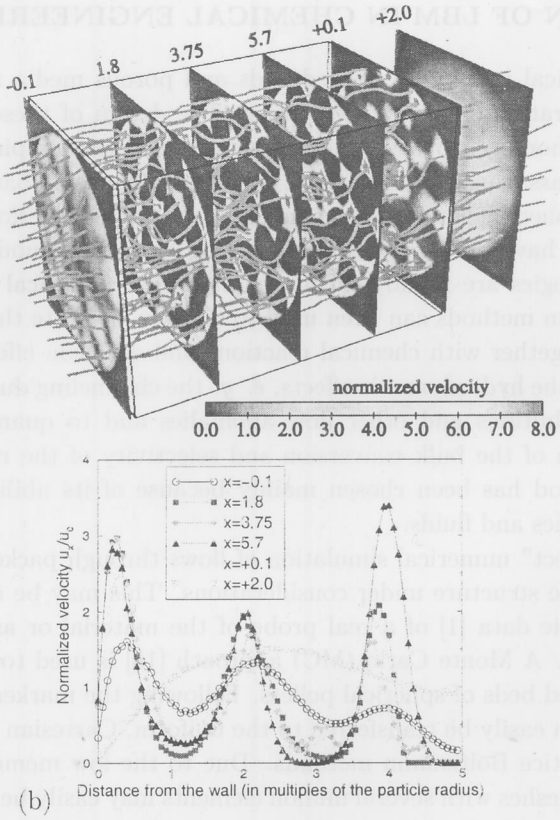

Figure 2. Snapshot of the flow field (a) through the MC generated geometrical structure of the packed bed simulated by the LBA approach and radial velocity distribution (b) in the different cross sections along the axial direction. $Re_p = 6.5$ (laminar flow regime). The axial positions $x = -0.1$ and $+0.1$ and $+2.0$ specify the distance in multiples of the particle diameter in front / behind the packed structure. All other positions give the distance from the beginning of the bed

to be fast compared to the convection resulting in a mass transport limitation. The Dahmköhler number, *i. e.* the ratio of reaction rate to flow rate is Da $\approx$ 100; the Reynolds number based on the particle diameter is Re $\approx$ 10. The structure consists of particles, randomly distributed in a confining cylinder with a diameter ratio (cylinder/particle) of 5. The computational domain is discretised by a $150 \times 150 \times 750$ regular grid, *i. e.* more than $16 \cdot 10^6$ elements. In order to obtain a converged steady state solution, about 40,000 propagation (=iteration) steps were necessary for the

present laminar flow conditions, which took about $2h$ CPU time on six NEC SX 5e shared memory processors. The simulation of the velocity field has been discussed previously [18, 33] and therefore, only the main characteristics are summarized here. In the geometries under consideration, strong variations of the local porosity become dominant, in particular close to the confining cylinder surface leading to severe flow inhomogeneities. This can be seen from the velocity contour plots along cross sections inside the packing at various x-positions (Fig. 2a). Predominantly close to the walls, velocity spikes are observed with a magnitude up to eight times higher that the averaged flux. The corresponding circumferentially averaged radial profiles of the velocity are depicted in Fig. 2b and show the same trend known as the wall effect or wall channeling. This effect is due to the fact that the structure of the packing close to the wall is "ordered", which leads to high local porosities. The simulated local concentrations of species A (the reactant) along cross sections are shown in Fig. 3. As can be seen, reactants are still present in high concentrations close to the exit of the reactor which is due to the fact of the low local flow residence times close to the wall and consequently, the low local conversion rates of A. This breakthrough of species A would lead to a decrease in conversion and degradation of selectivity.

The above approach allows to analyse transport phenomena in more complex geometries such as porous media including reaction or diffusion phenomena. Again, this requires the detailed representation of the geometry of the media. Here, a three dimensional X-ray computer tomography is used to provide a 3D "bitmap" of the geometry. Figure 4 shows a detail of this medium together with streamribbons to show the tortuosity of the flow. In order to analyse more quantitatively the flow and dispersion in porous media, the transport of a passive scaler is simulated using the Flekkøy model [23]. A Gaussian concentration profile is prescribed upstream of the porous media undergoing dispersion as it passes through the structure. From the rate of change of the variance of the concentration profiles a dispersion coefficient may be defined and related to the dispersion due to molecular diffusion. Figure 5 shows the velocity and concentration distribution along a cross section though the porous media. As can be seen, for higher molecular diffusivities (*i. e.* higher Peclet numbers) the effect of the convective dispersion is less pronounced. A quantitative comparison of the predicted dispersion coefficient is shown in Figure 6.

