

Simulating Hydrodynamics: a Pedestrian Model

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A Hele Shaw cell contains two fluids separated by an interface. Because the fluids are held in narrow regions between two plates the cell can be described by a set of two-dimensional hydrodynamic equations, which determine the velocity fields in the fluids as well as the motion of the interface between them. A discretized version of these equations can be implemented in terms of the motion of random walkers. The walkers have the effect of carrying pieces of the fluid from one place to another. They simulate a discrete version of the Laplace equation and obey the appropriate boundary conditions for the fluid. The walker-hydrodynamic connection is explored in the limiting situation in which the viscosity of one of the fluids vanishes. An algorithm is constructed and a few exemplary simulations are shown.

KEY WORDS: Chaos; interface; hydrodynamic instability; random walk; Hele Shaw; Green's function.

1. INTRODUCTION

One of the very simplest problems illustrating hydrodynamic stability and instability involves two immiscible fluids moving through a porous medium. The two-dimensional version of this problem seems particularly accessible. It can be studied experimentally using the Hele-Shaw⁽¹⁾ cell: a flow contained between narrowly spaced glass plates. This cell has a behavior which is described by the very same set of equations as those for two-dimensional flow in a porous medium. The basic equations are very simple. They involve the pressure, p , the velocities in the two fluids, v_1 and v_2 , and the common normal flow velocity at the interface, u , which is also the velocity of interfacial motion. Because of the friction, the flow velocities

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are proportional to the pressure gradients, with different constants of proportionality, κ_i , in the different media. Thus, we have

$$v_i = -\kappa_i \nabla p \quad (1.1)$$

Here κ is an abbreviation for the permeability of the porous medium divided by the viscosity of the fluid. If we view Eq. (1.1) as an analog of Ohm's law, $j = \sigma \mathbf{E}$, then we say that κ is analogous to a kind of conductivity for the fluids. Equation (1.1) holds everywhere except right at the interface. The fluids are considered to be incompressible so that the divergence of the velocity fields vanish. In terms of the pressure this is the statement that

$$\nabla^2 p = 0 \quad (1.2)$$

except right at the interface. We set up two boundary conditions to define the behavior at the interface. One of these is the statement that the normal components of the fluid velocities are equal and are exactly the interfacial velocity:

$$(v_1)_n = (v_2)_n = u \quad (1.3)$$

The other boundary condition defines the pressure discontinuity across the boundary. This capillarity condition states that the discontinuity depends upon the radius of curvature of the surface, i.e., that at the surface

$$p_1 - p_2 = \alpha/R \quad (1.4a)$$

Here α is a material-dependent constant while R is the radius of curvature of the surface. The right-hand side of Eq. (1.4a) is termed the *surface tension*. In a quasi-two-dimensional geometry in which the flow is held between two glass plates, the wetting angle of the film with the glass produces the largest curvature in the problem. In that case one⁽¹⁾ rewrites Eq. (1.4a) in the form

$$p_1 - p_2 = \beta + \alpha/R \quad (1.4b)$$

Here β is α times the curvature produced by the glass. So long as β is independent of position it drops out of the flow problem. However, as we shall see, the dependence of the pressure difference upon the orthogonal curvature (the α term) is all important.

That is all there is to the basic equations for this system. Very simple. But the solutions. Not so simple. When a less viscous material, one with larger k , is pushing a more viscous material there is a long-wavelength

instability⁽²⁾ on a flat surface set perpendicular to the flow. As a result, at first, the surface ripples. After a time, the ripples can get complicated and produce beautiful and apparently chaotic² patterns. This behavior has been illustrated in, for example, the experiments of Saffman and Taylor⁽³⁾ and the simulations of Tryggvason and Arel.⁽⁴⁾ However, when the fluids are confined in a channel of finite width, W , the chaotic behavior is only present for a finite period of time.⁽³⁾ If the pushing velocity is constant, after a time, one of the ripples turns into a very long finger, which dominates the channel, and the resulting long-time behavior is quite orderly. Figure 1 is a sequence of pictures which illustrates this effect.

This behavior is well known but only partially understood. The present paper will have very little to add to the understanding of the basic phenomena at hand. But, this problem provides a prototypical situation with behaviors ranging from chaotic to orderly. It then furnishes a beautiful case on which we can test our analytical, computational, and simulational methods. It is the purpose of this paper to set out a somewhat novel computational method.

Clearly, one test of any approach to this class of problems is that it should lead to the qualitative results described above (and more completely in the references). However, this problem is particularly nice in that there

² Here the word “chaotic” is used to suggest that the patterns are complex and sensitively dependent upon initial conditions.

