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LATTICE-GAS SIMULATIONS OF TWO-PHASE FLOW IN POROUS MEDIA

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SUMMARY

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 computational fluid dynamics (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 automation concept of John von Neumann. 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 therefore often two orders of magnitude more cells are used for a simulation with LGS than ‘elements’ in a finite element computation. LGS are explicit time-stepping procedures; no equation systems have to be solved. Thus every time-step is extremely cheap in terms of CPU power compared to standard procedures, yet again much shorter time-steps have to be used. LGS are inherently parallel and are suitable to coarse-grain as well as to fine-grain parallelization.

The paper will discuss some advantages and disadvantages of lattice-gas solvers and present LG simulation results of two-phase flow with moving boundaries on a microscope scale for a two-dimensional test geometry of randomly distributed equally sized disks where the effect of surface tension on the steady-state saturation will be demonstrated. © 1998 John Wiley & Sons, Ltd.

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1. LATTICE-GAS METHODS: THE BASIC CONCEPT

The principle idea of cellular automata dates back to John von Neumann. Following Toffoli, a cellular automaton (CA) is a dynamical system, the ‘universe’ is a uniform grid with each ‘cell’ containing a few bits of data. Time is advancing in discrete steps and the ‘laws’ of the universe are defined in a small look-up table, through which in each time-step each cell determines its new state from that of its neighbors.

A famous example for a cellular automaton is John Conway’s ‘game of life’, yet for a long time CA was seen more as a basic concept of theoretical computer science rather than a method being applicable to engineering problems. This view has changed significantly, since special types of CA, so-called lattice-gas methods (LG methods) have been investigated in computational physics, and some very promising features concerning the simulation of complex fluid flow have been demonstrated. We will summarize in the following only the basic ideas of LG methods; for more detailed discussions see, for example, References 3–5.

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The simplest useful LG simulates a strongly idealized particle flow on a hexagonal grid as shown in Figure 1. Particles are drawn as arrows on the left side of the picture. The right part shows a binary equivalent of the particle model, where a 1 at a grid node denotes a particle being present in a corresponding direction and a 0 defines the absence of a particle. For simplicity, no binary numbers are drawn at nodes where no particles are present. All particles have uniform weight and collision of particles is allowed at grid nodes, conserving the number of particles, energy and momentum. The evolution of the system is performed in discrete time-steps within which each particle can move within one time-step exactly from one node to one of its neighbours. Therefore all particles have a uniform velocity. In a more advanced variant of LG methods particles at rest are also allowed. In this case, energy conservation is observed only in the mean.

At every instance, the state of each node or ‘cell’ can uniquely be defined by a 6-bit number as shown in Figure 2. The update of the state of each cell, to be applied uniformly on the whole grid, consists of collision rules and of propagation rules. In the setting of the 6-bit state of each cell, the collision rule is a mapping of an integer to another where usually one of several possible resulting states is chosen randomly. In Figure 2 one of the two possible post-collision states is chosen with probability $A_1$ or $A_2$. Propagation shifts individual bits from one cell to the according neighbours.

To be more precise, define a microscopic Boolean variable $n_x(\vec{r}, t)$, being 1, if at time $t$ and location $\vec{r}$ a particle is present in direction $\alpha$, $\alpha$ ranging from 1 to 6. Macroscopic observables can then be introduced as mean values of specific quantities in a neighbourhood $K$ of $\vec{r}$:

$$f_\alpha(\vec{r}, t) = \frac{1}{Z} \sum_{\vec{r'}-\vec{r} \in K} n_\alpha(\vec{r'}, t)$$

(1)

Figure 2. Two possible post-collision states with their binary coding.

where \( f_x(\vec{r}, t) \) is a mean particle population in direction \( \alpha \) and \( Z \) is the number of grid points in \( K \);

\[
\rho(\vec{r}, t) = \sum_{x=1}^{6} f_x(\vec{r}, t)
\]

is the particle density and

\[
\vec{u}(\vec{r}, t) = \frac{1}{\rho(\vec{r}, t)} \sum_{x=1}^{6} \vec{e}_x f_x(\vec{r}, t)
\]

is the macroscopic flow velocity, \( \vec{e}_x \) being the unit vector in direction \( \alpha \).

