CELLULAR AUTOMATA MODELS FOR EXCITABLE MEDIA

by

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(ABSTRACT)

A cellular automaton is developed for simulating excitable media. First, general “masks” as discrete approximations to the diffusion equation are examined, showing how to calculate the diffusion coefficient from the elements of the mask. The mask is then combined with a thresholding operation to simulate the propagation of waves (shock fronts) in excitable media, showing that (for well-chosen masks) the waves obey a linear “speed-curvature” relation with slope given by the predicted diffusion coefficient. The utility of different masks in terms of computational efficiency and adherence to a linear speed-curvature relation is assessed. Then, a cellular automaton model for wave propagation in reaction diffusion systems is constructed based on these “masks” for the diffusion component and on singular perturbation analysis for the reaction component. The cellular automaton is used to model spiral waves in the Belousov-Zhabotinskii reaction. The behavior of the spiral waves and the movement of the spiral tip are analyzed. By comparing these results to solutions of the Oregonator PDE model, the automaton is shown to be a useful and efficient replacement for the standard numerical solution of the PDE’s.
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1. Introduction

Excitable media support undamped traveling waves of excitation, such as waves of membrane depolarization in nerve axons [12], waves of excitation in chemical reaction systems [32,34], and waves of star formation in galactic dust clouds [25]. In physical and chemical systems these waves provide striking examples of spontaneous symmetry breaking and spatiotemporal organization, and in biological systems they serve essential roles in cellular communication and organization. Although some of the first models of excitable media were based on the discrete cellular automaton (CA) approach [1,10,11,16,20,26,27,31], continuous partial differential equation (PDE) models have dominated recent theory of spatiotemporal organization in excitable media [2,6,13,14,21,22,23,29,32,37,38]. This hegemony of PDEs has come about because the original CA models lacked several essential features of excitable media [7,33]:

- Curvature. In two- and three-dimensional media, curved waves travel at speeds different from planar waves: concave waves travel slower, convex waves travel faster [15,35,36].
- Dispersion. The speed of a planar wave front depends on the extent of recovery of the medium immediately in front of the wave [3,19].
- Isotropy. In a homogeneous isotropic excitable medium, the speed of planar wave propagation should be the same in all directions, but early CA models exhibited gross anisotropies in wave speed relative to the underlying grid.

Many of these problems are rooted in the fact that classical CA models propagate waves at a single speed of one cell per time step (in the direction of the grid). To overcome this problem, it is necessary to introduce larger neighborhoods over which diffusion of excitation can operate in one time step. Several different groups have independently proposed CA models with expanded neighborhoods [4,7,8,9,17,18].
For instance, Gerhardt, Schuster, and Tyson [7,8,9] sum up all the excited cells within a square neighborhood of area \((2r + 1)^2\), \(r = \) integer \((1, 2, \ldots, 6)\). If this sum exceeds a certain threshold, then the central cell becomes excited in the next time step. They show that many effects of curvature are introduced merely by such an increase in the size of the neighborhood over which excitation can propagate in one time step. Furthermore, by making the threshold a function of the extent of recovery of the central cell, they incorporate dispersive effects into the CA rules. Though curvature effects ameliorate the anisotropy of wave propagation in this CA, they do not completely eliminate it.

Markus and Hess [17,18] show that anisotropy can be almost completely eliminated by somewhat randomizing the grid of cells. Like most other investigators, they adopt a rectangular lattice, but instead of placing each grid point at the center of a unit cell, they assign each grid point to a random location within its unit cell. In this way they obtain a semi-random grid that covers the spatial domain in a rather uniform fashion, without the "clumps" and "bald spots" characteristic of a truly random distribution. Then they define the neighbors of cell \(i\) as all those grid points that lie within a circle of radius \(R\) centered on \(i\). They sum up the total number of excited neighbors of a resting or recovering cell, and, if this sum exceeds a threshold, the central cell becomes excited. As for the uniform square neighborhoods of Gerhardt, Schuster, and Tyson, so here wave speed becomes linearly dependent on wave front curvature, but the circularity and slight nonuniformity of the Markus-Hess neighborhoods make wave speed nearly independent of direction relative to the underlying rectangular lattice. However, one must pay a steep price for isotropic wave propagation. Total excitation sums in the square neighborhoods of Gerhardt, Schuster, and Tyson can be computed by only four additions per grid point independent of the "radius" \(r\) of the neighborhood, but the sums for the random-circle neighborhoods of Markus and
Hess require approximately $\pi R^2$ table lookups and $\pi R^2$ additions per grid point. The computational inefficiency of this method cancels the most important advantage of the CA approach.

Fast and Efimov [4] take a third approach. They point out correctly that the effect of an excited cell at a distance $z$ from a resting cell should drop off with $z$. Thus, when calculating the sum-of-excitation in the neighborhood of a resting cell, the contribution from an excited cell at distance $z$ should be weighted by a factor $w(z)$. Reasonable would be the choice

$$w(z) = \left[ C e^{-\frac{z^2}{4d}} \right],$$

where $\lfloor \zeta \rfloor$ denotes the largest integer $\leq \zeta$; $z^2 = (x-x_0)^2 + (y-y_0)^2$, $(x_0, y_0)$ = location of central cell; and $C$ and $d$ determine the range of interaction ($R = \lfloor \sqrt{4d \log C} \rfloor$). Although such “Gaussian” masks give good results, as I shall show, they are also computationally inefficient, demanding a large number of additions and multiplications per grid point.