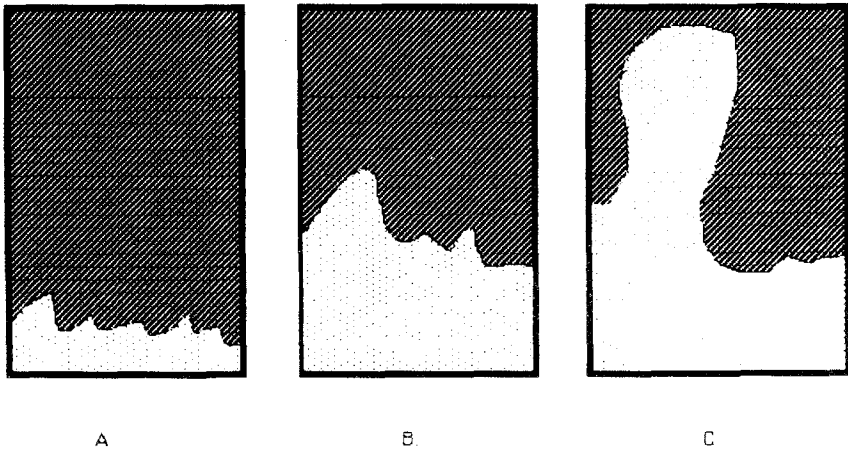


Fig. 1. Three successive states in the motion of the interface. In the first view, the instability produces a few small fingers. Then, the biggest ones tend to grow, leaving the others behind. Finally, in part C one finger has outstripped the others.

are quantitative but only partially understood results to serve as a basis of comparison. There exist experimental results which plot the shape and width of the steady-state tongue in terms of the two dimensionless parameters which define the problem. One of them is an asymmetry parameter, A , which describes the difference in viscosities between the two fluids

$$A = \frac{\kappa_2 - \kappa_1}{\kappa_2 + \kappa_1} \quad (1.5)$$

In addition, one needs a dimensionless version of the surface tension. This parameter has been defined in Ref. 3 to be

$$B = \frac{2\alpha\kappa_1\kappa_2}{u_\infty W^2(\kappa_1 - \kappa_2)} \quad (1.6)$$

Here W is the width of the channel (see Fig. 2) and u_∞ is the velocity of fluid 2 at the far end of the channel. (In Ref. 3, the velocity in fluid 1 is actually chosen as the reference, but this is a trivial difference.) The parameter, B , has a very simple physical interpretation. The surface tension and channel width, W , together set a characteristic velocity: the speed of motion of an interface with curvature of order W set a distance of order W from a flat surface. In view of Eqs. (1.1), (1.2) and (1.4) this characteristic speed is $\alpha\kappa/W^2$. Then Eq. (1.2) defines B to be the ration of this surface-tension characteristic velocity to the pushing velocity, u_∞ .

Another parameter, which is perhaps even more relevant to our understanding of given physical situation is the characteristic length,

$$\xi = 2\pi w(B)^{1/2} \quad (1.7)$$

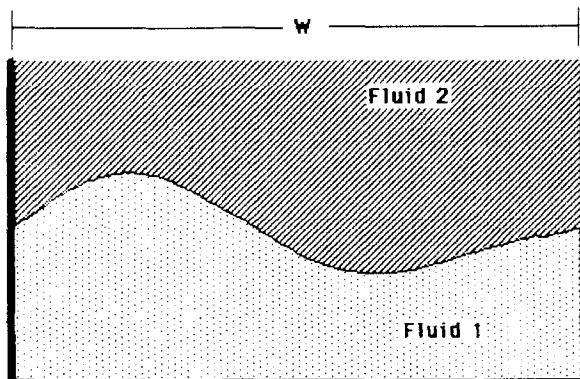


Fig. 2. A portion of a Hele Shaw cell. The fluids move toward the top of the page and are bounded by the walls shown.

This quantity, ξ , is the wavelength of marginally stable perturbations upon a flat interface. If the perturbations have a wavelength longer than ξ they grow; if shorter they decay.

Clearly ξ is only one of several quantities which we should monitor in trying to understand the system. This quantity describes the behavior of flat surfaces. Another involves the long-time domain in which the system settles into a steady flow in which one fluid forms a tongue within the other (see Fig. 1). A very simple parameter to measure is λ , the ratio of the tongue width to channel width. Saffman and Taylor measured λ for small B and found it to be close to $1/2$. McLean and Saffman⁽⁶⁾ then found λ as a function of B by doing a full numerical calculation of the steady-state velocity pattern. They then found λ to be $1/2$ in the limit as B goes to zero. Hence at least in this point, experiment and calculation agree. However, later work showed this “steady-state” profile to be totally unstable. In fact, when the surface tension parameter, α , is zero, all possible patterns seem to show instabilities for arbitrarily small wave vector.⁽⁷⁾ Shraiman and Bensimon have solved an initial value problem at $B=0$ and found that in a finite interval of time the solution leads to cusps in the surface profile, and that, after this time their $B=0$ solutions makes no sense.⁽⁷⁾ Subir Sarkar⁽⁸⁾ has proven that, in one particular geometry, cusps seem to arise from “almost all” initial conditions. Hence, even though we have a solution at $B=0$, we have an insufficient understanding of what the solution really means.

