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Interfacial Phenomena in Boltzmann Cellular Automata.

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Abstract. - A two-dimensional two-colour, nonlinear, Galilean-invariant, Boltzmann cellular automaton is developed and used to study two-fluid hydrodynamics and to model fluid interfaces. The interfacial tension and interface width are flexibly controlled by the parameters defining collision rules for the colored particles. Results of studies of both the static and dynamical relaxation of the surface tension and wetting properties are presented.

The interface between two immiscible fluids has been a subject of intense interest from several points of view including thermodynamics, pattern formation, and phase separation. Perhaps the simplest approach for mimicking two-fluid phases is the Ising model with its up and down states. However, it is well known that such simplified spin models do not incorporate hydrodynamic modes and are therefore in a different dynamical universality class [1]. Conventional methods of study include the numerical integration of the Navier-Stokes equation and molecular-dynamics (MD) simulations entailing the integration of Newton's laws of motion for the interacting fluid molecules. These methods are computationally intensive, however. Hydrodynamic equations follow from the presence of certain conservation laws at the microscopic scale. Thus, fictitious particles on a lattice—cellular automata (CA)—that, in collisions with each other, satisfy the desired (and not any spurious) conservation laws behave hydrodynamically at coarse-grained length and time scales [2-5]. An advantage of CA is that even though the microscopic physics is not accurately captured, the macroscopic behavior is correctly reproduced and often with less computational effort. The advent of CA as a viable technique has provided new insights into the behavior of fluids and often yields information complementary to that obtained from other methods [5].

In this letter, we develop a variant of the CA technique for studying a pair of fluids in two

dimensions with a desired degree of miscibility. Our approach follows the standard treatment—the system is made Galilean-invariant using a judiciously chosen maximum possible number of rest particles [6]; the noise is eliminated by use of the Boltzmann cellular automata (BCA) [7] in which ensembles of microscopic configurations are considered simultaneously by ascribing probabilities of occupation to each of the discrete velocity states (the individual event collision rules correspond to FHP II suggested by Frisch, Hasslacher and Pomeau [4]); and the prescription for having fluids of two colors follows the pioneering work of Rothman and Keller [8] with two key differences. First, instead of maximizing the scalar product of the color gradient with the color momentum, we redistribute the color after a color-blind collision in such a way that the difference between the densities of the two colors along the α -th direction depends continuously on the angle ϕ_α between the α -axis and the color gradient. Second, the interfacial tension and the width of the interface are flexibly controlled by two microscopic parameters, β_1 and β_2 , which are related to the energy barrier and the interface stiffness in a classical description of the interface.

With the machinery in place, we have carried out studies of static interfacial properties, wetting properties in the presence of a wall and the dynamical relaxation of the surface tension of two initially immiscible fluids on turning off the surface tension. Taken together, these results show that the BCA technique is a valuable tool for describing a variety of phenomena in fluids. Important differences between real fluids and these toy models are also demonstrated, especially relevant to studies of the dynamics of phase separation [9].

The BCA model. – Our method is most similar to that of Gunstensen *et al.* [7] with the following differences:

1) We do not assume that the local densities of the two fluids are close to their steady-state values—such an assumption would allow one to linearize the equations to lowest order in the density difference.

2) Our coloring scheme involves two steps. Following ref. [7], we determine the color gradient vector \mathbf{g} at each node and increase the total state density along the axis defined by the color gradient with a decrease in the density in a direction perpendicular to the axis,

$$f'_\alpha = f_\alpha + \beta_1 |\mathbf{g}| \cos 2\phi_\alpha, \quad (1)$$

where f_α refers to the initial state density, f'_α the density after the redistribution, ϕ_α is the angle between the α -th axis (on a triangular lattice, α takes on one of 6 values) and \mathbf{g} . This first step is the same as in ref. [7]. Our second step for the reassignment of colors is according to the equations

$$r'_\alpha = \frac{R_t}{R_t + B_t} f'_\alpha + \beta_2 \frac{R_t B_t}{(R_t + B_t)^2} \cos \phi_\alpha, \quad (2)$$

$$b'_\alpha = \frac{B_t}{R_t + B_t} f'_\alpha - \beta_2 \frac{R_t B_t}{(R_t + B_t)^2} \cos \phi_\alpha, \quad (3)$$

for the moving states ($\alpha = 1, 2, \dots, 6$) and

$$r'_0 = \frac{R_t}{R_t + B_t} f'_0, \quad b'_0 = \frac{B_t}{R_t + B_t} f'_0, \quad (4)$$

for the states at rest, where R_t and B_t refer to the total red and blue densities at a node (r and

b stand for red and blue, respectively). The parameters β_1 and β_2 typically take on values of the order of 0.001 and 0.2 and control the values of the surface tension and interfacial width, respectively.