In this thesis I present a general theory of “masks” as discrete approximations to the diffusion equation. I show how to calculate the effective diffusion coefficient of a mask from its weights. Then I assess the reliability of certain classes of masks by investigating their properties with regard to the propagation of wave fronts in excitable media. According to singular perturbation theory of traveling waves in two-dimensional excitable media [15,29, 35,36], the normal velocity ($N$) of a wave front should be linearly related to its curvature ($K$): $N = c - D K$, where $c$ is the velocity of a planar wave and $D$ is the diffusion coefficient of the excitation variable. I show that only some classes of masks give a linear speed-curvature relation with slope $D$ independent of the threshold for activation. Of these “good” masks, one class is especially noteworthy because it is computationally efficient.
Following the analysis of these masks, I introduce a new cellular automaton model for reaction-diffusion systems based on the new masks for the diffusion component and on singular perturbation analysis for the reaction component. The automaton is tested by simulating spiral waves in excitable media and following the movement of the tip of the spiral. Comparison with PDE solutions obtained with standard numerical techniques shows that the automaton can be used to replace the standard numerical methods for solving this PDE system.

2. Finite difference approximations to the Laplacian

The standard finite difference approximation to the Laplacian in two dimensions is the 5-point-cross

\[
\text{cross} := \begin{bmatrix}
    0 & 1 & 0 \\
    1 & -4 & 1 \\
    0 & 1 & 0 \\
\end{bmatrix}.
\]

Using this operator, the diffusion equation

\[
\frac{\partial u}{\partial t} = D \nabla^2 u
\]

can be solved using the finite difference scheme

\[
u^{k+1} = u^k + \frac{\Delta t}{h^2} D \cdot \text{cross} \ast u^k,
\]

where \(\Delta t > 0\), \(h > 0\), \(u_{i,j}^k\) is the computed approximation to the solution \(u(k \Delta t, x_0 + i h, y_0 + j h)\), and \(\ast\) denotes the convolution operation \((\text{cross} \ast u^k)_{i,j} = u_{i,j+1}^k + u_{i,j-1}^k + u_{i+1,j}^k + u_{i-1,j}^k - 4 u_{i,j}^k\). Here and from now on \(u^k\) is a 2-dimensional array at time \(k \Delta t\), which consists of elements \(u_{i,j}^k\). There is no reason why other masks might not be used.
instead of the 5-point-cross. In the following the implications of using different masks are investigated.

All masks considered here are assumed to have the following symmetry properties, where $a_{m,n}$ denotes the weight at position $[m,n]$ in the mask, which is centered around $[0,0]$:

$$\forall m,n \geq 0 : a_{m,n} = a_{-m,n} = a_{m,-n} = a_{-m,-n} = a_{n,m}. \tag{3}$$

For example, a mask of radius 2 has the general shape

$$a = \begin{bmatrix}
a_{2,2} & a_{1,2} & a_{0,2} & a_{1,2} & a_{2,2} \\
a_{1,2} & a_{1,1} & a_{0,1} & a_{1,1} & a_{1,2} \\
a_{0,2} & a_{0,1} & a_{0,0} & a_{0,1} & a_{0,2} \\
a_{1,2} & a_{1,1} & a_{0,1} & a_{1,1} & a_{1,2} \\
a_{2,2} & a_{1,2} & a_{0,2} & a_{1,2} & a_{2,2}
\end{bmatrix}.$$

These symmetries are necessary to make the mask operator a valid finite difference approximation to the Laplacian.

The result of the application of the mask $a$ to an array $u^k$ of values is described as the convolution of $a$ and $u^k$

$$\begin{equation}
(a * u^k)_{i,j} = \sum_{m=-r}^{r} \sum_{n=-r}^{r} a_{m,n} u^k_{i+m,j+n}. \tag{4}
\end{equation}

Think of $u^k_{i,j}$ as being obtained from a continuous function $u(t, x, y)$ evaluated at $t = t_k = k \Delta t$, $x = x_i = h i$, $y = y_j = h j$. Expand $u(t, x, y)$ in a Taylor series and use the symmetry
properties (3) of the mask to obtain

\[ (a \ast u^k)_{i,j} = \sum_{m=0}^{r} \sum_{n=1}^{r} \left[ 4 u(t_k, x_i, y_j) + (m^2 + n^2) \left( u^{(0,0,2)}(t_k, x_i, y_j) + u^{(0,2,0)}(t_k, x_i, y_j) \right) \right] h^2 \]
\[ + \frac{h^4}{12} \left( (m^4 + n^4) u^{(0,0,4)}(t_k, x_i, y_j) + 12m^2n^2 u^{(0,2,2)}(t_k, x_i, y_j) \right) \]
\[ + (m^4 + n^4) u^{(0,4,0)}(t_k, x_i, y_j) \right] a_{m,n} + a_{0,0} u(t_k, x_i, y_j). \]