All of the above is intended to say that the problem under consideration is sufficiently interesting to merit some serious effort. In particular, this paper is aimed at numerical methods of expressing and solving this problem. And indeed there have been, in the recent past, a reasonable number of other numerical calculations aimed at this class of problems.^(4,6) The novelty of the method proposed here is that it is based upon representing the solution to Laplace’s equation in terms of random walks. It is well known, of course, that the probability that a random walker will land at a given point obeys the Laplace equation. In discussing the behavior of the random walker, one can reach for the experience in an entirely different branch of theoretical knowledge: the study of the kinetic behavior of aggregating particles. Here, a seminal piece of work was provided by Witten and Sander,⁽⁹⁾ who studied the problem which has come to be known as diffusion-limited aggregation, DLA. In DLA an aggregate is defined to occupy some region of space. A “drunken” or random walk is performed, starting from far away from the cluster. As the walker touches the aggregate, it is absorbed by the aggregate, which thus grows. In this way, a very disorderly and chaotic structure is produced. It is easy enough to show that random walks have a probability density which

is described by Laplace's equation. Hence there must be some connection between the Hele Shaw problem and DLA. A part of this connection has been pointed out by L. Patterson.⁽¹⁰⁾ But Patterson's proposed answer is only partial and heuristic. Section 2 of this paper is devoted to describing in a precise manner a lattice problem which in one limit is DLA and which might well have as its continuum limit the hydrodynamic problem under discussion. Section 3 contains a discussion of algorithms which might be used to implement a simulation of the lattice problem and then shows some simulation results.

2. A RESTATEMENT AS A LATTICE RANDOM WALK

To define a solution to Laplace's equation one can specify the fields on the exterior boundary of a region U of space. The fields on the exterior will determine the fields everywhere inside. One formal way of setting up this boundary value problem is to define a Green's function, $g_u(\mathbf{r}, \mathbf{s})$, which depends upon two points, \mathbf{r} and \mathbf{s} . Here \mathbf{r} may lie either in the interior of U or on its boundary ∂U , while \mathbf{s} is required to lie on the boundary. (See Fig. 3.) In a lattice version, the Green's function obeys

$$\square g_u(\mathbf{r}, \mathbf{s}) = 0 \quad (2.1)$$

Here \square is the lattice version of the Laplacian, i.e.,

$$\square f(x, y) = 4f(x, y) - f(x+1, y) - f(x-1, y) - f(x, y+1) - f(x, y-1) \quad (2.2)$$

and δ is the usual δ symbol. Equation (2.1) is to be solved with the boundary condition that g vanishes whenever \mathbf{r} is on the exterior boundary of

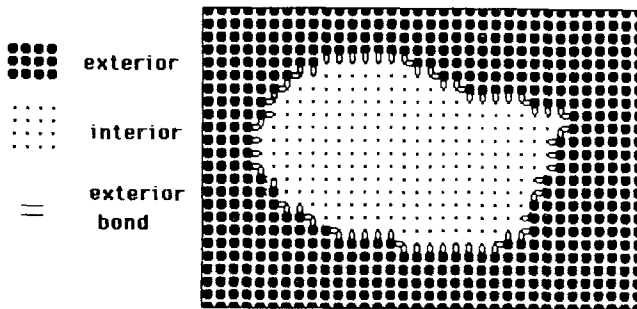


Fig. 3. The lattice used in this work.

the region—except that, at \mathbf{r} equals \mathbf{s} , $g_{\mathbf{u}} = 1$. In symbols, when \mathbf{r} is on the boundary

$$g_{\mathbf{u}}(\mathbf{r}, \mathbf{s}) = \delta(\mathbf{r}, \mathbf{s}) \tag{2.3}$$

