43. PROPAGATION OF CHEMICAL WAVES IN DISCRETE EXCITABLE MEDIA: ANISOTROPIC AND ISOTROPIC WAVE FRONTS

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1. Introduction

Cellular automaton theory has been recognized as a useful tool for the study and the simulation of wave processes in excitable media (see [2]) and presents an alternative to the integration of partial differential equations (pde), as used by Tyson et al. [10]. By incorporating only the most important characteristics of the dynamical system into the automaton rules, one can reproduce the dynamical properties of a large system of coupled nonlinear oscillators within a fraction of the computing time that is needed to integrate numerically corresponding partial differential equations.

For the purpose of a computer simulation one divides an excitable medium into a large array of elements. For ease of programming, these elements are arranged on a regular quadratic lattice. Since such a lattice breaks the isotropy of the medium, anisotropic and thus "unrealistic" wave geometries can result. In the framework of pde's this problem of "spatial stiffness" is overcome by dividing the excitable medium into a sufficiently fine mesh. Simulations typically use lattices with a lattice constant of the order of 1/50 of the wavelength of the resulting wave (see e.g. [10]).

The dynamics of excitable media are given by the local properties of the elements and by the coupling of elements. This coupling, i.e. the response of one element to the action or state of another element, is usually assumed to decrease with growing distance between the elements. Different directions with respect to the lattice axes will exhibit different nearest neighbour spacings and, as a result, one excitable element will elicit different responses along these axes.

The more sensitive the response of excitable elements is to small variation in the elements' stimulation, the more a resulting wave pattern will reflect the anisotropy of the lattice. Near their excitation threshold, excitable media show such sensitivity, and therefore the wave fronts resulting from computer simulations are prone to reflect the geometry of the underlying lattice. This is in sharp contrast to simulations of diffusion or heat flow, the dynamics of which is not sensitive to small fluctuations of any dynamical variable.

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In the cellular automaton approach to the simulation of excitable media, the problem of artificial wave geometries is accentuated by the discrete dynamics of the excitable elements. For example, if the automaton rules are such that one automaton can excite a finite set of neighbouring automata and does not affect other automata, the polygonal outline of the set of neighbouring automata will be reflected by the excitation wave front.

In simulations based on the integration of pde's one can alleviate this problem by using finer lattices of excitable elements and shorter time steps. Similarly, in automaton simulations, one can go over to models with more states, with more elaborate rules and with interactions involving larger neighbourhoods. However, such procedure is in contrast to the original aim of the cellular automaton approach which is to reduce the complexity of the system and the computing time.

The question arises then, how simple modifications of the lattice automata models can lead to natural, i.e. isotropic, lattice-independent geometries of the excitation wave front.

2. Random distributions of excitable elements

Isotropic wave fronts arise in nature in the case of homogeneous isotropic excitable media, e.g. in the case of the well-known Belousov-Zhabotinsky reaction. However, the underlying homogeneous conditions cannot be reproduced on a digital computer. But there exist in nature also systems with a blatantly discrete character that give rise to isotropic wave fronts, an example being colonies of slime mold amoebae. A single amoeba can be considered a discrete excitable element. In an amoeba colony, isotropic wave fronts are not achieved because of an underlying homogeneous excitable medium, but are achieved rather because of a random distribution of amoebae. Such a system, however, can be readily reproduced in computer simulations by a lattice with a larger fraction of empty lattice sites. Figure 1 compares two extreme situations: the left side shows a regular lattice of excitable elements, that will give rise to polygonal wave fronts, whereas the random distribution on the right on a large spatial scale side will yield isotropic wave fronts.