Therefore the total effect of the mask \( a \) in terms of values \( u^k \) and \( \nabla^2 u^k \) is

\[ a \ast u^k = S \cdot u^k + h^2 D \nabla^2 u^k + \frac{h^4}{12} E(u^k) + \mathcal{O}(h^6). \]

with

\[ S = a_{0,0} + 4 \sum_{m=0}^{r} \sum_{n=1}^{r} a_{m,n}, \]
\[ D = \sum_{m=0}^{r} \sum_{n=1}^{r} (m^2 + n^2) a_{m,n}, \]
and

\[ E(u(t_k, x_i, y_j)) = \sum_{m=0}^{r} \sum_{n=1}^{r} a_{m,n} \left[ (m^4 + n^4) \left( u^{(0,0,4)}(t_k, x_i, y_j) + u^{(0,4,0)}(t_k, x_i, y_j) \right) \right] \]
\[ + 12m^2n^2 u^{(0,2,2)}(t_k, x_i, y_j) \right], \]

where \( S \) and \( D \) are independent of \( u(t, x, y) \). The characteristics of the finite difference scheme can be described in terms of \( S \) and \( D \), which are dependent only on the mask, and \( E \) to describe the error. \( S \) is the sum of all entries in the mask and \( D \) is one-fourth of the weighted sum over all entries of the squared distances from the center of the mask.
Consider an updating scheme where the data at time \( t + \Delta t \) is the result of the convolution of the data at time \( t \) and a mask:

\[
u_{i,j}^{k+1} = (a * u^k)_{i,j} = S \cdot u_{i,j}^k + h^2 D \cdot (\nabla^2 u^k)_{i,j} + \mathcal{O}(h^4) \\
\approx u_{i,j}^k + D \Delta t \left( \nabla^2 u^k \right)_{i,j}.
\]

(8)

The last part is the demand from the differential equation for diffusion (1). It is immediately obvious that this requires \( S = 1 \) and

\[
D = D \frac{h^2}{\Delta t} \iff D = \frac{h^2}{\Delta t} \sum_{m=0}^{r} \sum_{n=1}^{r} a_{m,n} \left( m^2 + n^2 \right).
\]

(9)

An argument similar to the one in [24 page 12] can be used to show that this finite difference method is stable at least if \( \forall i, j : a_{i,j} \geq 0 \).

New masks can be created as convolutions of smaller masks. Let mask \( a_3 \) be the convolution of masks \( a_1 \) and \( a_2 \). The effect of applying \( a_3 \) to \( u \) is

\[a_3 * u = (a_1 * a_2) * u = a_1 * (a_2 * u),\]

since convolution is an associative operator. Now according to (6), \( (a_2 * u) \) is described as

\[u' = (a_2 * u) \]

(10)

\[= S_2 \ u + h^2 \ D_2 \nabla^2 u + \frac{h^4}{12} E_2(u) + \mathcal{O}(h^6).\]

The mask \( a_1 \) can also be described in terms of \( S_1 \) and \( D_1 \):

\[u'' = (a_1 * u') \]

(11)

\[= S_1 \ u' + h^2 \ D_1 \nabla^2 u' + \frac{h^4}{12} E_1(u') + \mathcal{O}(h^6).\]
Then
\[ u'' = (a_1 \ast u') = a_1 \ast a_2 \ast u \]
\[ = S_1 \cdot S_2 \cdot u + S_1 \cdot h^2 \mathcal{D}_2 \nabla^2 u + S_2 \cdot h^2 \mathcal{D}_1 \nabla^2 u + \mathcal{O}(h^4) \]
\[ = S_1 \cdot S_2 \cdot u + h^2 (S_1 \cdot \mathcal{D}_2 + S_2 \cdot \mathcal{D}_1) \nabla^2 u + \mathcal{O}(h^4) \]
\[ = S_3 \cdot u + h^2 \mathcal{D}_3 \nabla^2 u + \mathcal{O}(h^4). \]

(12)

Therefore \( S_3 = S_1 \cdot S_2 \) and \( \mathcal{D}_3 = S_1 \cdot \mathcal{D}_2 + S_2 \cdot \mathcal{D}_1 \).

The same result is obtained when the algebraic expressions for the convolution are inserted into the definitions of \( \mathcal{D} \) and \( S \) (7). For my updating scheme (8), we have \( S_1 = S_2 = 1 \) and therefore \( S_3 = 1 \) and \( \mathcal{D}_3 = \mathcal{D}_1 + \mathcal{D}_2 \).

When used as finite difference methods, big masks have an error in the same order as the simple 5-point operator. The advantage of big masks is that they allow larger time steps, as it is obvious in (9) that a larger \( \mathcal{D} \) (while \( D \) is fixed) leads to a larger \( \Delta t \).

3. Neighborhood operators used

Since we are looking at large neighborhoods, the application of the neighborhood operators needs to be very fast even for large neighborhoods. There are some neighborhoods that have the property that the computation time required is essentially independent of the neighborhood size. The simplest of these operators is the square mask:

\[
\text{square}(1) = \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{bmatrix}
\]

(here radius 1), which is constructed as the convolution of

\[
\begin{bmatrix}
1 \\
1 \\
1
\end{bmatrix}
\text{ and } \begin{bmatrix}
1 & 1 & 1
\end{bmatrix}.
\]
In general, a square mask of radius \( r \) has size \((2r + 1)^2\) and can be generated by the convolution of row and column vectors of length \(2r + 1\). Each of these operators can be implemented as a column-wise (respectively row-wise) scan through the grid where a running count is kept, and, in going from one cell to the next, one cell at the top (right) is added and one cell at the bottom (left) subtracted from the current count. In this way the effect of a square mask of radius \( r \) can be calculated by just four additions per grid point, independent of the size of the mask. Square masks were favored by Gerhardt, Schuster and Tyson [7,8,9].

Another mask can be constructed by applying the square mask to the neighborhood count which resulted from another square mask. In other words, this new mask is a convolution of two square masks with radii \( r_1 \) and \( r_2 \). For \( r_1 = 1 \) and \( r_2 = 1 \) this results in the mask

\[
\text{square}(1) * \text{square}(1) = \begin{bmatrix}
1 & 2 & 3 & 2 & 1 \\
2 & 4 & 6 & 4 & 2 \\
3 & 6 & 9 & 6 & 3 \\
2 & 4 & 6 & 4 & 2 \\
1 & 2 & 3 & 2 & 1
\end{bmatrix}.
\]

The computation necessary to perform this neighborhood count operation is approximately double that necessary to compute the simple square mask, since it is applied two times. The time is also almost independent of the radii \( r_1 \) and \( r_2 \).