This Green’s function serves to solve the boundary value problem, since if we set the value of the potential, p , to be ψ on the boundary of region U , then the solution of the Laplace equation, will be simply that

$$p(\mathbf{r}) = \sum_{\mathbf{s}} g_{\mathbf{u}}(\mathbf{r}, \mathbf{s}) \psi(\mathbf{s}) \tag{2.4}$$

where the sum runs over all points on the boundary. Once one has $g_{\mathbf{u}}$, then one has the solution. The solution is manifestly correct. For our later work, we shall need a slightly different Green’s function, one which is connected with the bonds lying on the boundary of our region. We call these particular links between the interior and the remaining world, exterior bonds. These bonds are depicted in Fig. 3. Each exterior bond, b , is connected with one and only one interior point \mathbf{r} , but an interior point neighboring the boundary may be connected with more than one such bond. We define a bond, bond Green’s function, $G_U(b_1, b_2)$. G is defined only for surface bonds, and is essentially a special case of $g_{\mathbf{u}}$. In particular, $\sum_{b_2} G_U(b_1, b_2)$ is identical with $g_{\mathbf{u}}(r_1, r_2)$, with the condition that bond b_1 has its interior end be r_1 and that all summed bonds, b_2 have interior ends r_2 . Unlike $g_{\mathbf{u}}$, which is defined asymmetrically, the bond Green’s function G_U obeys the symmetric condition

$$G_U(b_1, b_2) = G_U(b_2, b_1) \tag{2.5}$$

Now one can see the connection to random walks very simply. Consider N random walkers who all start out at \mathbf{s} . They walk at random, obeying but one condition: when they reach the boundary of U , they disappear. Their only contact with the boundary or the exterior is at the very first step. Now, measure the number of times any walker lands upon \mathbf{r} . Call this $N(\mathbf{r})$. In the limit as N goes to infinity, I claim that the ratio $P(\mathbf{r})$ defined to be $N(\mathbf{r})/N$ will approach $g_{\mathbf{u}}(\mathbf{r}, \mathbf{s})$. Why? In the interior, since the sites get occupied by hopping from one site to its neighbor, the occupation probability must obey the discrete Laplace equation. On the boundary, by construction, we have $P(\mathbf{r})$ being 1 or 0. All that is being said is the well-known statement that the random walk probabilities solve the Laplace equation. Along the same lines, the bond Green’s function $G_U(b, c)$ also has a very simple probabilistic interpretation. Given a random walk which is known to enter the region via external bond c , $G_U(b, c)$ is the probability

that the walk will leave the region via the bond b . This interpretation at once implies the sum rule

$$\sum_c G_U(b, c) = 1 \quad (2.6)$$

It is time to translate our considerations into statements appropriate to the porous medium flow problem. The connection we shall draw is between a random walk problem and a particular version of the fluid problem. Specifically we consider the situation in which the filled sites or the aggregate represent the vacuum or a void and the region through which the walkers wander is the one filled by actual fluid. This describes the situation in which the first "fluid" has very low viscosity so that it can respond very easily to pressure changes. In this extreme situation, the A of Eq. (1.5) equals -1 .

The reader should notice that there is some ambiguity about how to take the limit in which the viscosity of one fluid goes to zero. The difficulty can best be seen by considering a drop of this fluid. If the "fluid" is actually vacuum and hence infinitely compressible, then the size of this drop may expand and contract. If the drop is composed of an incompressible fluid it cannot change its volume. If, however, the drop is connected via a channel, no matter how narrow, to a reservoir of this fluid held at constant pressure, then the very slender neck permits the drop's volume to vary. As long as the topology is of two infinitely large regions of fluid connected at a simple interface then there is no ambiguity in the zero viscosity limit. As soon as these are inclusions and droplets, an ambiguity arises. In this paper, we resolve the ambiguity in the limiting process, κ_1 goes to infinity, by allowing "fluid 1" to be compressible.

As an additional simplification, let the remaining fluid (fluid 2) be completely surrounded by boundaries (Fig. 3) and for the moment assume that the pressure on the exterior is the predefined function, $\psi(\mathbf{s})$. Then, the pressure in the interior of the fluid is exactly given by the right-hand side of Eq. (2.4). To actually generate the fluid problem, we must also define the motion of the interface. This motion is, in the continuum fluid, proportional to the gradient of the pressure normal to the surface. To get the lattice version of this motion, isolate a bond at the surface (as in Fig. 4) and say that in the end the velocity of motion along this bond will be proportional to the difference in pressures between the point on the bond just exterior to the region, \mathbf{s} , and the point just within the region \mathbf{r} . In symbols,

$$\begin{aligned} u &= -C[\psi(\mathbf{s}) - p(\mathbf{r})] \\ &= C \sum_{\mathbf{s}_1} g_U(\mathbf{r}, \mathbf{s}_1) \psi(\mathbf{s}_1) - C \sum_{\mathbf{s}_1} g_U(\mathbf{s}, \mathbf{s}_1) \psi(\mathbf{s}) \end{aligned} \quad (2.7)$$