The question is how to implement random distributions best on a computer. Mackay [4] distributed 1000 excitable elements randomly on a 2D surface to simulate successfully the cAMP wave propagation in slime mold colonies. He distributed the excitable elements without any regard to an underlying lattice, i.e. the coordinates of elements were chosen continuous insofar as this was possible on a computer. Another implementation was realized by Markus & Hess (see their contribution in this book [5]). In their approach, one cell

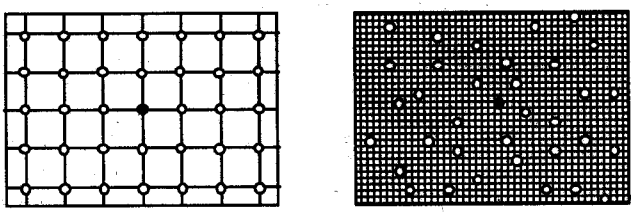


Figure 1. Fully occupied lattice of excitable elements (left side) and random distribution of excitable elements (right side). The situation on the right side will be interpreted as a partially occupied lattice.

was put randomly anywhere in each of the cells of a square lattice. Also in the approach of these authors, elements are essentially represented by a continuous position. In comparison to regular lattices, in these approaches the information about the neighbourhood of an excitable element is totally or partially lost. The distances between the excitable elements can have any values; thus the strength of the interaction has to be evaluated for every pair of excitable elements within a certain neighbourhood.

In this contribution we like to suggest a new approach which is reflected in the partially occupied lattice in Fig. 1. In our approach, automata are distributed on the lattice points of a fine-grained lattice with a low number of lattice points occupied. Each automaton is then represented by a discrete lattice position. In our approach, the simple neighbourhood relations typical of automaton simulations are preserved, with the only extension that some sites will not response to stimuli by neighbouring sites because they do not contain an excitable element. As the occupancy, i.e. the fraction of lattice sites occupied by excitable elements, is lowered, the distance over which automata interact has to be gradually increased such that an automaton remains to interact with approximately the same number of neighbouring automata.

Our approach not only benefits from having very simple neighbourhoods, but also allows the degree of randomness and isotropy to increase continuously by lowering the occupancy of a lattice. It would be ideal to use in simulations a lattice occupancy that is low enough to ensure isotropic wave propagation, and is high enough to limit the additional computational effort caused by the use of large, sparsely occupied lattices.

We have therefore investigated the properties of the transition from polygonal wave fronts of fully occupied lattices to isotropic wave fronts for sparsely occupied lattices. Our study has been based on the realization that the aforementioned transition in partially occupied lattices of excitable media is closely related to the phenomenon of percolation.

3. Coupling of excitable elements

Chemical media capable of generating spontaneous spatio-temporal order can be generated by chemical reactions with nonlinear kinetics involving activating and inhibiting substances [9,7,6]. The coupling between the local nonlinear kinetics is realized in most natural systems by diffusion of either the activating or the inhibiting substance, or of both substances. In fact, diffusion is itself a nonlinear process. This means that the diffusing substances reach nearby neighbours not only earlier than more distant ones, but the nearby neighbours are also reached with a higher velocity. More distant neighbours will either be reached with a very slow velocity or not be reached at all.

For our investigations, we described the propagation of the excitation from one element to the neighbouring elements by a law that is typical for diffusive processes, namely a $\sqrt{t}$-law. In this case the time needed for the excitation of one element to reach another element at a distance d is described by the power-law

$$t \sim d^2. \qquad (1)$$

This law might not be realistic for all excitable media, but it yields a good model to investigate the effect of lowering the occupancy of a lattice of excitable elements. Equation (1) ensures that only the nearest neighbours of

an excitable element are reached with maximal velocity. Furthermore, this property implies that besides the nearest neighbours, only a few next-nearest neighbours contribute to the propagation of the excitation wave, because distant neighbours take much longer to be reached directly by the cell originally excited than to be reached by relayed propagation involving nearest and next-nearest neighbours.

The use of a power-law ensures that as the occupancy of the lattice is varied, the size of the effective neighbourhood of an automaton, i.e. the distance over which direct excitation between automata is relevant to the propagation of the wave front, is automatically adjusted so that it always contains approximately the same number of cells. The number of cells in the neighbourhood is thus independent of the lattice occupancy; however it can be varied by changing the exponent in the power-law (decreasing the exponent will increase the size of the effective neighbourhood). Furthermore, the selection of the exponent in the power law (1) not only simulates diffusive coupling very well, but also ensures that neighbours are reached only at discrete times that are multiples of the time necessary to reach the nearest lattice point. This is very convenient for an automaton description.