The same technique of scanning through the grid and keeping a running total can also be applied in directions other than horizontal and vertical. Our next mask is constructed by scanning in both diagonal directions. This results in a diamond shaped mask (but with holes inside):

\[
diamond(1) = \begin{bmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0
\end{bmatrix}.
\]
The computational complexity of this mask is almost independent of its size and it is about the same as that for the simple square mask.

Convolutions of diamond masks and square masks give masks that almost have a round shape. These diamond-square masks seem very useful. For example, the convolution of a square mask of radius 1 and a diamond mask of radius 1 yields

\[
diamond(1) * \text{square}(1) = \begin{bmatrix}
0 & 0 & 1 & 1 & 1 & 0 & 0 \\
0 & 1 & 2 & 3 & 2 & 1 & 0 \\
1 & 2 & 4 & 4 & 4 & 2 & 1 \\
1 & 3 & 4 & 5 & 4 & 3 & 1 \\
1 & 2 & 4 & 4 & 4 & 2 & 1 \\
0 & 1 & 2 & 3 & 2 & 1 & 0 \\
0 & 0 & 1 & 1 & 1 & 0 & 0
\end{bmatrix}.
\]

All masks used here are constructed to model diffusion processes in one way or another.

The effect of diffusion on a unit pulse can be described as

\[
\frac{1}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4\sigma^2}},
\]

where \(D\) is a diffusion coefficient. This suggests using a mask whose elements drop off in magnitude like a Gaussian function of distance from the origin. It is not possible to compute the effect of such a mask in a time independent of its size. Instead the computational effort required is proportional to the number of elements in the mask. These masks are created using the formula

\[
a_{m,n} = C e^{-\frac{(m^2+n^2)}{4\sigma^2}}.
\]

In [4] a mask was used that differs only slightly from the mask obtained with this formula and parameters \(C = 11, \sigma = 3.5\). The combination mask \(\diamondsuit(2) * \text{square}(3)\), which I find very useful, can almost be obtained by this formula with parameters \(C = 21.5\) and
Figure 1: Comparison of (a) Gaussian mask without truncation to integers and (b) combination mask \( \text{diamond}(2) \ast \text{square}(3) \).

\( d = 5.125 \). The combination mask and the true Gaussian mask differ only in 16 out of 225 entries. None of the entries differs by more than one. In Figure 1, both masks are shown. Combination masks are similar to Gaussian masks because each time step can be thought of as two sub-steps using simpler (non-gaussian) masks. As I have just shown, these simpler masks, when iterated, model the diffusion operator, and consequently they smooth a unit pulse into a Gaussian distribution. Clearly, the alternation of diamond and square masks is quite effective at generating a nearly Gaussian distribution in only one compound step. The only purpose of the Gaussian masks in the current setting is to compare their performance with that of the other proposed masks which are computationally feasible.

The fifth type of mask I consider is the random circle mask, proposed and used by Markus and Hess [18].

In order to use these masks, it is necessary to find the mask diffusion coefficient \( D \), denoted by \( D_m \) in the sequel. It can be easily calculated from (7) for any given mask. For some mask types it is possible to determine a general formula that gives the value \( D_m \) as a
function of the parameters (e.g., radius) of the mask. For the square mask we get
\[
D_m = \frac{r (r + 1)}{6}
\]
and for the diamond mask
\[
D_m = \frac{r (r + 1)}{3}.
\]

For the convolutions of square and diamond masks, \(D_m\) can be calculated from the sum rule \(D_{m3} = D_{m1} + D_{m2}\).

For the Gaussian and random circle masks, \(D_m\) cannot be calculated easily in closed form, but it is easy to obtain integral approximations to \(D_m\). In general, \(D_m\) can be approximated as
\[
D_m \approx \int_0^\infty \int_0^\infty a(m, n) (m^2 + n^2) \, dm \, dn.
\]

The functions \(a(m, n)\) for the different masks are

- **square mask:** \(a(m, n) = \begin{cases} \frac{1}{(2r + 1)^2}, & \text{if } |m| \leq r + \frac{1}{2} \text{ and } |n| \leq r + \frac{1}{2}, \\ 0, & \text{otherwise}; \end{cases}\)

- **circle mask:** \(a(m, n) = \begin{cases} \frac{1}{\pi r^2}, & \text{if } m^2 + n^2 \leq r^2, \\ 0, & \text{otherwise}; \end{cases}\)

- **Gaussian mask:** \(a(m, n) = \frac{1}{2\sqrt{\pi d}} e^{-\frac{m^2 + n^2}{4d}}\).

These functions are normalized so that
\[
S = \int_{-\infty}^\infty \int_{-\infty}^\infty a(m, n) \, dm \, dn = 1.
\]
Table 1: Diffusion coefficients for Gaussian masks.

<table>
<thead>
<tr>
<th>$C$</th>
<th>$d$</th>
<th>$D_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>3.5</td>
<td>2.399</td>
</tr>
<tr>
<td>21.5</td>
<td>5.1</td>
<td>4.072</td>
</tr>
<tr>
<td>10</td>
<td>5</td>
<td>3.460</td>
</tr>
<tr>
<td>100</td>
<td>5</td>
<td>4.617</td>
</tr>
<tr>
<td>1000</td>
<td>5</td>
<td>4.924</td>
</tr>
<tr>
<td>10000</td>
<td>5</td>
<td>4.988</td>
</tr>
<tr>
<td>100000</td>
<td>5</td>
<td>4.998</td>
</tr>
</tbody>
</table>

Table 2: Diffusion coefficients $D_m$ for commonly used masks.

