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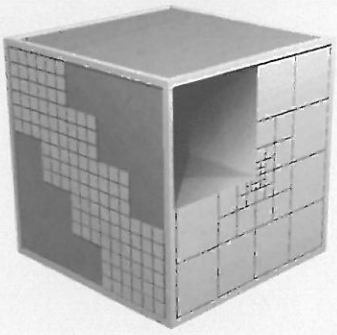

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Abstract

The last decade has seen the development of Lattice-Gas (LG) schemes as a complementary if not alternative method for the simulation of moderate Reynolds-Number Navier-Stokes-Flow. After a short introduction we present a specific 2D-LG algorithm for simulation of chemically reacting flows which runs in parallel on a workstation-cluster and discuss simulation results and efficiency . Finally, we point out present problems and perspectives of these algorithms.

1 Introduction

Nearly all CFD-methods can be considered as discretization methods for partial differential equations, such as finite difference, finite volume, finite element, spectral or boundary integral element methods. Virtually unrecognized by the scientific mainstream in CFD during the last decade, a completely different approach to flow simulation has been developed in Computational Physics. The basic idea of *Lattice-Gas Solvers* (LGS) goes back to the Cellular Automaton (CA) concept of John von Neumann [8]. A CA is a dynamic system represented by a grid of arbitrary dimension. The state of the system is represented by the discrete states of all of its gridpoints. Dynamic development of the state of a gridpoint is a function of the states of a (predefined) local neighbourhood and its own present state. The mapping of a present state to a subsequent state is defined by time independent, predefined rules covering the whole phase space of a neighbourhood. The phase space of a single grid point is usually taken to be very small, eventually binary. Such a class of systems is known to show arbitrarily complex behaviour and to simulate a variety of natural phenomena, provided that an adequate definition of rules is given. As the rules can be applied to the gridpoints simultaneously, CA algorithms are inherently parallelizable, an advantage that might gain significant importance in future.

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2 Description

We present simulations using a particular member of a special class of CA, the so-called Lattice-Gases. An extensive bibliography about this topic can be found e.g. in [1], a detailed description of our implementation is given in [6] which is based on ideas of [4]. LGS use objects ('cells') being extremely simple compared to finite boxes or finite elements. The state of a cell is usually described by only a few bits to represent the existence of particles. These states are subject to simple logical operations defining collision and motion of particles on the grid. Frisch, Hasslacher and Pomeau showed [3], that under certain limitations and for special classes of lattices in such systems large ensembles of particles mimic fluid flow described by the incompressible Navier-Stokes equations. LGS are *explicit* time stepping procedures; *no equation systems* have to be solved. As there is only strictly local interaction between cells, LGS are *inherently parallel*, being suitable to coarse grain as well

as to fine grain parallelization. They are very promising for *dynamic* flow phenomena, multi component flow and flow through geometrically very complex structures (e.g. porous media). In this paper we examine the possibility to model incompressible reactive two-component flows for simulation of etching processes where the flow is influenced by time-dependent boundaries which are subject to etching caused by one of the flow components.

Basically the idea is very simple: A lattice-gas system consists of boundary cells where particles are reflected in a specified manner (see e.g. [7]) and system cells on which particles collide and travel through the system. The introduction of particles of different 'colours' representing different flow-components does not change the mean dynamics given by the incompressible Navier-Stokes equations as long as there are no additional rules which lead to surface-tension effects on a macroscopic scale (see [9]) and which, for simplicity, are not included here. Etching is introduced as an additional collection of rules besides the collision-look-up table so that boundary cells become system cells with a certain probability that is weighed by the number of particles of the etching component being present on such a boundary cell at a given timestep. The 'etching probability' can be scaled according to reaction-rates of the chemical components to be simulated.

3 Implementation

As lattice-gas algorithms allow for fine and coarse grain parallelization we implemented a domain decomposition method as the number of computing nodes in a typical workstation-cluster is relatively small (O(10)). The implementation was done on a cluster of HP 9000/715/50 machines using the EXPRESS parallel environment [2] under the programming language C. In [5] it was shown that due to the inherent structure of lattice gases it is possible to reduce the communication between computing nodes in a way that allows an efficiency of about 85 % using thirty machines. This leads to a maximum nominal performance of about one Gflops in our system. A collection of EXPRESS routines effectively hides the virtual parallel machine from the user by means of automatic domain decompositioning.