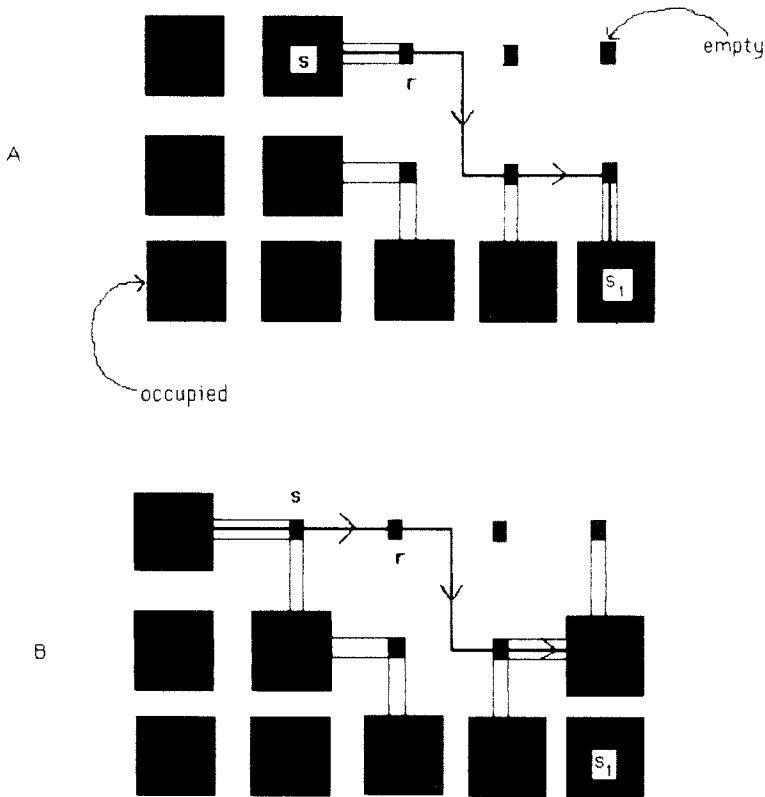


Fig. 4. Motion in the lattice system. Part A shows the situation just before the move; part B is just afterward. The motion is driven by differences between the pressure on occupied cells (e.g., s in part A) and that on neighboring unoccupied ones (e.g., r). These can then be converted into differences between two occupied sites (e.g., s and s_1).

The last sum in Eq. (2.7) is exactly unity in virtue of Eq. 2.6. Convert Eq. (2.7) into a statement about bonds. Connect with the points a bond b , and with s_1 a bond b_1 . Then write Eq. (2.7) as

$$u = C \sum G_U(b, b_1) \Psi(s_1) - C \sum G_U(b, b_1) \Psi(s) \tag{2.8}$$

Now, let us give a random walk interpretation to Eq. (2.8). Consider $\Psi(s)$ to be positive for all values of s . Visualize independent random walkers entering our region at a rate equal to $C\Psi(s)$, walking through the region, hitting the boundary, and disappearing. As each such walk is completed, see Fig. 4, one bit of fluid is removed on the exterior end of the entry bond

and added at the interior end of the exit bond. In this way, the random walk process almost fully simulates the hydrodynamics.

Almost. There is, of course, a modest difficulty. The lattice and the random walkers are grainy, "quantized." The real hydrodynamics is continuous. If fluctuations are not important and if there is a well-defined continuum limit, then the walkers give it. If, however, the continuum limit is ill defined, then there are no statements about the hydrodynamics to be made. Soon, we shall discuss how this works out.

But, before turning to this crux of the matter, a bit more effort must be spend upon boundary conditions. To simplify the analysis, we are considering the case in which only one of the fluids feels an appreciable frictional resistance. The other fluid has κ equal to infinity and might be visualized as vacuum. In this fluid, the pressure is constant. Take it to be zero. Then, Eq. (1.4) gives the preasure in the other fluid as

$$p = \beta + \alpha/R \quad (2.9)$$

We are about to replace this fluid problem with a mathematically equivalent random walk problem. In the latter, instead of a pressure one has a probability. The vacuum region of the fluid problem translates into the region filled by aggregate in the random walk problem. The walkers do their random motion in the region filled by the finite- κ fluid. Equation (2.9) now translates into a statement about the probability of finding a walker at site s at the edge of the aggregate, $\psi(s)$. Assume that we can define a local radius of curvature, $R(s)$ in a lattice situation.⁽¹¹⁾ Then to make contact with the fluid problem we shall want $\psi(s)$ to obey

$$\psi(s) = \beta + \alpha/R(s) \quad (2.10)$$

At this point, one version of the hydrodynamics problem has been described in terms of walkers. To see what this come to, consider specifically the case in which a constant flux of walkers proceeds from infinity toward a finite aggregate. To get the simplest possible set of equations, let us—for the moment—assume that the surface tension of Eq. (2.10) is 0. The resulting model is very simple indeed. Random walkers are released at infinity. They walk along until they hit an aggregate. When they hit they stick. This is exactly the DLA model of Witten and Sander⁽⁹⁾ with the trivial, and unimportant, difference that, in their model, when a walker arrives at a site neighboring the aggregate it sticks there while, in this model, the walker hits the aggregate and is the placed upon the previous (unoccupied) site upon its path. Earlier simulations⁽¹²⁾ have shown that such tiny differences do not affect the qualitative properties of the resulting structure. It can then be expected to be fractal,⁽¹³⁾ scale-

invariant,⁽¹⁴⁾ and consequently cannot be the continuum limit of anything. It will be both highly ramified and highly chaotic.