<table>
<thead>
<tr>
<th>radius</th>
<th>square</th>
<th>diamond</th>
<th>random circle (from (13))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.33</td>
<td>0.66</td>
<td>0.125</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>0.5</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>4</td>
<td>1.125</td>
</tr>
<tr>
<td>4</td>
<td>3.33</td>
<td>6.66</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>10</td>
<td>3.125</td>
</tr>
<tr>
<td>6</td>
<td>7</td>
<td>14</td>
<td>4.5</td>
</tr>
<tr>
<td>7</td>
<td>9.33</td>
<td>18.66</td>
<td>6.126</td>
</tr>
<tr>
<td>8</td>
<td>12</td>
<td>24</td>
<td>8</td>
</tr>
</tbody>
</table>

The result of carrying out the integration for the square mask is

\[ D_m \approx \frac{(2r + 1)^2}{24} = \frac{r(r + 1)}{6} + \frac{1}{24}, \]

for the random circle mask

\[ D_m \approx \frac{r^2}{8}, \]

and for the Gaussian mask

\[ D_m \approx d. \]

For the Gaussian mask, this approximation is good only if $C$ is sufficiently large. In Table 1 several different parameter combinations for the Gaussian mask are listed, together with the value $D_m$ one obtains from carrying out the summation in (7) explicitly.

The value $D_m$ is important for further simulations, therefore it is listed for several masks in Table 2.
4. Wave propagation and curvature effects

Several researchers are using comparable cellular automata models to simulate excitable media \([4,7,8,9,18]\). All these models have two features in common: 1. They all have a resting and an excited state. 2. The transition from resting to excited state occurs when the number of excited cells in some neighborhood exceeds a threshold \(k\). The neighborhoods and the threshold vary from model to model.

In this section, I seek to verify numerically the curvature relationship \(N = c - DK\), where \(N\) is the normal velocity of the wave front, \(c\) is the speed of a planar wavefront, \(D\) is the diffusion coefficient of the excitation variable and \(K\) is the curvature of the wavefront. To simulate excitable media reliably, it is desirable that this relationship be linear in \(K\) and that \(D\) be independent of the threshold \(k\) of the cellular automaton.

In order to investigate the validity of the curvature relationship, the following simple experiment is set up:

On a grid of size \(150 \times 150\), all cells are set to 0 except for a circular area, which is initialized to 1. Since there is an inherent symmetry in the masks used here, only one quarter circle is used, where the center of the circle is near coordinates \((0,0)\). Mirror boundary conditions complete the circle according to the size of the mask. The circular area has a radius \(r\), which is equivalent to having curvature \(K = \frac{1}{r}\). This situation is depicted in Figure 2, where the center of the circle is at \((0.3, 0.3)\), the boundary is 2 cells wide (for use with a mask of radius 2) and the circle has radius 10. Grey squares indicate the cells (centered at the mesh points) that are 1. The criterion is that the mesh point (intersection of vertical and horizontal lines) must be inside the circle or on the circle.

Now the mask under consideration is applied to this array, giving a count of the number of excited (value = 1) neighbors for each cell. Then a thresholding function is applied.
Figure 2: Circle of 1-cells with radius 10.

which replaces a cell’s value by 1 if the neighborhood count $S$ is greater than the specified threshold $k$. Otherwise the cell value becomes 0. This procedure mimics the spread of excitation in cellular automaton models of excitable media.

An average normal velocity is determined by calculating the average distance to the center $(0,0)$ of all cells that lie on the border of the resulting region of 1’s. Specifically, the average of all cells that are either 1 and have immediate neighbors which are 0 or that are 0 and have immediate neighbors that are 1, is taken. (Immediate neighbor here means that exactly one coordinate differs by exactly one.) From the resulting value the radius of the original circle is subtracted. This is the speed a wavefront with curvature $K$ would have if the threshold were $k$ in the region of the wavefront.

It is important to recognize the discreteness of the underlying grid. Small radii lead to regions of 1’s on the grid that look far from circular. To reduce this effect, the experiment is repeated many times with different origins of the circle with respect to the origin of the
Figure 3: Two examples of normal speed $N$ as a function of curvature $K$: (a) for random circle(5) with threshold 10 and (b) for diamond(2)+square(3) with threshold 200.

grid. The setup used here is to take all positions of the origin in $(x, y) \in \{0, \delta, 2\delta, 3\delta, \ldots, 1 - \delta\} \times \{0, \delta, 2\delta, 3\delta, \ldots, 1 - \delta\}$. Mostly, $\delta$ is chosen to be 1/3 or 1/4. Symmetry considerations lead to the elimination of the cases where $y < x$, so that $1/\delta \cdot (1/\delta + 1)/2$ positions of the origin are simulated and the results averaged. The result is the speed that is reported for the given initial radius $r$ and threshold $k$.

To determine the relationship $N = c - DK$, this experiment is repeated for many different curvatures of the initial circle. As was stated earlier, it is desirable that the $N$ vs. $K$ relationship be linear for all thresholds, and that the slope of the line ($D$) be independent of threshold. For the simulations, the units of space and time are $\Delta t = 1$ and $h = 1$. These are the units that $N, c, K,$ and therefore also $D$ are measured in. Therefore from (9), we expect that $D$ should be close to $D_m$, the theoretical diffusion coefficient of the mask.