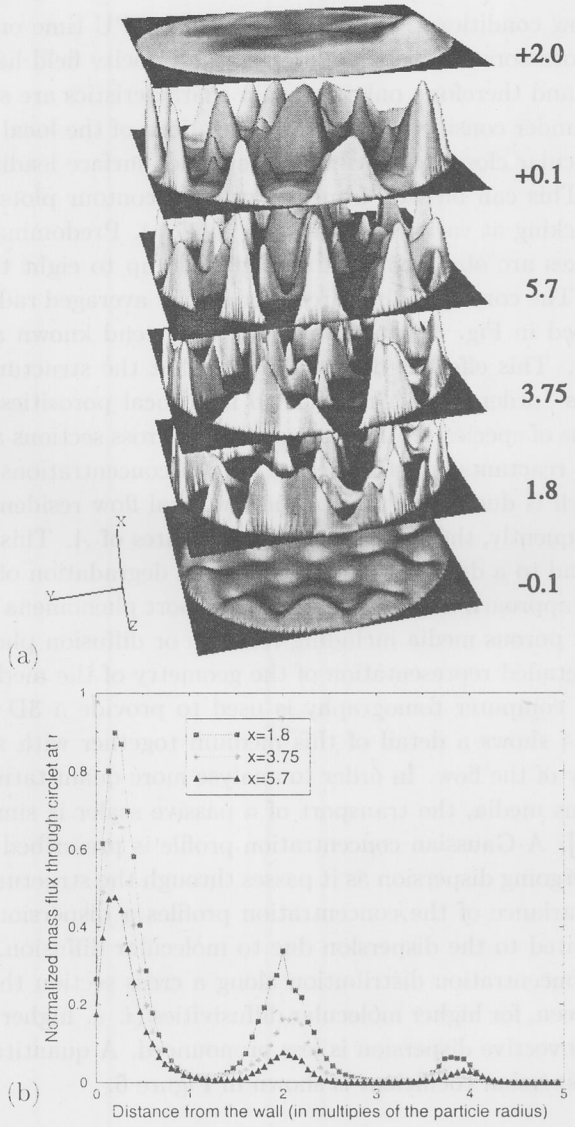

Figure 3. Snapshot of the concentration field of reactant A (a) simulated by the LBA approach and the radial averaged mass flux (b) in the different cross sections along the axial direction. The corresponding flow field is shown in Fig. 2. The Schmidt number of species A is Sc = 18.5 and the reaction occurs only at the surface of the spheres. The reactant is continuously injected over the complete cross section at $x \approx -0.5$. All axial positions are given as multiples of the particle diameter

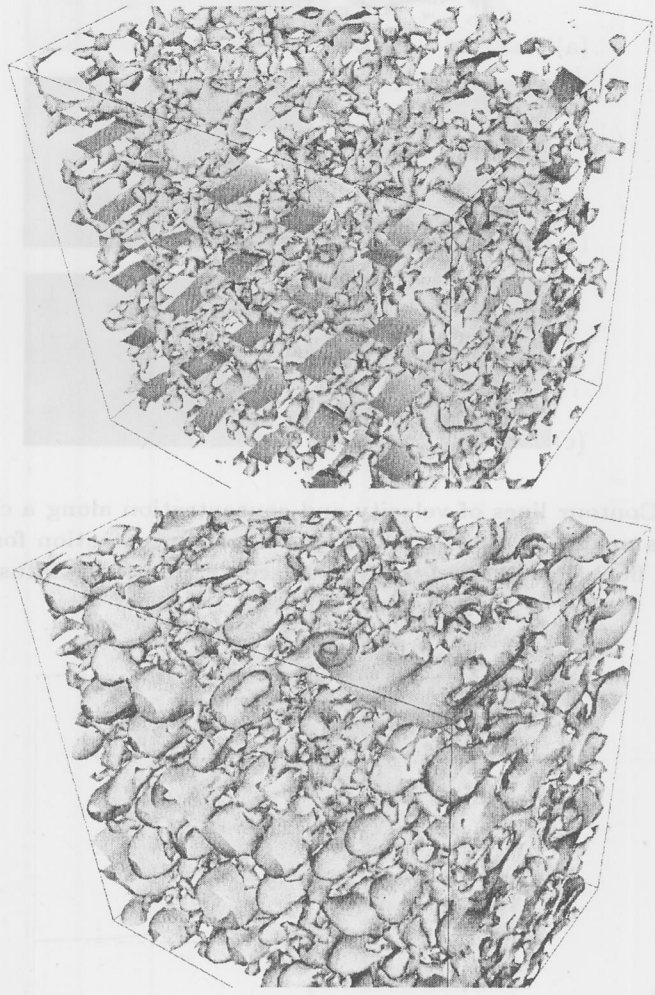

Figure 4. Snapshot of the structure and the flow in a porous media. The geometry is obtained from a computer tomographic scan of a ceramic, foamlike structure. The flow is calulated with the LBM for Re $\approx$ 1. (a) streamribbons, (b) isosurface of velocity

