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Simulating Fully Three-Dimensional External Flow by Lattice Gas Methods.

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Abstract. – We have built a three-dimensional 24-bit lattice gas algorithm with improved collision rules. Collisions are defined by a look-up table with 2^{24} entries, fine-tuned to maximize the Reynolds number. External flow past a circular plate at Reynolds number around 190 has been simulated. The flow is found to evolve from axi-symmetric to fully 3D. Such simulations take a few minutes of CRAY-2 per circulation time (based on plate diameter and upstream velocity).

1. Introduction.

Lattice gas methods using fictitious Boolean microworlds for the simulation of hydrodynamics have been introduced by Frisch, Hasslacher and Pomeau [1] (see also [2]). Mass and momentum conservation and a «sufficiently» large crystallographic symmetry group ensure that the large-scale and low-speed behaviour is indistinguishable from that of a real fluid in an incompressible regime. No three-dimensional Bravais lattice has the required symmetry (isotropy of fourth-order tensor is needed). D'Humières, Lallemand and Frisch [3] observed that the face-centred-hyper-cubic (FCHC) four-dimensional lattice possesses such symmetries. From this, they constructed the *pseudo-4D* model, which has microscopically four space dimensions; it extends only one lattice constant in the fourth dimension, and has three-dimensional macroscopic behaviour. The pseudo-4D model can be viewed as a *cellular automaton* residing on a ordinary 3D cubic lattice with a 24-bit state for each node, 24 being the number of nearest neighbours on the 4D FCHC lattice. Rivet [4] has validated the pseudo-4D model for 3D Navier-Stokes simulations. Transport coefficients were measured and comparisons were made with spectral calculations for the Taylor-Green vortex.

Efficiency of lattice gas simulations has two aspects. First, there is the viscosity, which inherently depends on the collision strategy [5], and must be made as small as possible to achieve the highest Reynolds numbers. As shown in ref. [2], the latter can be written as the product of three factors, the characteristic size (in lattice constants), the Mach number, and a «Reynolds coefficient» $R_*^{\max}$ (dimensionless form of the maximum inverse viscosity), dependent only on the collision rules. Necessary computational resources, for a given physical 3D situation, scale like $(R_*^{\max})^{-4}$. The second aspect is the actual efficiency which can be achieved in the implementation on a given computer; this is a function both of the chosen collision strategy and of the hardware.

The early validations [4] were done with the *isometric collision rules* [6], in which the output state is obtained from the input state by an appropriate isometry, and which has $R_*^{\max} = 2.0$. Its implementation on a CRAY-2, requiring considerable logic and memory accesses, had low efficiency (0.5 million node updates per second). We have developed a new, more efficient strategy, which has $R_*^{\max} = 7.13$ and a speed of approximately 30 million node updates per second. The first ingredient for this is the fine-tuning of collision rules.

2. Collision rules.

For basic concepts and notation, we refer the reader to [2, 5]. The Reynolds coefficient is given by

$$R_*^{\max} = \max_d R_*(d), \qquad R_*(d) = \frac{g(d)}{\nu(d)} c_s . \tag{2.1}$$

Here, $c_s = 1/\sqrt{2}$ is the speed of sound, d is the (reduced) density, $g(d)$ is independent of the collision rules (as long as semi-detailed balance holds), and ν is the kinematic viscosity, which depends both on the density and the collision rules. It has been shown that, for nonpathologically small or high densities, the *Boltzmann approximation* gives fairly accurate predictions for the viscosity in two dimensions [7] and even better ones in three dimensions [4]. In all subsequent optimizations, we thus use the Boltzmann approximation for the viscosity, which allows an explicit expression in terms of the density and the collision rules [5]. Thereby, the optimization of the Reynolds coefficient becomes a local problem.