4. Our simulations

For our simulations we used the following automaton rules: if one automaton k is excited, it will fire immediately. The automata that are at a distance of one lattice constant from automaton k will be excited in the next time step. Automata at a distance of n lattice constants from automaton k will be excited after n^2 time steps. In our investigations, we focused on the geometric properties of the wave front. We were thus only interested in the time at which a given cell was reached for the first time by an excitation and consequently had fired. After firing, our automata entered the refractory period and would not fire again.

We started with simulations of 10^4 excitable elements which we distributed on lattices of varying sizes, thus obtaining different lattice occupancies. As an example, Fig. 2 shows a typical result of a simulation of wave fronts at equally spaced instances for a lattice with 50 per cent of the sites occupied. The wave fronts presented, except for a scatter due to random occupation of lattice sites, exhibit clearly isotropic propagation. We consider this a key result of this contribution. This isotropic propagation has been achieved at small computational expense.

In order to analyse how isotropic propagation arises for a sufficiently low lattice occupancy we need to consider the convergence of propagation velocities in the axial and diagonal directions of the lattice. To monitor

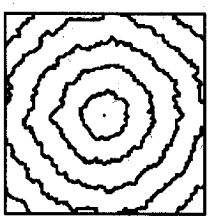


Figure 2. Simulation of wave fronts on lattices with 50 per cent occupancy. The diagrams show the wave front at equally space instances.

this convergence we consider mean propagation velocities in different lattice directions. Accurate values for these velocities can be obtained by averaging. For this purpose we have averaged wave front propagation over 150 runs like the one represented in Fig. 2. We also averaged over the eight equivalent octants in order to obtain smooth polar plots. The results are presented in Figs. 3 and 4. We would like to point out that the averaging procedure has only been adopted for the following mathematical analysis, but is not needed when our method is used for a simulation of isotropic propagation.

Figure 3 compares some averaged wave fronts obtained by simulations on lattices with 100 per cent, 70.7 per cent and 50 per cent occupancy. It can be observed that by reducing the occupancy of the lattice from 100 per cent to 50 per cent, the initially strong anistropy of the wave fronts virtually disappears. To detect a small remaining anistropy, Fig. 4 presents the velocities with which the automata surrounding the centre are reached. Below occupancies of 25 per cent, even the propagation velocities do not reveal any significant anisotropy.

For simulations of waves travelling **repeatedly** through an excitable medium, one would have to introduce a finite refractory period τ_{ref} into the automaton rules. Simultaneously, the time span during which one automaton affects neighbouring automata would have to be limited to an even shorter period than τ_{ref} to avoid artificial self-excitation in the trail of the wave front. As discussed previously, excitations which involve distant neighbours and which are slow, do not contribute to the propagation of wave fronts. Therefore, the above extensions of the automaton rules would not alter the propagation of the wave front.

Figure 4 also demonstrates a relationship between the curvature of the propagation front and propagation velocity. For a lattice occupancy of 25 per cent, this relationship can be described by the heuristic formula

$$v(r) = c - \frac{n}{r + m} \qquad (2)$$

where $c = 0.5$, $n = 3.5$ and $m = 16.5$, and where the radius r, expressed in units of the lattice constant, measures the curvature of the wave front. $v(r)$ is the velocity of the wave front in units of lattice constants per time step. c is the **asymptotic wave propagation velocity** for planar wave fronts. Equation 2 reproduces qualitatively the relations discussed in [1] for the curvature dependence of the propagation velocity of a wave front in an excitable medium. The constant m in our formula is needed to account for the discrete nature of our excitable medium.

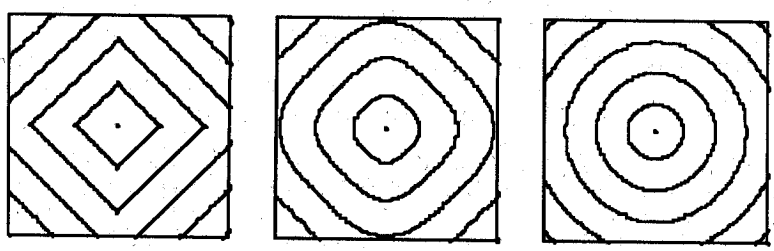
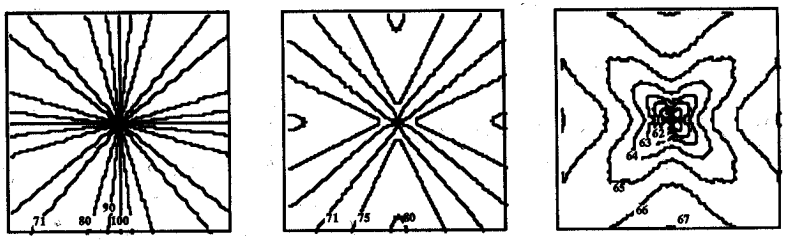