Frisch et al.\(^3\) showed in 1986 that the macroscopic dynamics of the lattice gas is described by the Navier–Stokes equations:

\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \vec{v}) = 0
\]

and

\[
\frac{\partial (\rho v_j)}{\partial t} = -\frac{\partial}{\partial x_j} (g(\rho) \rho v_j v_k) - \frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \nu S_{ijkl} + \zeta \delta_{ij} \delta_{kl} \right) \frac{\partial (\rho v_j)}{\partial x_k}
\]

where \( g(\rho) \) is a model-specific function, \( \zeta \) is the bulk viscosity, \( \nu \) the kinematic viscosity and \( S_{ijkl} = \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} + \delta_{ij} \delta_{kl} \).

In contrast to classical methods, a lattice gas is not a discretization of the Navier–Stokes equations, but an artificial physical system whose evolving dynamics can be described (up to second order) by these equations. An important consequence of this observation is that the kinematic viscosity \( \nu \) and bulk viscosity \( \zeta \) are implicitly defined by density and collision rules, and are not, as in discretization methods, numerical parameters to be plugged into a model. These quantities can be approximately calculated but usually have to be measured for a specific LG implementation in a very similar way as they are measured in a physical system.

As \( \zeta \ll \nu \) the flow of an LG can be considered incompressible for small Mach numbers, and for models including non-moving (so-called rest-) particles \( g(\rho) \) can be adjusted to 1, so that lattice artefacts of the simplest model described above disappear.

Further consequences of the basic principles of LG are the following:

1. There is a maximum mean velocity of a lattice gas, measured in units of grid space and time steps: \( u_0 \ll 1 \) (small Mach number limit).
2. By \( Re = (\rho \nu) / \nu \) there is a linear relation between the number of grid points in each space direction and the (maximum) Reynolds number to be simulated for a given grid.
3. The computational complexity of an LG algorithm grows more than quadratic with the Reynolds number.

Therefore LG-algorithms show poor efficiency for ‘standard’ flow simulation at higher Reynolds numbers (\( \geq 500 \)), compared to implicit state-of-the-art discretization techniques. The use of grid refinement techniques (see, for example, Reference 6) to overcome this problem is not feasible for multiphase flows as the surface tension of the LG methods found in the literature to date depends on the local grid size and thus forbids non-uniform grids. Yet, they show very significant
advantages in applications where a higher geometric resolution is mandatory, e.g. in porous media flow simulation on a microscopic scale, or in problems with free and moving interfaces. Recently there have been extensions to LG methods resulting in so-called lattice–Boltzmann techniques which will not be discussed here. The interested reader is referred to References 7–10 and the references therein.

2. SIMULATION OF TWO-PHASE FLOW

In 1988 Rothmann and Keller\textsuperscript{11} suggested an LG model for simulating two-phase flow of immiscible fluids, introducing particles of different ‘colours’ and choosing from all possible post-collision states those which locally separate the colours.

More formally, for an LG with ‘red’ and ‘blue’ particles, a local colour flux

$$\vec{q}(\text{red}(\vec{r}), \text{blue}(\vec{r})) = \sum_{a=1}^{6} \vec{e}_{a}(\text{red}_{a}(\vec{r}) - \text{blue}_{a}(\vec{r}))$$  \hspace{1cm} (6)

and a local colour gradient

$$\vec{f} = \sum_{a} \vec{e}_{a} \sum_{b} (\text{red}_{b}(\vec{r} + \vec{e}_{a}) - \text{blue}_{b}(\vec{r} + \vec{e}_{a}))$$  \hspace{1cm} (7)

are defined, where red\textsubscript{a} and blue\textsubscript{a} are the microscopic Boolean variables n\textsubscript{a}(\vec{r},t) for the respective colours.