Paterson⁽¹⁰⁾ has already made some arguments along these lines. He discusses that the removal of particles from a preexisting aggregate via the DLA algorithm gives a very close correspondence with the hydrodynamics equations. This process, which he called anti-DLA, gives a orderly structure with an apparently well-defined continuum limit. By the arguments given here, anti-DLA should have a very close correspondence with hydrodynamic behavior in the small surface tension limit. Indeed, Paterson argued for this point of view, but without the detailed Green's functions treatment given here. He also argued that DLA in its raw form might be applicable to real flow through a real and somewhat disordered porous medium. The point of view outlined here does not really permit us to comment upon whether or not the two kinds of fluctuations, (i) the random behavior of walkers and (ii) the pore size distribution in random media, are effectively interchangeable.

It is not too difficult to introduce surface tension into the problem. Previous workers^(9,11,15) have introduced analogs of surface tension by allowing the probability that a DLA particle will stick to depend upon the curvature of the surface or of the density of particles near the surface. The argument given here strongly suggests that a better representation of surface tension is to allow walkers to move from point to point on the aggregate with the probability or frequency of a given random walk being proportional to the difference in ψ between the beginning and the end of the walk. In the next section of this paper, algorithms for realizing this idea will be discussed.

3. ALGORITHMS AND SIMULATIONS

3.1. The Walks

Here we consider methods for converting the ideas outlined in the previous chapter into real simulations. The specific geometry under consideration is a channel which is closed on three sides and open at the top (Fig. 5). The walkers are free to enter from the top. At the side and bottom walls, the walkers obey reflecting boundary conditions.

The approach is based upon the consideration of two kinds of walks³:

i. Some walks (see A in Fig. 5) representing the flux from outside the region under consideration. This walk starts at "infinity" and terminates

³ Nigel Goldenfeld has informed me that Eshel Ben-Jacob, Len Sander, and he have also been thinking about the relation of interface motion to DLA and that they independently had the idea that surface tension should be represented by "moves."

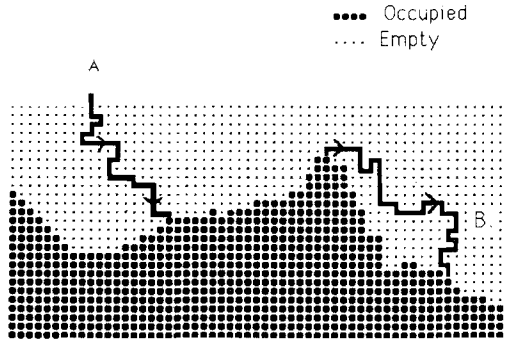


Fig. 5. The two kinds of paths. Path A adds a particle from outside; path B produces a motion of a particle already in the cluster.

when the walker lands on the occupied region. When the landing occurs, a new “particle” is placed upon the edge of the aggregate. Specifically, it is put upon the last unoccupied site visited by the walker. We term these walks “additions,” since they add particles to the aggregate.

ii. Other walks (see B in Fig. 5) start upon a boundary bond of the lattice and continue until the walker lands upon the aggregate. We term these walks “moves.”

There is a parameter, m , in the model which sets the relative frequency of these two kinds of walks. Let w be the width of the channel and let N_b be the number of exterior bonds in the system. The probability of a walk of type one will then be given in terms of these quantities as

$$p_i = w/(w + mN_b) \quad (3.1)$$

To describe the effect of the move-type walk, one specifies the values of the surface tension, ψ_1 and ψ_2 at the two ends of the walk. One can think of at least two different ways to use the walks to construct the surface tension boundary condition. The conceptually simplest one is to choose ψ to always lie between 0 and 1. Associate a direction (the arrows in Fig. 5) with each walk. Take the ψ -value at the beginning of the walk. Interpret the ψ as a probability that the walk will occur. Then if a use of the random number generator determines that the walk does take place, remove a particle from the tail end of the walk and place it at the head end. Note the full correspondence between this description and Eq. (2.8).

Actually it is probably slightly more efficient to use an almost equivalent algorithm. Determine

$$\Delta = (\psi_1 - \psi_2)/2 \quad (3.2)$$

If Δ is positive then let the motion go from 1 to 2, if Δ is negative the motion will go in the opposite sense. If Δ is smaller than unity in magnitude, allow the random number generator to determine whether the motion will actually occur. If Δ is greater than unity, take a number of particles equal to the integer part of Δ from a neighborhood of the beginning of the path and move them along the path and put them at unoccupied points in the neighborhood of the end of the path, then finally use the random number generator to determine whether a motion will occur in virtue of the remaining, fractional, part of Δ .