Figure 3. Simulation of averaged wave fronts on lattices with different occupancies. The diagrams show the wave fronts at equally space instances.



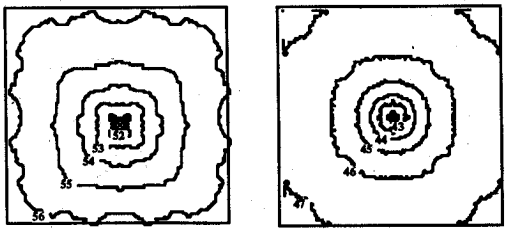


Figure 4. Simulation of averaged wave velocities on lattices with different occupancies. The contour lines denote positions that are reached with the same velocity, which is given as a percentage of the maximal propagation velocity in a fully occupied lattice.

5. Analysis of the transition to isotropic wave fronts

Figure 3 shows that wave fronts in an almost completely occupied lattice propagate fastest along the lattice axes and slowest along the lattice diagonals. Figure 5 presents and compares the asymptotic wave propagation velocities for axial and diagonal propagation as a function of lattice occupancy. The following properties emerge:

- The velocity of axial wave propagation varies with the square root of the lattice occupancy. This dependence is expected for two-dimensional media with random distributions of excitable elements. (This expectation is based on the fact that the mean velocity for diffusion is inversely proportional to the average distance between elements and that, for two-dimensional media, this distance is inversely proportional to the square-root of the occupancy.)
- The velocity of diagonal wave propagation assumes a value of $\sqrt{1/2}$ lattice units per time step for lattice occupancies between 100 and 60 per cent.
- For occupancies below 50 per cent, the difference between the velocities for propagation along the diagonal and the axial directions is very small, i.e. one can speak of virtually isotropic wave fronts.

The fact that the velocity of wave propagation along the diagonal remains constant over a wide range of occupancies plays a key role in the fast convergence of axial and diagonal propagation velocities for occupancies below 50 per cent. We want to investigate in the following how this convergence arises. In particular, we will investigate the behaviour near the occupancy of 60 per cent at which the diagonal propagation velocity starts to decrease. We will show that this behaviour corresponds to that of a percolation transition [8].

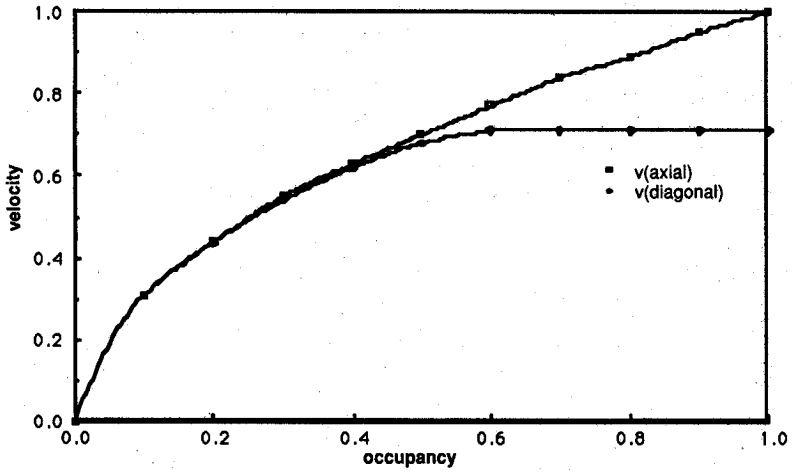


Figure 5. Occupancy dependency of asymptotic wave velocities for a quadratic lattice.