The colour separation rule chooses a post-collision state which maximizes colour flux in the direction of the colour gradient:

$$\vec{q}(\text{red}(\vec{r}), \text{blue}(\vec{r})) \cdot \vec{f} \overset{!}{=} \text{max}$$  \hspace{1cm} (8)

On a macroscopic scale, this rule generates a density-dependent surface tension $\sigma$ which can be calculated by measuring the pressure difference in- and outside a bubble of given colour and radius $R$ in a sea of the other colour and fitting the data to the Laplace law,

$$\Delta P = \sigma/R$$  \hspace{1cm} (9)

3. POROUS MEDIA FLOW

It is well known that for a large variety of flow phenomena in porous media Darcy’s law is applicable, linearly relating flow rate and driving forces (or pressure gradients) via the geometrical properties of the medium (permeability) and the fluid (viscosity). Non-linear deviations are known for Re$\gg$1 and, for example, for multiphase flow with Re $<$ 1, where capillary pressure and wettability effects are responsible for non-linear behaviour of the flow. Due to their high geometric resolution LG methods have been used to gain understanding of

Figure 3. Three snapshots of the transient saturation at times-steps 10,000, 30,000 and 100,000 with suppressed surface tension (miscible fluids)

these regimes. The simulations in this paper using a model of Reference 14 are intended to support the usefulness of LG simulations for these non-linear regimes.

4. RESULTS AND DISCUSSION

We have defined an artificial porous geometry by a random distribution of discs with a radius of ten cells in a system of 900 × 600 cells resulting in a porosity of 60 per cent. The system is topologically connected as a torus. A standard domain-decomposition approach was used to split the system into equal parts. The simulation was done on a workstation cluster of nine HP-715s using the parallelization software EXPRESS (similar to PVM). The update rate was about 560,000 cells per second, gaining an efficiency of about 80 per cent. For implementation details the reader is referred to Reference 15. Although the porosity in real 3D systems is usually much smaller, one has to keep in mind that in 2D the permeability is much lower for a given porosity than in 3D. So we used a porosity of 60 per cent as a compromise between the complexity of the geometry and the resulting simulation time. The lattice was initially filled with particles of the wetting ‘color’ to simulate the phenomenon known as drainage (a non-wetting fluid invading a porous medium filled with a wetting fluid). A driving body force (‘gravity’) was superimposed by changing the direction of particles towards the negative y-axis with a small probability in each time-step. This resulted in an average velocity giving a Reynolds number of about 1 related to the disc-radius. The colour of ‘dark’ particles which reach the lower bound of the system was changed to white. This ensured that we have an exact conservation of the particle number in the system during simulation. The system evolves for 100,000 time-steps. Figures 3 and 4 show the transient saturation of the dark fluid evolving to a steady state for different choices of the probability \( p \) to apply phase-separating instead of colour-blind collision rules at each cell and time-step. The phase-separating rules imply a surface tension of

\[
0.085 \pm 0.008 \left( \frac{\text{lattice-units}}{\text{time-step}^2} \right)
\]

whereas the colour-blind rules lead to an inter-species diffusion with a diffusion-constant that can be determined to be

\[
0.00911 \pm 0.0008 \left( \frac{\text{lattice-units}^2}{\text{time-step}} \right)
\]

for the model used. Snapshots of the saturation at three distinct time-steps (10,000, 30,000 and 100,000) for \( p = 0 \) (Figure 3) and \( p = 1 \) (Figure 4) are shown, with the small arrows indicating the local magnitude and direction of the flow velocity. Figure 5 shows saturation curves (mass volume percentage of dark fluid in the system) for \( p = 1, 0.75, 0.5, 0.25, 0.15, 0.1, 0.0 \) during the simulation time. One can clearly see the non-linear effect of this parameter on the steady-state saturation. In this paper we did not quantify this non-linear relationship because the use of a 2D geometry is somewhat artificial and it is difficult to compare these results to experimental data. The future goal is to extend the simulations to three-dimensional realistic geometries which

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Figure 4. Three snapshots of the transient saturation at time-steps 10,000, 30,000 and 100,000 with maximum surface tension (immiscible fluids)

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can be obtained by microtomography (see, for example, References 16 and 17) to allow for experimental feedback. Nevertheless the results so far indicate that the use of LG methods for simulation of non-linear flow phenomena in porous media will become a valuable tool to obtain parameters like permeabilities for particular geometries as well as to gain insight into non-linear relationships between macroscopic attributes of complex multiphase flows. The striking ability of LG simulations to model the transient and complex dynamics of phase-interfaces can be demonstrated when looking at animations of the system evolution. An example of such animations is available from the authors.

REFERENCES