In our actual simulations, to ensure that the clusters formed are reasonably compact, when adding a particle we consider all possible unoccupied sites within the “most immediate neighborhood” of the site which terminates our path and actually perform the addition upon the unoccupied site with the largest number of nearest neighbors. Similarly, when a particle is removed the “most immediate neighborhood” of the removal site is polled to find the occupied site with the smallest number of nearest neighbors. In cases of ties, a random choice is made among the “equally good” sites. For the simulations shown below, we give an operational definition to the “most immediate neighborhood” of a given point by taking this to mean the point itself and the eight points nearest to it.

When the random walk passes far from the aggregate, the walker may take many steps in a region far from the one of interest. The calculation of these steps tends to lengthen the simulation. Fortunately the methods of the previous section enable one to set an algorithm for dealing with such walks through regions of little direct interest. Let this uninteresting region be V . Consider $G_V(b_1, b_2)$, the Green’s function for this region as defined in Section 2. Let the walker enter the region V via the bond b_1 . Then $G_V(b_1, b_2)$ is the probability that the walker will leave via bond b_2 . If V is simple enough, one can calculate G_V analytically and never have to deal numerically with walks in this region.

For example, let V be the upper portion of our cell: all coordinates (i, j) with j greater than a maximum height H . Then a walker enters the region via an upward step starting from (i_0, H) and returns via a downward step ending at (i_f, H) . If $g(i-i', j-j')$ is the Green’s function of the infinite lattice, the Green’s function for the region V is

$$g_V(i, j; i', j') = g(i-i', j-j') - g(i-i', j+j'-2H) \tag{3.3}$$

Given the form (3.3) g_V automatically obeys the discrete Laplace equation in U and vanishes at the boundary, $j=H$. Then the bond-bond function G_V is simply given by putting j and j' on the external boundary to find

$$G_V(i-i') = g(i-i', 0) - g(i-i', 2) \tag{3.4}$$

Since we know the Fourier transform of g to be $(4 - 2 \cos k_x - 2 \cos k_y)^{-1}$, we thus know G_V and need not compute any walks in the upper region of our system.

3.2. Radius of Curvature Estimates

To calculate the surface tension in the neighborhood of a given point, I use a variant of a method originally due to Vicsek.⁽¹¹⁾ Consider a circle of diameter L centered about the site in question. Let the number of occupied sites within the circle be N . Then the radius of curvature, R , is very large in comparison to L one can estimate R by using the formula

$$N/L^3 = c_1 + c_2/R \quad (3.5)$$

Here N is the number of occupied sites. The constant c_2 is $32/5$. The other constant c_1 is quite irrelevant to the remaining calculation since the moving probability depends upon the difference between values of ψ at two different points while ψ is chosen to be proportional to the inverse of the radius of curvature,

$$\psi(r) = \Gamma/R(r) \quad (3.6)$$

where Γ is one of the parameters of our model. To relate our parameters, m and Γ , to the original system parameter, B , we should notice that in the "time" it takes the computer to add w particles to the aggregate, the computer will have examined each bond in the system $2m$ times to see whether it should be involved in a rearrangement [see Eq. (3.1)]. Let us choose the lattice constant to be our unit of length and this "time" to be our unit interval. Thus, we have chosen units in which the basic velocity u_∞ is 1. The other fundamental velocity is the speed of a surface with curvature R set at a distance X from a flat surface. In our model, this velocity is $m\Gamma/RX$. In the real fluid, this same velocity is $\alpha\kappa/RX$. Hence, we have found B in terms of the model parameters as

$$B = 2\Gamma m/W^2 \quad (3.7)$$

3.3. The Simulations

Figures 6 and 7 show two examples of simulations constructed with the algorithms discussed above. Each of the simulations starts from a flat interface. In each case, reflecting boundary conditions are used at the bottom and side walls. Figure 5 shows a low B simulation. To form this simulation, we choose $m = 10$, a cell width, W , of 256 lattice constants, and