6. Percolation theory approach

Figures 6 and 7 show the propagation of planar waves in axial and diagonal lattice directions. Let us first discuss the propagation in the axial direction, which is schematically illustrated in Fig. 6. On the left side of this figure, the wave front propagates one lattice step forward for every time step. The wave front itself propagates in this situation with maximal velocity. If some of the excitable elements are missing, as on the right side, some parts of the wave front beyond the unoccupied sites will only be reached with some delay, because they take more time to be reached by more distant neighbours or through longer paths. The more empty sites the lattice of excitable elements has, i.e. the lower the occupancy of the lattice is, the more often such delay will occur, which translates into a decreasing propagation velocity.

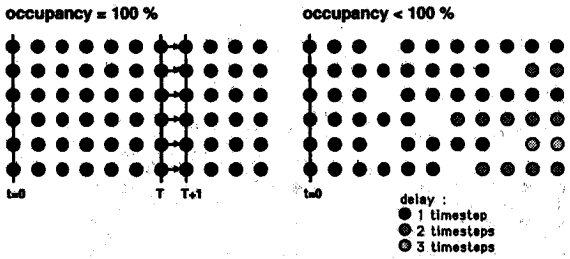


Figure 6. Schematic representation of the wave propagation in axial direction for a fully and partially occupied lattice. The left diagram shows the wave front at different times t = 0, t = T and t = T +1, and the direction from where the cells in the in the column eight will be excited at time T. The right diagram illustrates how unoccupied sites lead to a gradually increasing delay of the wave front, the latter being coded by increasigly lighter shaded cells.

The situation is different for the case of wave propagation along diagonals, which is represented in Fig. 7. In the case of a fully occupied lattice, the wave front advances $\sqrt{1/2}$ lattice constants per time step. However, along the diagonal direction, every cell can be reached by three of its neighbours. When the lattice occupancy is decreased slightly, there will still be enough connected paths left to each lattice site such that the wave front can propagate without delay, as shown on the right of Fig. 7. In the situation presented in Fig. 7, only two cells are reached with delay.

We have seen that along the diagaonal direction three lattice sites can be reached without delay from every lattice site that is occupied with an excitable element. In a figurative way one could say that one element is connected with three other sites by a **fast** link. If one of these three sites is occupied, it will again be connected with three further sites by **fast** links. In this way, clusters of cells are formed that are all connected by successive **fast** links to the original cell.

At low lattice occupancies, only a few cells might be reached by one specific cell through fast links. In this case the wave front often has to propagate directly to the next-nearest neighbours, a propagation mode that causes a delay of the wave front. At higher occupancies, the average number of cells that can be reached from one specific cell will steadily increase so that delays of the wave fronts will become more and more infrequent. This translates into an increasing mean propagation velocity. As long as a lattice contains an infinite cluster of cells connected by fast links, the wave front will propagate with maximal speed. Therefore, a knowledge of the dependence of the average size of clusters connected by fast links on the lattice occupancy will provide important clues to the understanding of the dependence of the wave velocity on the lattice occupancy: at occupancies for which infinite clusters exist, the diagonal propagation velocity should be at a maximum, at occupancies for which clusters are only finite, wave fronts should slow down in the diagonal direction.

The theory that deals with the size of clusters in partially connected lattices is percolation theory [8]. For our purposes, we define a cluster of cells as the set of all those cells that can be reached through fast links from a given set of initial cells. Percolation theory predicts that the mean size cs of a cluster, i.e. its linear dimension in the direction of the wave propagation, diverges with a power law behaviour

$$cs = const_1 \cdot (p_c - p)^{\gamma_1}, \qquad (3)$$

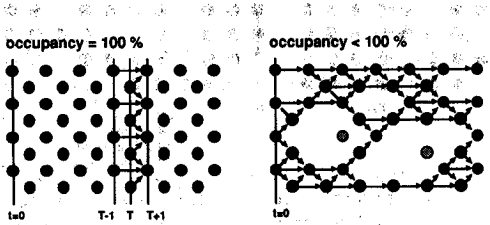


Figure 7. Wave propagation in a diagonal direction for a fully and partially occupied lattice. The left picture shows the wave front at different time steps and the directions, from where the cells have been excited for the first time. In the right picture, one can see that a limited amount of unoccupied space does not lead to a delay of the wave front.