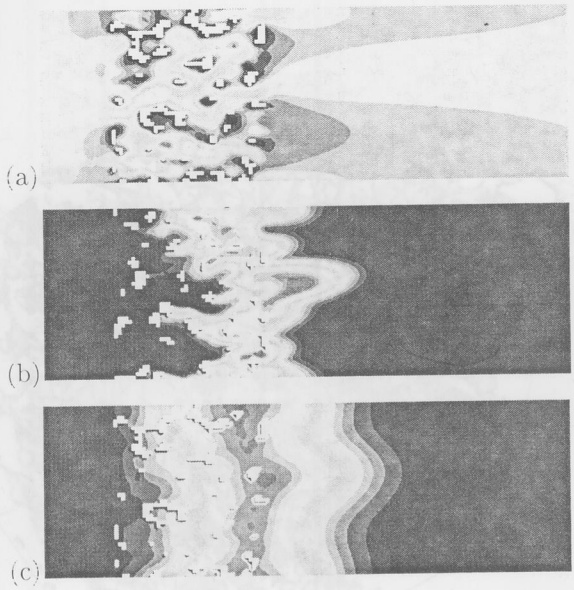

Figure 5. Contour lines of velocity and concentration along a cross section of the porous media. (a) velocity and (b) tracer concentration for a convection dominated flow (Pe = 124), (c) tracer concentration for a diffusion dominated flow (Pe = 12,4)

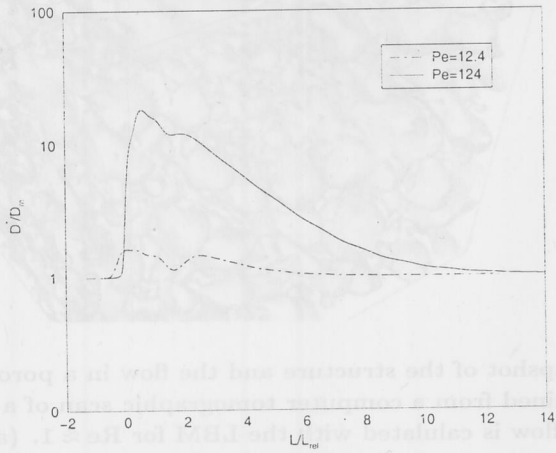

Figure 6. Nondimensional dispersion coefficient for the flow through a porous media (see Fig. 5). The porous media is located between $L/L_{ref} = 1$ and $L/L_{ref} = 2$

APPLICATION OF LBM IN AERODYNAMICS AND TURBULENCE

In aerodynamics, CFD codes based on the approximative solution of the Navier Stokes eqautions are used since a quite long time but have not yet led to a breakthrough with respect to the integration in the overall aerodynamic design process. This is mainly due to the long turn around times and the integration in the workflow [26]. Here, the lattice Boltzmann methods may provide a promising alternative to the classical grid based methods since it allows a nearly automatic preprocessing of geometries of arbitrary complexity, as has been shown in the previous section. The approach is based on a mapping the CAD representation of three dimensiosin spacenal objects on the voxel data structure. In the meantime, in several automotive companies this approach is already realized based on EXA's PowerFLOW code. Thus, an increasing interest is focused on the application of LBM for high Reynolds number turbulent flows. In that context, several questions have to be adressed in order to qualify the LBM as a reliable tool with high predictive accuracy and efficiency. It can be shown, that the dynamics of turbulent flows can be correctly simulated, *e. g.* within a DNS. Figure 7 shows a snapshot of the vorticity field computed with