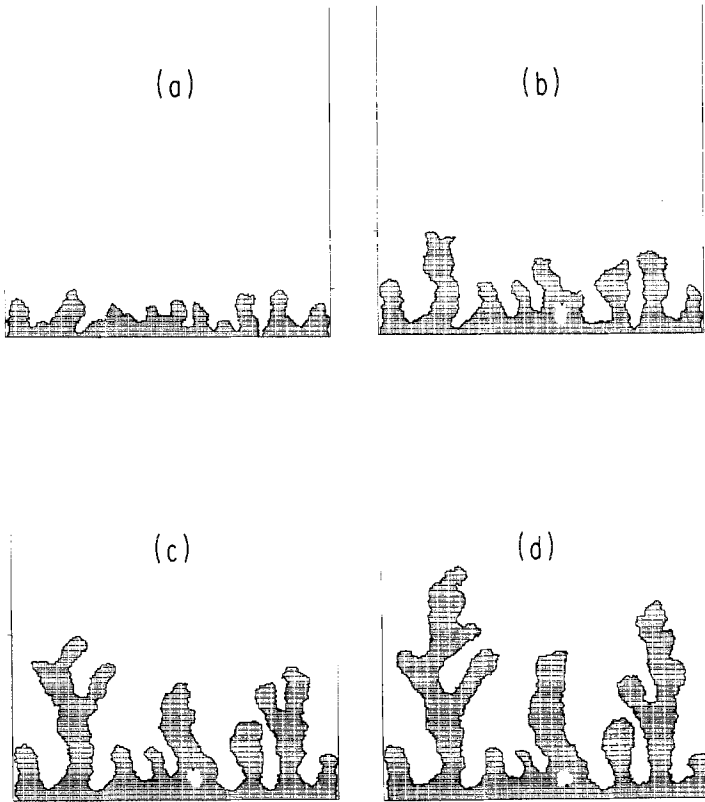


Fig. 6. Successive stages in a low B simulation. Some features of this result are probably affected by “computer noise.”

$L = 3$. We end up with $B = 0.0007$. The snapshots shown in Fig. 6 successively contain 4656, 8256, 12 256, and 16 256 particles. At first (see Fig. 6a) many fingers are formed. Later snapshots, Figures 6b–d, show a competition in which the fingers which reach out higher can grow and the others cannot. Because the system is relatively unstable, the details of the succession shown are probably considerably affected by the fluctuations in the Monte Carlo simulation.

The simulation shown in Fig. 6 runs, starting from a flat interface at the bottom of the area shown, in about two hours on an FPS 164 array processor.

Figure 7, however, shows a case in which I believe the development of the simulation is not much affected by noise. Here we depict a case in which L is 6, $m = 10$, and $W = 64$. Now the B value is considerably larger, $B \approx 0.03$. At the stage shown, the number of particles is 4864. In this high B

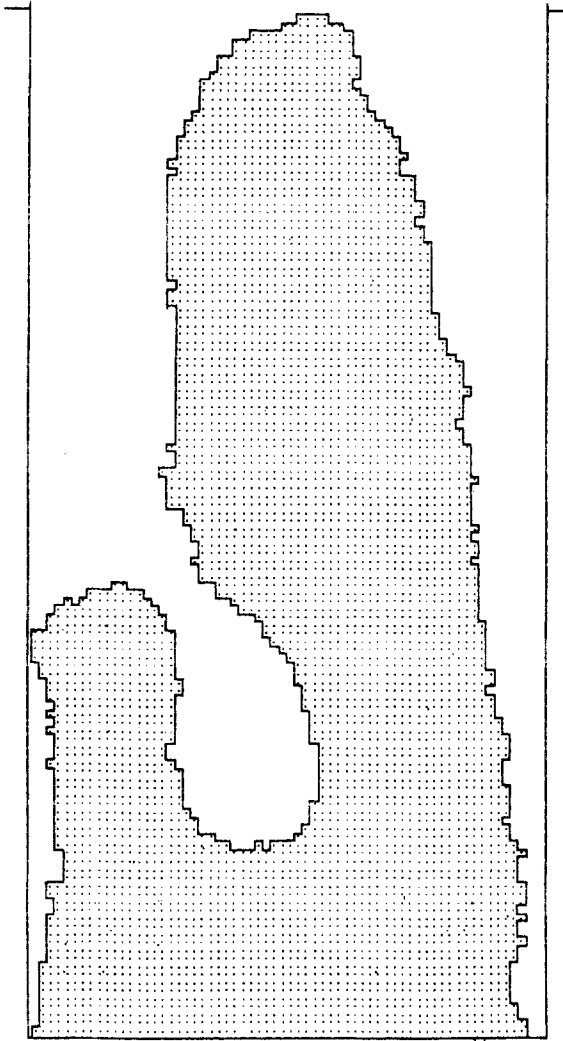


Fig. 7. A simulation in which the system forms a single finger. Noise probably does not affect this run very much.

simulation, only two fingers form themselves. The snapshot shows the situation in which one of these fingers has gotten ahead and fills over half the channel. Henceforth, the longer finger will grow.

These simulations show that a program built upon the principles discussed in this paper can be made to give results in qualitative agreement with the results of Hele Shaw experiments. Further papers will describe more quantitative tests of this kind of model.

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