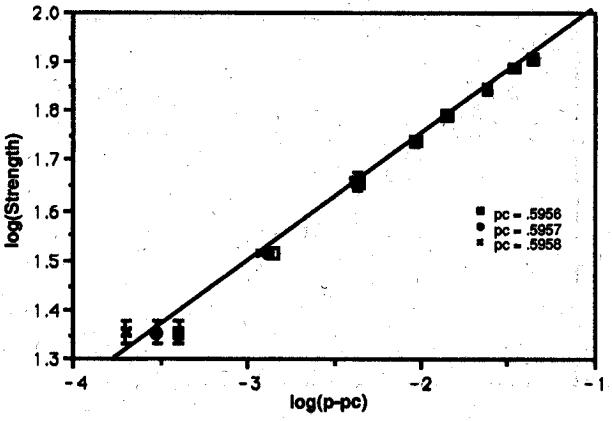


Figure 8. Strength st of the infinite cluster as a function of the lattice occupancy. The data are plotted for three different assumed percolation thresholds. A threshold $p_c = .5957$ and exponent $\gamma_2 = .255$ reproduces best the power-law (4).

as the lattice occupancy p approaches a critical value p_c, which is also called the percolation threshold. γ_1 is called a critical exponent. Above the percolation threshold, there will always be a cluster of infinite size. The strength st of the infinite cluster, which is defined as a ratio of cells that belong to the infinite cluster decreases from 1 down to 0 according to the power-law

$$st = const_1 \cdot (p - p_c)^{\gamma_2}, \qquad (4)$$

as the occupancy p is lowered from 1 down to p_c. Laws (3) and (4) can be used to extrapolate the percolation threshold from values of the cluster size or strength near the percolation threshold by matching a log-log-plot of the respective quantities to a straight line.

We performed simulations to determine the strength of the infinite cluster and mean cluster size for different lattice occupancies. Through resulting log-log-plots reproduced in Figs. 8 and 9 the percolation threshold and the critical exponents were determined to

$$\begin{aligned} p_c &= 0.5957 \pm 0.0001 \\ \gamma_1 &= -1.50 \pm 0.05 \\ \gamma_2 &= 0.255 \pm 0.015 \end{aligned} \qquad (5)$$

The value $p_c = 0.5957$ signifies that there will always be an infinite cluster in lattices with an occupancy higher than 59.57 per cent. For occupancies

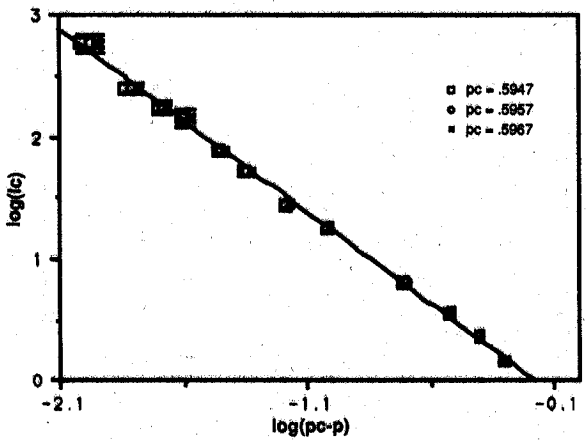


Figure 9. Mean cluster size cs as a function of the lattice occupancy. The data are plotted for three different assumed percolation thresholds. The threshold $p_c = .5957$ and exponent $\gamma_1 = -1.50$ reproduces best the power-law (3).

higher than this critical value, the propagation velocity in diagonal lattice directions will always assume its maximum value. Put another way, lowering the occupancy of an initially fully occupied lattice will only decrease the faster axial wave propagation velocity until the percolation threshold p_c is reached (see Section 5 above). At this point, the anisotropy of the wave fronts has already been reduced significantly. As the occupancy is lowered further, both axial as well as diagonal wave propagation velocities will decrease. Therefore, as the occupancy is lowered below p_c, the anisotropy will decrease more slowly. From this behaviour one can derive the important practical conclusion that a lattice occupancy just below the percolation threshold will represent the best compromise to minimize anisotropy as well as minimize computational effort.