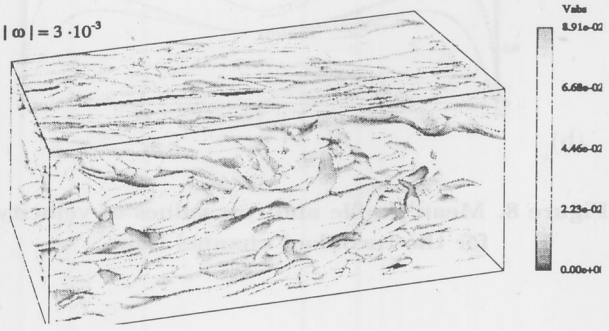

Figure 7. Isosurfaces of vorticity for the flow in the minimal channel. See [14] for the flow parameters

the LBM. The geometry and flow parameters have been chosen according to the well known benchmark test case of Kim et al. [14]. In the present calculations, the computational mesh consists of $600 \times 300 \times 300$ lattice sites. Figure 8 shows the mean velocity profile and the RMS values of velocity predicted with the present LBM in comparison with exiting results obtained using a spectral code. In technical aerodynamic applications of LBM, however, the use of turbulence models is unavoidable. Besides the transport models, such as the $k - \varepsilon$ Model [20], the focus is mainly on

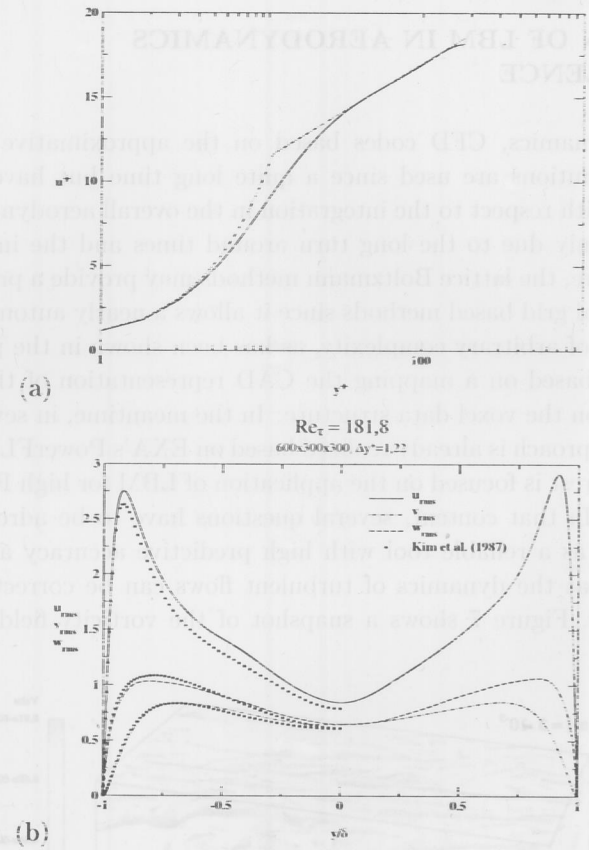

Figure 8. Mean profile and rms values of velocity for the turbulent channel flow

the application of subgrid models. The combination of LES and LBM is promising, as usually larger computational domains with high resolution may be realised with LBM. The implementation of the subgrid model is in fact straighforward, since the second moment of the distribution function already represents the stress tensor, see eq. 6. The input for *e. g.* a Smagorinsky model is thus readily available. After modifying the subgrid viscosity, the relaxation parameter (eq. 8) in the BKG eq. 3 has to be adapted. As a result of this approach, the flow past the AMSO configuration is shown in Figure 9.

CONCLUSION

The lattice gas cellular automata and lattice Boltzmann methods emerged just 15 years ago as new techniques to describe the motion af a fluid based on the simplified transport equations. During that time, remarkable improvements to the methods have been introduced that allow the prediction of complex flows, *i. e.* fluids with chemical reactions, diffusion processes, turbulent flows, among others. A conceptual advantage of the LBM is the algorithmic structure, which can be efficiently implemented on digital computers. Thus, the resulting codes require in general less memory and CPU time compared to classical CFD methods.

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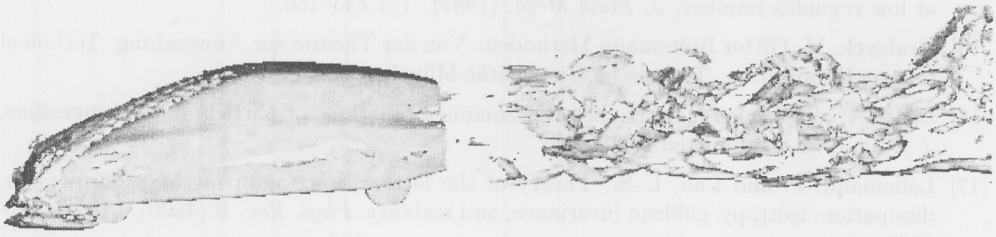

Figure 9. Contour lines of vorticity in the flow past the ASMO body

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