The experiment is repeated for each mask for each threshold. To illustrate the resulting dependence of speed on curvature, Figure 3 shows exemplary plots of speed vs. curvature. Fig 3(a) is from the random circle mask with radius 5, using 94 different curvatures from $-0.1$ to $0.1$, where $\delta = 0.34$ and the threshold $k = 10$. Fig. 3(b) is for a convolution of
a square mask with radius 3 and a diamond mask with radius 2. The threshold here is \( k = 200 \), all other parameters are the same. For both examples it is obvious that a linear fit is a good approximation to describe the data sets. In (a) one would get \( N \approx 3.09 - 2.33K \), where the 99% confidence interval for the slope is \( 2.33 \pm 0.28 \). The corresponding values for (b) are \( N \approx 2.93 - 3.67K \) where the confidence interval for \( D \) is \( 3.67 \pm 0.13 \).

The first question to be solved is the range of curvatures that should be used. In a small series of experiments, different ranges of curvatures are used to calculate a linear fit to the obtained normal velocities (as a function of curvature). Also, a confidence interval for the slope of the obtained fit is calculated. The results are presented in Figure 4 for a square mask of radius 6.

Two important points should be mentioned: large curvatures (small radii) are limited by the fact that the number of 1’s in the initial circle needs to be big enough to exceed the threshold of the mask. Otherwise it is not possible to calculate a speed. The other limitation is for small curvatures (large radii). Since the size of the array used for these simulations is 150 \( \times \) 150, radii above \( (150 - 3 \cdot \text{masksize}) \) are not possible, because the resulting circle would exceed the simulation domain. Therefore, curvatures between \(-0.01\) and \(0.01\) are not possible. The range of curvatures used should be at least \(-0.03 \cdots 0.03\), so that the measured points form a line for both positive and negative curvatures. (The negative curvature experiments start with the exterior of the circle excited.)

From the graphs we see that using the range of curvatures from -0.1 to 0.1 seems to be the most suitable for determining the diffusion coefficient, since here the graphs are smoother and the errors are smaller than for other curvature ranges.

Using this range and six different centers with \( \delta = 1/3 \), many different masks are tested. Although most masks have a fairly flat \( D \)-curve for high thresholds and exhibit a
Figure 4: Diffusion coefficient vs. threshold for square mask radius 6 for different curvature ranges. Error bars indicate 99% confidence interval and the horizontal line marks $D = D_m$. (a) Curvature $-0.2 \ldots +0.2$, increment 0.01. (b) Curvature $-0.1 \ldots +0.1$, increment 0.005. (c) Curvature $-0.05 \ldots +0.05$, increment 0.002. (d) Curvature $-0.025 \ldots +0.025$, increment 0.0008.

linear curvature relationship for almost all thresholds (most error bars are fairly small), the result shows that most masks do not have a constant slope $D$ over all thresholds $k$. For all masks, very small thresholds result in a slope that is much too small. In order to be able to compare experiment and theoretical prediction, the average of $D$ for all thresholds $k$ is
Figure 5: (a) Diffusion coefficient vs. threshold and (b) speed vs. threshold for square mask of radius 8. The linear fit used 87 curvatures between −0.1 and +0.1 in steps of 0.002 (δ = 1/3).

calculated as $D_{av}$.

5. Diffusion coefficients for different masks

5.1. Square mask

For square masks the slope $D$ is not independent of threshold; rather, $D(k)$ is clearly an increasing function. Figure 5 shows the function $D(k)$ for radius 8, as well as the speed curve, $c(k)$, for this mask. Although $D$ increases with $k$, the average value of $D$ over all thresholds is not far from the expected value ($D_m$):

<table>
<thead>
<tr>
<th>radius</th>
<th>$D_{av}$</th>
<th>$D_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.23</td>
<td>3.33</td>
</tr>
<tr>
<td>6</td>
<td>7.14</td>
<td>7</td>
</tr>
<tr>
<td>7</td>
<td>9.77</td>
<td>9.33</td>
</tr>
<tr>
<td>8</td>
<td>12.94</td>
<td>12</td>
</tr>
<tr>
<td>9</td>
<td>16.71</td>
<td>15</td>
</tr>
</tbody>
</table>
**Figure 6:** (a) Diffusion coefficient vs. threshold and (b) speed vs. threshold for random circle mask of radius 8. The linear fit used 94 curvatures between $-0.1$ and $+0.1$ in steps of 0.002 ($\delta = \frac{1}{3}$). The horizontal line marks $D = D_m$.

### 5.2. Random circle mask

The random circle mask exhibits very strong irregularities for small thresholds. Here there is no linear relationship between $N$ and curvature $K$, so that the error in the linear fit is very large. Beyond some point, the curve for this mask looks almost exactly like that for a square mask of slightly smaller radius. This is not surprising, since the center part of a circle looks similar to the center part of a square. The close similarity comes from the fact that in both cases the weight of all cells is 1. The random mask is not a good choice if the aim is to achieve a threshold-independent $D$. Figure 6 shows the $D$ plots and the speed plots for radius 8. The value $D_{av}$ compares as follows to the theoretical value:

<table>
<thead>
<tr>
<th>radius</th>
<th>$D_{av}$ averaged over all $k$</th>
<th>Average over all but first 8</th>
<th>$D_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>6.63</td>
<td>5.01</td>
<td>4.5</td>
</tr>
<tr>
<td>8</td>
<td>9.73</td>
<td>8.99</td>
<td>8</td>
</tr>
</tbody>
</table>
Figure 7: Diffusion coefficient vs. threshold for diamond mask of radius 5. Same conditions as in Figure 6.