7. Comparison with the hexagonal lattice

We have carried out the above investigations also for the hexagonal lattice. Figure 10 shows the results of a simulation of the asymptotic propagation velocities in axial (0°, 120° or 240°) and diagonal (60°, 180° or 300°) directions. For a fully occupied lattice, wave propagation is less anisotropic in a hexagonal lattice than in a square lattice, the diagonal propagation velocity

$$v_{diag,hex} = \sqrt{3/4} \cdot v_{axial,hex} = 0.866... \cdot v_{axial,hex} \qquad (6)$$

being closer to $v_{axial,hex}$ than in the case of the square lattice, for which

$$v_{diag,sq} = 0.707... \cdot v_{axial,sq} \qquad (7)$$

holds. Furthermore, the two extreme velocities $v_{diag,hex}$ and $v_{axial,hex}$ for a

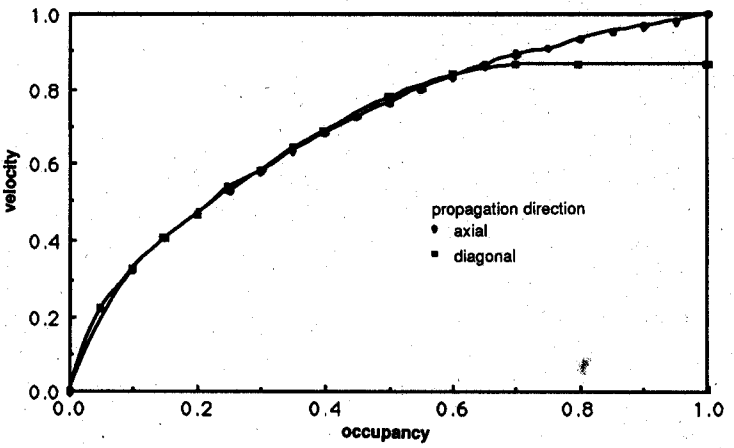


Figure 10. Simulation of the asymptotic wave velocities for different lattice occupancies for a hexagonal lattice.

hexagonal lattice converge already below occupancies of 70 per cent. This advantage of the hexagonal lattice over the quadratic lattice in producing isotropic propagation comes at the expense of a higher computational effort needed to code and handle a hexagonal lattice and at the expense of a larger number of lattice points per area for this lattice. From a computational point of view there is, therefore, no reason to prefer either one of these lattices.

The mechanism that leads to a rapid convergence of axial and diagonal propagation velocities below occupancies of 70 per cent is the same for the hexagonal lattice as for the quadratic lattice. This convergence can again be attributed to a percolation transition, i.e. there exists a critical occupancy above which the diagonal propagation velocity remains constant. For a hexagonal lattice and for the case of diagonal wave front propagation, a cell can be reached by only **two** cells through fast links, i.e. there are only two neighbouring sites that contribute to the fastest propagation of wave fronts in the diagonal direction. Therefore, one can expect that the percolation threshold, i.e. the occupancy below which an infinite cluster no longer exits, lies at a higher value than for the case of the quadratic lattice, for which every cell could be reached by **three** cells through fast links.

Numerically the percolation threshold and the critical exponents for the hexagonal lattice have been determined to be

$$p_{c,hexa} = 0.7055 \pm 0.0002$$

$$\gamma_1 = -1.377 \pm 0.020 \qquad (8)$$

$$\gamma_2 = 0.250 \pm 0.007$$

(The value for $p_{c,hexa}$ is in agreement with earlier calculations by Kinzel & Yeomans [3].) In hexagonal lattices, occupancies just below the value of $p_{c,hexa} = 0.7055$ thus will be best suited in terms of isotropy and

computational effort for simulations of isotropic wave front propagation in a hexagonal lattice.

8. Conclusion

In this contribution, we have investigated an approach to obtain isotropic geometries in automata simulations of discrete excitable media. The approach involves lattices with randomly occupied sites. We have demonstrated that relatively few unoccupied lattice sites, i.e. around 50 per cent for a square lattice and around 33 per cent for a hexagonal lattice, suffice to obtain isotropic wave propagation. We have argued that the nature of the convergence to isotropic behaviour can be attributed to a percolation transition. We propose that lattices with randomly occupied lattice sites provide a computationally effective avenue to the study of spatial dynamical systems.

Acknowledgements

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