Our flexible prescription for the introduction of immiscibility allows us to avoid having an abrupt interface whose properties are sensitive to its orientation with respect to the underlying lattice.

Static interfacial properties. – We have verified that our model accurately reproduces the correct behavior. We focus on the Galilean-invariant case of 18 allowed particles at rest on a site and with the total density of $1/3$ per state (the density per site is 8). Our rules generate an isotropic surface tension—an initial square drop of blue fluid within a sea of red is found to become circular (modulo the discreteness of the lattice) within 800 time steps. Further, a stable interface extends over several nodes of the lattice (fig. 1). Indeed, on varying the parameters, we have been able to tune the interface width from 2 to 40 lattice spacings without losing the interfacial identity. The interfacial thickness (estimated as the width of the region corresponding to a relative concentration variation between 0.25 and 0.75) δx is found to be substantially independent of β_1 , but varies inversely with β_2 ; we get $\delta x \sim (0.45 \pm 0.05)/\beta_2$. Our units are such that the lattice parameter, the time step and the particle mass are all one. Laplace's law relating the pressure difference, δP , between the inside and outside of a circular drop of radius l and the surface tension γ , $\delta P = \gamma/l$, is well satisfied. γ is found to be simply proportional to β_1 and substantially independent of β_2 ; we get $\gamma \sim (185 \pm 5)\beta_1$.

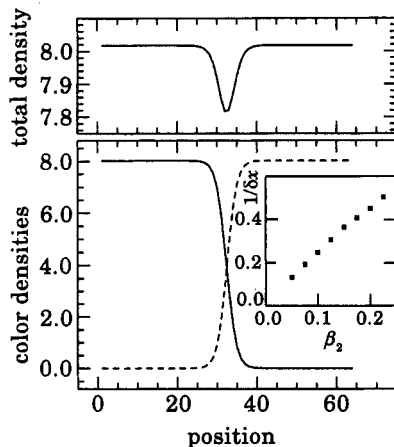


Fig. 1.

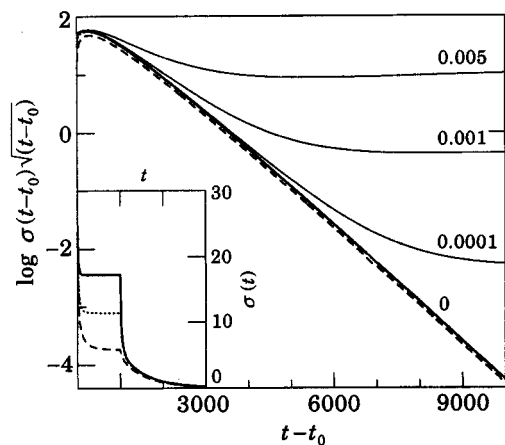


Fig. 2.

Fig. 1. – Top: plot of the total density (red + blue) on a line crossing an interface. The value of our control parameters are $\beta_1 = 0.0015$ and $\beta_2 = 0.15$. The depletion of the density in the vicinity of the interface arises from the effective repulsion of the two fluids below the consolute point. Bottom: same as in top figure but for the red (solid line) and blue (dashed line) densities. The inset shows that the inverse interface width varies approximately linearly with the control parameter β_2 .

Fig. 2. – The time-dependent surface tension. The inset is in linear scale and the main figure is log-linear. The thick solid, dotted and broken lines (that are parallel to each other for $t > 1000$) correspond to initial values of $\beta_2 = 0.25, 0.16$, and 0.08 , respectively ($\beta_1 = 0.001$). The final values of β_1 and β_2 in all three cases are 0. The time scale of the inset is the same as in the main figure and $t_0 = 1000$ is the switch time. The thinner solid lines correspond to a switch from $\beta_2 = 0.25$, $\beta_1 = 0.001$ to an unchanged value of β_1 and the value of β_2 shown in the figure.

Our model allows simple tuning of the surface tension by more than half an order of magnitude.

The two-parameter control of the interface is reminiscent of the classical approach to the interfacial properties of nonuniform systems [9] (for example van der Waals fluid): the continuous variable is the density and the two equilibrium states are the low- and high-density phases corresponding to gas and liquid, respectively. In our two-color BCA, the analogous equilibrium states are the fully red and fully blue liquids and the continuous variable is the relative density of one color. A free energy of a nonuniform system depends on the square of the density gradient through the interface. In the simplest model the surface