5.3. Diamond mask

Similar to the square mask is the diamond mask, with additional jumps, which are probably caused by the holes in the mask. Figure 7 shows the results for the diamond mask with radius 5. The results of the averaging are:

<table>
<thead>
<tr>
<th>radius</th>
<th>$D_{av}$</th>
<th>$D_{m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>8.43</td>
<td>6.66</td>
</tr>
<tr>
<td>5</td>
<td>12.83</td>
<td>10</td>
</tr>
<tr>
<td>6</td>
<td>17.89</td>
<td>14</td>
</tr>
</tbody>
</table>

5.4. Combination square-square

The convolution of two square masks shows a new effect: the curve of $D$ vs. $k$ is not monotone any more, but fluctuates up and down. On the other hand, the average over all thresholds is close to the theoretically predicted value. Figure 8 shows the result from the convolution of a radius 2 square mask with a radius 3 square mask. The averaged result is:

<table>
<thead>
<tr>
<th>radii</th>
<th>$D_{av}$</th>
<th>$D_{m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,2</td>
<td>1.85</td>
<td>2</td>
</tr>
<tr>
<td>2,3</td>
<td>2.89</td>
<td>3</td>
</tr>
</tbody>
</table>
Figure 8: (a) Diffusion coefficient vs. threshold and (b) speed vs. threshold for convolution mask square(2)*square(3).

5.5. Combination diamond-square

The convolution of a diamond mask with a square mask seems to be the best mask of those under consideration here. The curve of $D$ vs. $k$ is fairly flat and smooth for this mask. Also, the averaged $D$ is very close to the theoretical prediction. Figures 9 and 10 show the results for two such masks. I take into consideration only those combinations of radii where the radius of the diamond mask is not greater than the radius of the square mask. The other combinations have masks for which the weights are not monotonously decreasing from the inside to the outside. Experiment and theory compare as follows:

<table>
<thead>
<tr>
<th>radii</th>
<th>$D_{av}$</th>
<th>$D_{m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 2</td>
<td>1.49</td>
<td>1.66</td>
</tr>
<tr>
<td>2, 2</td>
<td>2.87</td>
<td>3</td>
</tr>
<tr>
<td>1, 3</td>
<td>2.52</td>
<td>2.66</td>
</tr>
<tr>
<td>2, 3</td>
<td>3.93</td>
<td>4</td>
</tr>
<tr>
<td>3, 3</td>
<td>6.10</td>
<td>6</td>
</tr>
<tr>
<td>2, 4</td>
<td>5.37</td>
<td>5.33</td>
</tr>
</tbody>
</table>
**Figure 9:** Diffusion coefficient vs. threshold for combination masks (a) diamond(2)\*square(3) and (b) diamond(2)\*square(4).

**Figure 10:** Speed vs. threshold for combination mask diamond(2)\*square(3).

5.6. Gaussian mask.

The Gaussian mask gives unexpectedly bad results in this experiment. The diffusion coefficient jumps in a very broad range and the average is not very close to the theoretical value. Some examples are shown in Figure 11 and some averaged results are shown in the table, where $D_m$ is the diffusion coefficient calculated from the actual mask (see also Table 1 and remarks in Section 3). Note that the Gaussian mask can only be tested for small $D_m$, because the computation gets too expensive for larger masks.
Figure 11: Diffusion coefficient vs. threshold for Gaussian masks with $C = 11, d = 3.5$ (a) and $C = 20, d = 3$ (b). The linear fit used 62 curvatures between $-0.1$ and $+0.1$ in steps of $0.003$ ($\delta = \frac{1}{3}$).

<table>
<thead>
<tr>
<th>parameters C, d</th>
<th>$D_{av}$</th>
<th>$D_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11, 3.5</td>
<td>2.16</td>
<td>2.40</td>
</tr>
<tr>
<td>20, 2</td>
<td>1.26</td>
<td>1.53</td>
</tr>
<tr>
<td>40, 3</td>
<td>2.32</td>
<td>2.54</td>
</tr>
<tr>
<td>20, 3</td>
<td>2.10</td>
<td>2.34</td>
</tr>
<tr>
<td>10, 2.5</td>
<td>1.39</td>
<td>1.65</td>
</tr>
</tbody>
</table>

6. Dependence of plane wave speed on propagation direction

One basic parameter in the design of a cellular automaton is the choice of the grid or lattice. Most researchers using cellular automata for excitable media choose a square lattice because it is easier to work with numerically.

For a given mask and a given threshold, the speed of a plane wave depends upon the direction of the wave in relation to the grid. A simple example with a small mask illustrates this in Figure 12. Here a square mask of radius 1 with threshold 0 (i.e., a cell becomes excited if $> 0$ neighbors are excited) gives rise to waves with speed 1 in the horizontal
Figure 12: Speed of planar waves in different directions. Dark grey is wave before updating, light grey after updating. (a) is a horizontal wave, (b) and (c) are diagonal waves with thresholds 0 for (b) and 1 or 2 for (c).

Table 3: Multiples of 1 and 1/\sqrt{2} (corresponding to possible speeds of planar waves in horizontal and diagonal directions).