For this it is convenient to divide the set of all possible input states into *packets*. Each packet contains all states which have a given number of particles p and a given momentum $\boldsymbol{q}$. A collision must change a 24-bit input state s into a 24-bit output state s' belonging to the same packet. Thus, each packet presents a separate optimization problem. The collision probabilities $A(s; s')$ should be chosen so as to minimize the quantity [5]

$$\sum_s \sum_{s'} A(s; s') W(s; s') , \tag{2.2}$$

where the sums on s and s' run over all states of the packet, and the weights $W(s; s')$ are defined by

$$W(s; s') = \sum_\alpha \sum_\beta (Y_{\alpha\beta} + Y'_{\alpha\beta})^2 . \tag{2.3}$$

$Y_{\alpha\beta}$ is the anisotropic part of the second-order momentum of the input state

$$Y_{\alpha\beta} = \sum_i s_i c_{i\alpha} c_{i\beta} - \frac{p}{2} \delta_{\alpha\beta} . \tag{2.4}$$

$Y'_{\alpha\beta}$ is defined similarly for the output state.

For reasons of simplicity, we restrict ourselves to *deterministic* collision rules; by this we mean that for a given input state s there is only one permitted output state s'. The rules are then defined by a function $s' = Z(s)$ (which is in fact a permutation of the states in each packet). We have $A(s; s') = 1$ if $s' = Z(s)$, $A(s; s') = 0$ if $s' \neq Z(s)$. The quantity (2.2) can be written

$$\sum_s W(s; Z(s)). \tag{2.5}$$

We also assume that the rules satisfy *detailed balance* (microreversibility), *i.e.* we have $Z[Z(s)] = s$ for any s.

Our problem reduces then to an instance of the classical *weighted matching problem* [8, 9]. Existing algorithms for the optimal solution require a computing time proportional to N^3, where N is the size of the packet. Since N can here be as high as 11 740, the necessary time is prohibitively large.

We settled for an approximate optimization. We used a simple form of «greedy algorithm» [10]: the two states of the packet for which the weight is smallest are matched and withdrawn from the packet, and this is repeated until the packet is exhausted. Computing time is proportional to N^2 only. Recent results indicate that this simple procedure gives results which are within 6% of the optimum.

Figure 1 shows $R_*(d)$, evaluated for the greedy collision rules. It should be compared to the corresponding figure for the isometric collision rules [6]. The Reynolds coefficient is now $R_*^{\max} = 7.13$. This represents an improvement by a factor 3.6 over the isometric rules. The maximum is reached for an average number of particles per node $24d = 7.90$.

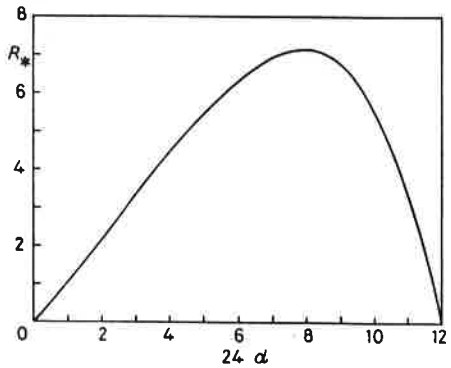

Fig. 1. – Quantity $R_*(d)$, defined by (2.1), as a function of the average number of particles per node, $24d$, for the greedy collision rules.

Our collision rules do not strictly satisfy the symmetry requirements [2, 5], *i.e.* they are not invariant under isometries, since this condition was not set to the greedy algorithm. Hence, the viscosity becomes a fourth-order tensor, which need not be exactly isotropic. From the collision rules, the viscosity tensor can be obtained by solving the linearized Boltzmann equation [2, 5], here, a system of 24 linear equations. To minimize possible anisotropies, the greedy algorithm has been randomized as follows. Observation shows that in most cases the minimum of W is achieved simultaneously by many pairs of states. This is because the quantity (2.3) can take only a restricted set of values. The pair to be matched is then randomly chosen.

All components of the resulting viscosity tensor differ by less than 1.5% from their isotropic values.

3. Practical implementation.

The pseudo-4D model has been implemented on a CRAY-2 machine. Large memory, hard-wired indirect addressing, very short clock period, and multitasking on four processors can be used to achieve very high efficiency. In single user situations, 30 million 24-bit nodes can be updated per second. Actual performances are down by 20% or less.