4 Results

As numerical examples we present simulation results of dynamic one- and two-component flows. Fig. 1 shows a one-component flow behind an obstacle at Re $\simeq$ 250 related to the width of the obstacle at timestep 100000. The system consists of 1.1×10^7 cells with about 0.9×10^8 particles. Velocity vectors are space-averaged over blocks of 50×50 cells and time-averaged over 50 timesteps. The width of the obstacle is 400 cells and the entrance velocity in horizontal direction is 0.0875 cells per timestep. Calculation time for the transient flow was about 10 h using 24 machines. Figure 2 shows a Driven Cavity at Re $\simeq$ 1000 where one can clearly see secondary vortices in the lower corners (note that the velocity vectors have unit length for optical reasons). The overall height of the system is 2000 cells, the inlet velocity is 0.1 cells per timestep and the velocities are time-averaged over 20000 timesteps and space-averaged over blocks of 40×40 cells. The overall calculation time was about 15 hours using 24 machines showing clearly that the presented LG-method is not competible with state-of-the-art CFD-Solvers with respect to computational time as long as one is only interested in the stationary flow problem. This changes completely, as soon as effects are included, which are difficult or impossible to model with classical methods as shown in the next example (Figure 3). It shows a time-series of a two-component flow simulation where the boundaries are changed by etching from the darker component which leads to a

drastic change of the flow-dynamics during the simulation. The Reynolds Number (related to the height of the upper left inlet) is about 50. The dark dots represent cells where the majority of particles belongs to the etching species. The system size is 250×250 cells, the calculation time for the whole series was about 30 minutes using *one* HP 9000/735/50.

5 Discussion and Conclusions

The ability of lattice-gas algorithms to model fluid flow at moderate Reyolds Numbers is known for some years, yet the efficiency up to now is not comparable to state-of-the-art multi-grid methods when e.g. looking at stationary problems. Still, the upcoming of multi-speed lattice-gases are expected to increase efficiency by about two orders of magnitude besides the fact that there are special classes of flow-problems which are principally difficult to handle for 'classical' numerical techniques of CFD like flows in porous media and chemically reacting multi-component-flows similar to the problem presented in this work.

The idea of simulating chemically reactive multi-component-flow using lattice-gases is generalizable to an arbitrary number of components and can be used for moderate Reynolds Numbers. Simple chemical reactions can be mapped onto additional rules in a quite straightforward manner.

The development of LG methods as a simulation tool has just begun. Yet it is not clear, how important this class of algorithms will become in the next years. The efficiency of future flow simulations depends apart from other problems on how effectively an algorithm can be mapped onto existing hardware. As future high performance hardware will surely be massively parallel, LG methods seem to offer at least a valuable extension to classical discretization methods, which are often hard to parallelize. The possibility to construct a virtual parallel machine from a workstation cluster using appropriate parallelizing software offers a low cost alternative for high performance simulations in this area.

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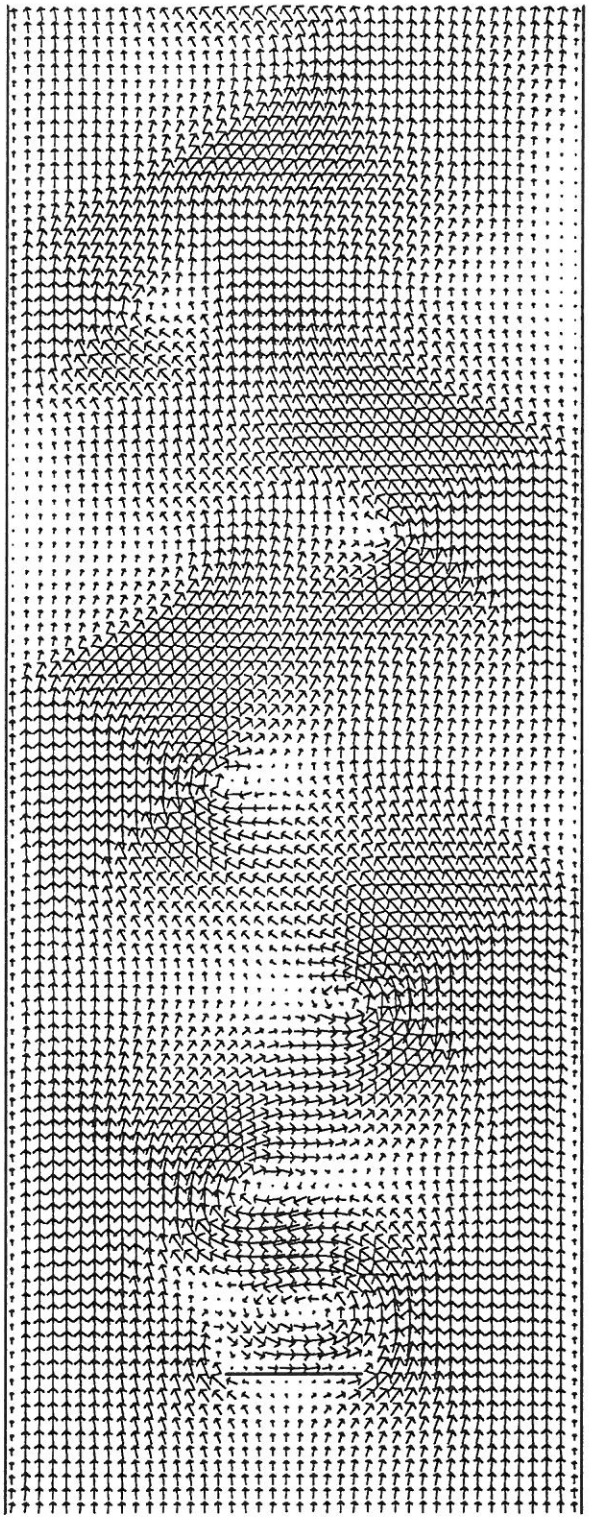