tension can be written as $\gamma = \int_{-\infty}^{+\infty} S(\partial\rho/\partial x)^2 dx$, where x is a direction across the interface and S the stiffness of the interface. We can readily compute the integral of the square of the density gradient, $\sigma = \sum_i (R_i - R_{i+1})^2 / 2a^2$, where R_i is the total red color corresponding to the i -th layer and a the layer-to-layer distance. The σ measurements correspond to the flat plateau of the inset of fig. 2. σ , i.e. $\gamma/2S$, is independent of β_1 whereas it is almost linear in β_2 : $\gamma/S \sim (145 \pm 10)\beta_2$. Since we have already determined γ independently, we get the interface stiffness as $S \sim (1.28 \pm 0.12)\beta_1/\beta_2$. Let us consider a simple situation [9] in which the two phases correspond to the minima of a double-well potential with an energy barrier W . The interfacial properties are then governed by the parameters S , W and the half-density jump $\Delta\rho$ between the two phases (ρ_0 is the mean density; in fig. 1 $\rho_0 = 0$ and $\Delta\rho = 4$). The density variation across the equilibrium interface is of the form $\rho(x) = \rho_0 + \Delta\rho \tanh(x/\delta x)$ and the interface thickness δx and γ are given by $\delta x = \Delta\rho \sqrt{S/2W}$ and $\gamma = 4 \Delta\rho \sqrt{2SW}/3$, respectively. From the latter we get an energy barrier $W \sim (470 \pm 80)\beta_1\beta_2$. Therefore, our two parameters are related to the inputs of van der Waals fluids. Moreover, this approach is predictive, since from the former we expect $\delta x \sim (0.15 \pm 0.02)/\beta_2$ in reasonable agreement with our measurement $\delta x \sim 0.45/\beta_2$ in the inset of fig. 1. Thus we find that β_1 and β_2 provide a simple connection between the microscopic and macroscopic parameters.

Dynamical surface tension. – Let us first set β_1 and β_2 both equal to zero: the surface tension vanishes, the fluids become miscible, and the interface is expected to spread because of molecular diffusion (diffusion coefficient D_m). We have performed a simulation with periodic boundary conditions where half of the lattice is filled with particles of one color, and the remaining half with the other color. The color-density profiles are well represented by error functions, which allows us to measure the molecular-diffusion constant. We find $D_m \sim 0.25 \pm 0.05$.

It is well known that the dynamics of spinodal decomposition of two immiscible fluids crucially depends on the conservation laws that are operational. Superficially, one may expect that since the two-color CA not only produces hydrodynamic behavior at coarse-grained scales, but also satisfies a local color conservation law, the dynamical behavior ought to be similar to that of two fluids. Recent studies [10,11] have shown that the dynamical behavior of the «surface tension» (measured by monitoring the integral of the square of the density gradient) on turning off the immiscibility between the two fluids provides a simple diagnostic of the nature of the operational conservation law. Thus, for a two-fluid system (with model-B or model-H dynamics [1] both with a conserved order parameter—model-H additionally incorporates the hydrodynamic modes) one expects γ to decay as $1/\sqrt{t}$, whereas for a liquid-vapor system (model-A dynamics) γ behaves as $\exp[-t]/\sqrt{t}$.

Our BCA allows for an accurate study of the dynamical behavior of γ on starting with an equilibrated profile at nonzero values of β_1 and β_2 and abruptly switching both β_1 and β_2 to

zero. Strikingly, the behavior is well fitted by the form $\exp[-t]/\sqrt{t}$, as shown in fig. 2. This surprising result arises, in spite of the local color conservation law, because the immiscibility is caused by kinetic collision rules and not due to any genuine repulsive interaction between the two colors. The exponential dependence signifies that, once the surface tension is switched off, the phenomenon is governed by viscosity—without the surface tension, the system is essentially a one-component fluid with an initial density inhomogeneity. Results of the dynamical evolution of γ on abruptly changing β_2 to a nonzero value are also shown in fig. 2.

Wetting properties. — Following the prescription of ref. [7], one may obtain desired wetting properties by setting the color content of the walls to the appropriate value. As usual, we employ bounce-back boundary conditions at the wall in order to impose no-slip. We have found that the contact angle behaves approximately linearly with the relative color content of the wall at long times, as demonstrated in fig. 3. Triangles, crosses and squares show the situation after 6000, 18 000, and 60 000 time steps, respectively, starting from a semi-circular blue drop surrounded by a red fluid which corresponds to a 90° initial contact angle. Equilibrium is reached at longer times for the nonwetting case. In order to measure the dynamical contact angle as a function of flow rate, a partially wetting red bubble was flushed between two walls by a flow. We find that the dynamical contact angle increases with the capillary number (fig. 4)—our results are qualitatively consistent with those obtained from other considerations [12].

In summary, we have developed and tested a two-fluid, fully nonlinear, Galilean-invariant Boltzmann cellular automaton. Our coloring rules allow for a flexible control of the degree of miscibility, the nonlinearity enables study of situations in which the densities take on arbitrary values, the Galilean invariance ensures that no spurious physics is produced due to the advection speed being different from the interfacial speed and the Boltzmann approach allows for the removal of noise and obviates the need for long-time averaging. Our studies of surface tension and wetting demonstrate that the BCA is a valuable laboratory for further investigation of such problems.