The key element in the implementation is the use of a look-up table with 2^{24} entries, corresponding to the collision rules described in sect. 2. This table is generated once for all and retrieved from mass storage before each run. There are three main steps in the lattice gas simulation.

First, the Boolean field is initialized, either by a Monte-Carlo procedure from macroscopic data, or from stored previous time-segments of the run. The Monte-Carlo generation is distributed between four balanced and independent tasks.

Second, there is the automaton updating, which has two steps, particle displacement and local operations: collisions, boundary bounces, particle injection and absorption. The former is done successively for the x, y, and z directions by mask operations and address shiftings. The latter, mostly collisions, is done by indirect addressing of the look-up table. Both steps are shared among four interdependent balanced tasks, synchronized by semaphore flags, in such a way that minimal idle-time results. The storage mode (involving two 24-bit nodes per CRAY word and other aspects) is chosen to reduce the number of memory accesses, to facilitate boundary treatment and future extensions of the model.

Third, the macroscopic information is extracted and processed. The hydrodynamic velocity and pressure fields are computed with full multi-tasking from suitable averages of the Boolean field over cubic cells containing typically 8^3 nodes. The resulting information (strongly packed in binary form) is transferred to local machines (VAX 785 and SUN 3/160) for the final processing and the graphical treatment.

Wherever possible (and useful) care is given to reduction of the various conflicts, to vectorization and parallelization. The latter corresponds to a suitable splitting up of the physical space into four subdomains. It would be simpler, but not correct to use the four processors to run four microscopically different versions of the flow. Indeed, in situations with macroscopic symmetry breaking, the averaging of the macroscopic fields over the four versions does not produce a solution of the Navier-Stokes equations.

4. Results.

We have chosen to study flow at Reynolds numbers of a few hundreds around an obstacle with an axial symmetry, such that three-dimensional motion results from spontaneous symmetry breaking. For internal flow (*e.g.*, channel flow) transition Reynolds numbers are about an order of magnitude larger, and thus quite unpractical for present lattice gas calculations.

We have set up a 3D «numerical wind-tunnel» with a controlled upstream flow, using particle emission/absorption as in ref. [11]. Our initial conditions are roughly equivalent to an impulsively started obstacle in a flow at rest. The lattice size (in number of nodes) for the reported run was $128 \times 128 \times 256$. Quadrupling of all three dimensions is, in principle, feasible on a CRAY-2. The simulations had periodic boundary conditions in the directions transverse to the upstream flow. We used as obstacle a circular plate ([1]) normal to the flow

([1]) Some early 3D results on flow past a plate have also been obtained by the Los Alamos group [12].

(arbitrary shapes can be handled). The plate diameter was 64 nodes, giving a solidity (obstruction of the transverse area) of 20%. The Mach number was $M = 0.42$. The Reynolds number, based on plate diameter and upstream velocity was $Re = 190$. The calculations took about 100s of CRAY-2 four-CPU time (645 automation steps) per circulation time. The latter is defined as plate diameter divided by upstream velocity.

Figure 2*a*) and *b*) represent details of axial slices of the flow at two different times. Figure 2*a*) corresponds to 400 automaton steps, that is 0.62 circulation times ([2]). At such early times the recirculation zone is a nearly perfect vortex ring, as observed experimentally, for example by Werlé [13]. Figure 2*b*) corresponds to 3500 automaton steps