Figure 1: Flow behind an obstacle at Re $\simeq$ 250 at t= 80000

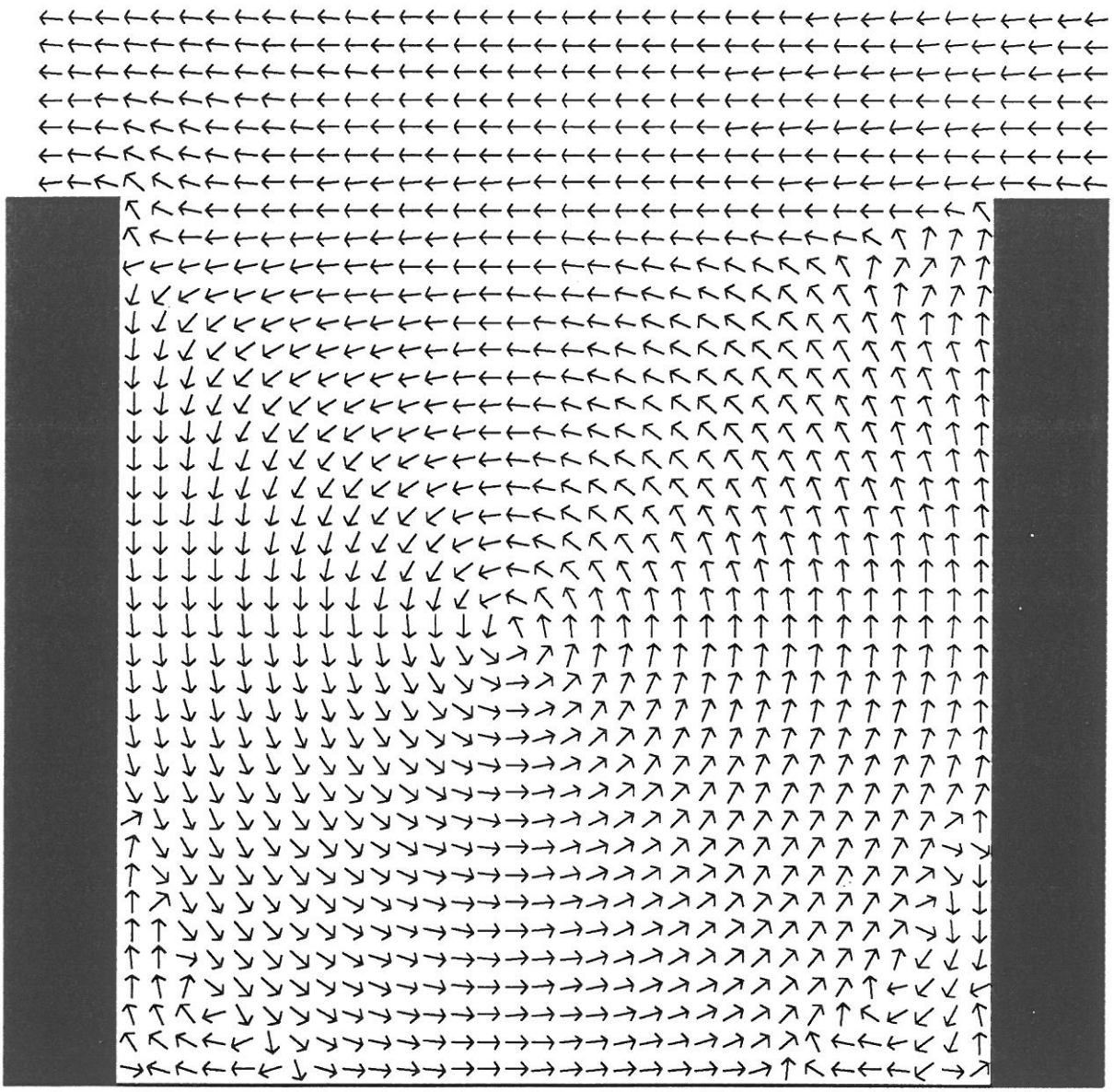

Figure 2: Driven Cavity at Re $\simeq$ 1000 