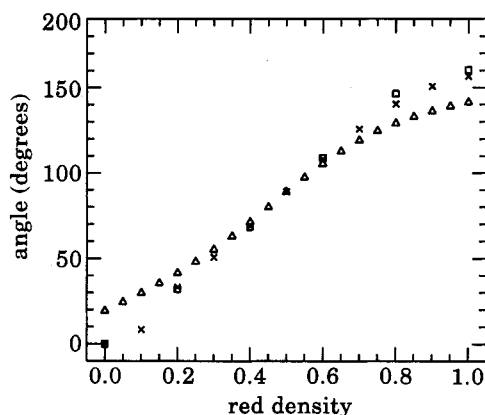


Fig. 3.

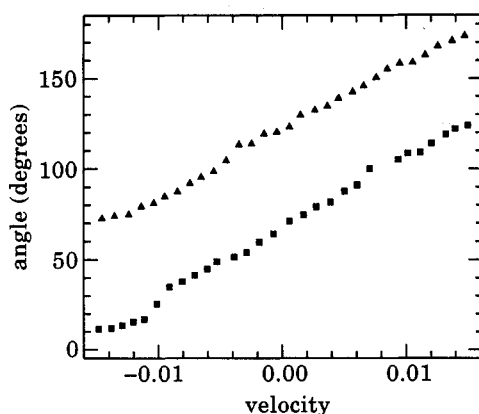


Fig. 4.

Fig. 3. — Plot of the contact angle *vs.* the relative color content of the wall. Triangles, crosses and squares show the situation after 6000, 18 000 and 60 000 time steps, respectively, starting from a semi-circular drop which corresponds to a 90° initial contact angle.

Fig. 4. — The dynamic contact angle *vs.* the reduced flow rate (capillary number). The static contact angles are 45° (bottom) and 135° (top).

* * *

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REFERENCES

- [1] HOHENBERG P. C. and HALPERIN B. I., *Rev. Mod. Phys.*, **49** (1977) 435.
- [2] FRISCH U., D'HUMIÈRES D., HASSLACHER B., LALLEMAND P., POMEAU Y. and RIVET J.-P., *Complex Systems*, **1** (1987) 649.
- [3] MANNEVILLE P., BOCCARA N., VICHNIAC G. Y. and BIDEAUX R. (Editors), *Cellular Automata and Modelling of Complex Physical Systems* (Springer Verlag, Berlin) 1989.
- [4] FRISCH U., HASSLACHER B. and POMEAU Y., *Phys. Rev. Lett.*, **56** (1986) 1505.
- [5] See, for example, APPERT C. and ZALESKI S., *Phys. Rev. Lett.*, **64** (1990) 1; ROTHMAN D., *Phys. Rev. Lett.*, **65** (1990) 3305; BENZI R., SUCCI S. and VERGASSOLA M., *Phys. Rep.*, **222** (1992) 145; ROTHMAN D. and ZALESKI S., *J. Phys. (Paris)*, **50** (1989) 2161.
- [6] GUNSTENSEN A. K. and ROTHMAN D. H., *Physica D*, **47** (1991) 53.
- [7] GUNSTENSEN A. K., ROTHMAN D. H., ZALESKI S. and ZANETTI G., *Phys. Rev. A*, **43** (1991) 4320 and references therein; see also McNAMARA G. R. and ZANETTI G., *Phys. Rev. Lett.*, **61** (1988) 2332. Gunstensen *et al.* consider a two-color BCA with Galilean invariance. The differences between their approach and ours is that our collision operators does not have a linearization approximation and the interface is governed by two control parameters rather than one.
- [8] ROTHMAN D. H. and KELLER J. M., *J. Stat. Phys.*, **52** (1988) 1119; see also BURGESS D., HAYOT F. and SAAM W. F., *Phys. Rev. A*, **39** (1988) 4695.
- [9] CAHN J. W. and HILLIARD J. E., *J. Chem. Phys.*, **28** (1958) 258.
- [10] MA W. J., KEBLINSKI P., MARITAN A., KOPLIK J. and BANAVAR J. R., *Phys. Rev. Lett.*, **71** (1993) 3465.
- [11] MAY S. E. and MAHER J. V., *Phys. Rev. Lett.*, **67** (1991) 2013 and references therein; the dynamical surface tension may play an important role in pattern formation in miscible fluids.
- [12] ADAMSON A., *Physical Chemistry of Surfaces* (John Wiley and Sons, New York, N.Y.) 1982; FERMIGIER M. and JENFFER P., *J. Colloid Interface Sci.*, **146** (1991) 227 and references therein.