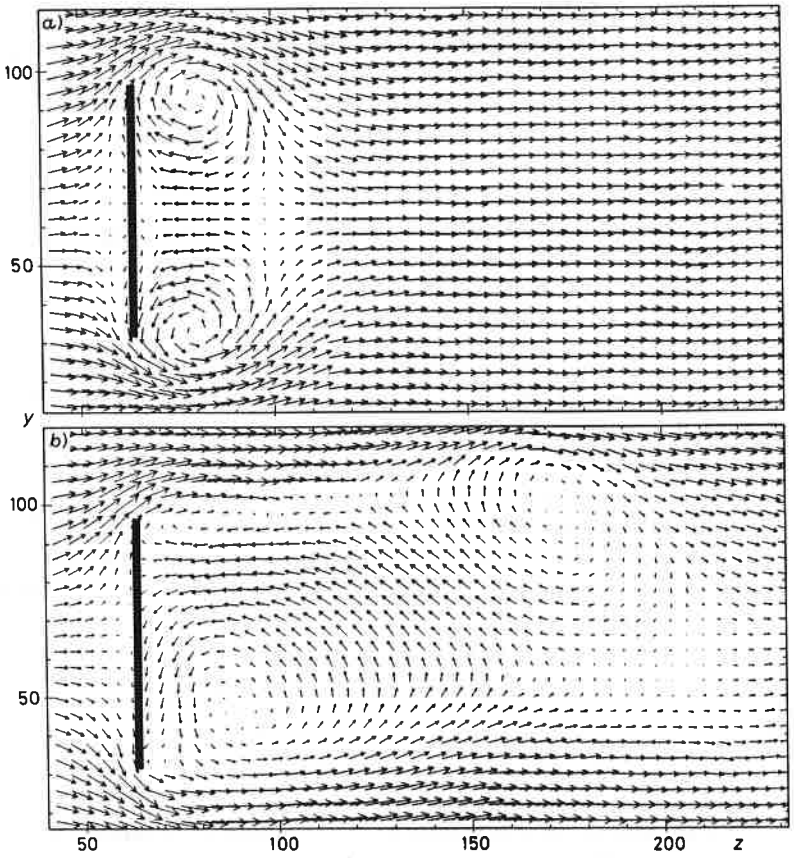

Fig. 2. – Flow past a circular plate at Reynolds number of 190. *a*) After 400 automaton steps (0.62 circulation times): axi-symmetric vortex ring; *b*) after 3500 automaton steps (5.43 circulation times): fully 3D flow.

(5.43 circulation times). The axial symmetry is now broken and the flow is fully three-dimensional; a detached vortex is seen in the upper right corner. Figure 3 gives some feeling for the three-dimensional vortical structure at 6.2 circulation times; it is a perspective view of high-vorticity modulus regions displaying a «basket and handle» structure; the figure also shows the plate and the full simulation domain.

Transition to three-dimensionality in external flow is poorly understood. It is

([2]) In computing physical times one must take into account the factor $g(d)$, here about 0.3 [2, 3].

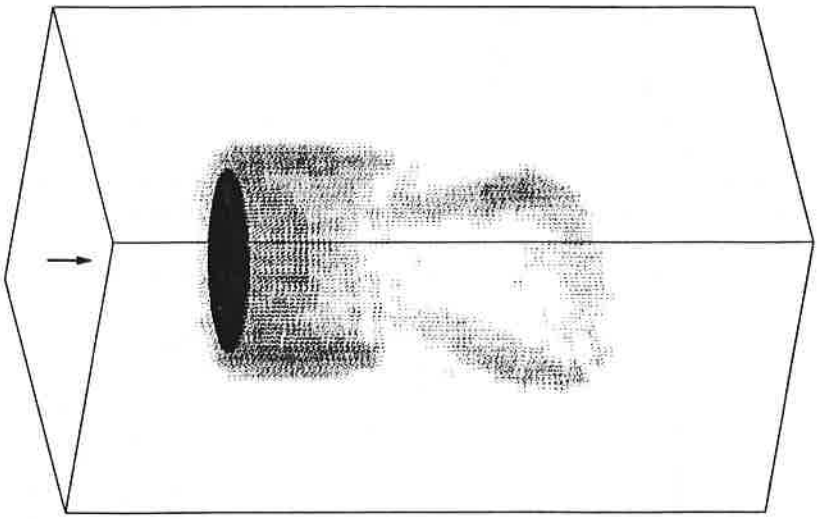

Fig. 3. – High vorticity regions (perspective view) after 4000 automaton steps (6.2 circulation times). Also shown: full simulation domain, mean flow (arrow), and circular plate.

considerably more difficult than, say, transition in convective internal flow. Lattice gas simulations are an attractive and efficient alternative to floating point methods for exploring this frontier of fluid dynamics.

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