averaged over 20000 timesteps

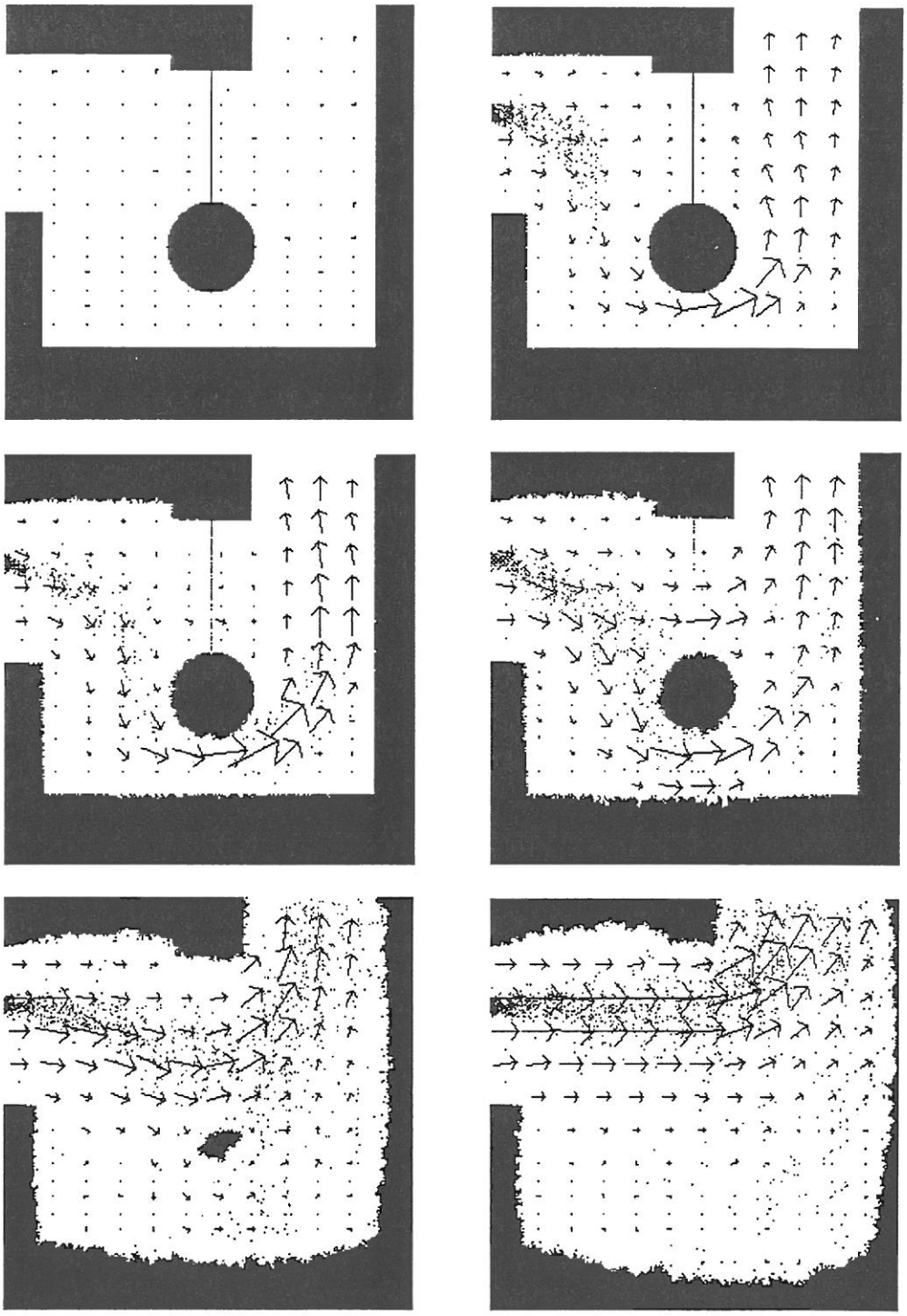

Figure 3: Etching simulation at timesteps 0, 1000, 2000, 3000, 6000 and 11000