<table>
<thead>
<tr>
<th>horizontal</th>
<th>diagonal</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>0.707</td>
</tr>
<tr>
<td>1</td>
<td>1.414</td>
</tr>
<tr>
<td>2</td>
<td>2.121</td>
</tr>
<tr>
<td>3</td>
<td>2.828</td>
</tr>
<tr>
<td>4</td>
<td>3.536</td>
</tr>
<tr>
<td>5</td>
<td>4.243</td>
</tr>
<tr>
<td>6</td>
<td>4.950</td>
</tr>
<tr>
<td>7</td>
<td>5.657</td>
</tr>
<tr>
<td>8</td>
<td>6.364</td>
</tr>
<tr>
<td>9</td>
<td>7.071</td>
</tr>
<tr>
<td>10</td>
<td>7.899</td>
</tr>
</tbody>
</table>

(Vertical) direction and speed \( \sqrt{2} \) in the diagonal directions. For thresholds 1 and 2, the horizontal speed is still 1, whereas the diagonal speed is \( 1/\sqrt{2} \). For thresholds 3,4 and 5, both speeds are 0.

In general, it is important to note that in the horizontal direction, the speed of a plane
Figure 13: Speed of planar waves as a function of the angle for threshold 246 (a) and 294 (b).

wave can only assume integer values. The speed in the diagonal direction can only assume multiples of \(1/\sqrt{2}\). Table 3 shows these values. It can be seen that there are certain wave speeds for which horizontal and diagonal speed can be very close together (e.g., 5) and others for which the difference is much bigger (e.g., 6). Similar arguments can be made for waves traveling with slopes \(\frac{p}{q}\), where \(p\) and \(q\) are small integers.

In a series of experiments, the propagation speed of plane waves is measured. Two examples of how the speed depends upon the angle of a wave are given in Figure 13. Both examples use the combination mask diamond(2)*square(3), at thresholds 246 and 294. It can be seen that in both cases the speed in the horizontal direction is 2. The speed in the diagonal direction is \(2.828 = 4/\sqrt{2}\) and \(2.121 = 3/\sqrt{2}\). For intermediate angles the speed is relatively constant even in (a). One way to assess the isotropy of wave propagation is to calculate the average planar wave speed over all angles and the variance about this average. Figures 14 and 15 show the results for some masks. It can be seen that the average speed is a monotonously decreasing function of the threshold (which is almost identical to the speed function derived from circular waves). The variance of the speed is very different for different thresholds.
**Figure 14:** Average speed and variance of speed for planar waves as a function of threshold for the square mask of radius 3.

**Figure 15:** Average speed and variance for planar waves as a function of threshold for the combination mask diamond(2)*square(3).

If isotropic behavior is very important, it might be useful to restrict the possible thresholds to those with small variance of the speeds. This reduces the number of available speeds, however. Figures 14 and 15 show that the variance is considerably smaller for the combination mask than for the simple square mask.

7. Possible extensions of masks into three dimensions

For three-dimensional simulations, the only change necessary for our automaton is to define a three-dimensional mask. For the square mask, the obvious extension is the cubic mask, a convolution of strips in the x-, y-, and z-directions. For the diamond mask,
Figure 16: **Scan directions for the three different possibilities for three-dimensional masks.**

Extensions are not so obvious, because in the three-dimensional case there are many more symmetries than in the two-dimensional case.

Two possibilities exist for convolutions of strips that are fully symmetric:

- Apply a diamond mask in each of the three planes, i.e., in the xy-plane, in the yz-plane, and in the xz-plane. This amounts to a total of six strip operations and is completely symmetrical.
- Do one strip in each of the four space diagonals of a cube. This amounts to four strip operations and is also fully symmetric.

Both possibilities of diagonal masks suffer from the same problem of the diamond mask in two dimensions: there are holes left in the mask. Therefore, both masks need to be combined with a cubic mask to eliminate these holes, the same way this is done in two dimensions. Figure 16 shows the three possibilities for symmetric masks by indicating the scan directions in a cube.
8. Construction of cellular automaton rules from the PDE model

Many PDE models of excitable media, when cast in dimensionless variables, take the following simple form

\[
\frac{\partial \hat{u}}{\partial t} = \epsilon \nabla^2 \hat{u} + \frac{1}{\epsilon} f(\hat{u}, \hat{v}),
\]

(14)

\[
\frac{\partial \hat{v}}{\partial t} = \epsilon \delta \nabla^2 \hat{v} + g(\hat{u}, \hat{v}),
\]

where $\epsilon$ is a small (positive) parameter representing the ratio of time scales for changes in $\hat{u}$ (the fast variable) relative to $\hat{v}$ (the slow variable). Space has been scaled so that the diffusion coefficient of $\hat{u}$ is simply $\epsilon$. Then $\delta$ is the ratio of diffusion coefficients of $\hat{v}$ to $\hat{u}$. The smallness of $\epsilon$ makes numerical solution of (14) difficult, but it can be exploited by singular perturbation theory [29] to show that

1. traveling wave solutions are possible for these systems;
2. away from the wavefronts and wavebacks, $\hat{u}$ changes very little, so that $f(\hat{u}, \hat{v}) \approx 0$;
3. within the wavefronts and wavebacks, $\hat{v}$ changes very little, since $\hat{v}$ is a slow variable.
It is typical of excitable media that the equation \( f(\hat{u}, \hat{v}) = 0 \) has three solution branches,

\[
\hat{u} = h_-(\hat{v}), \quad \hat{u} = h_0(\hat{v}), \quad \hat{u} = h_+(\hat{v}),
\]
two of which \((h_-(\hat{v}) \text{ and } h_+(\hat{v}))\) are stable. These two branches determine the value of \( \hat{u} \) in the regions between wavefronts and wavebacks.

The value of \( \hat{v} \) is limited by \( \hat{v}_{\text{min}} \leq \hat{v} \leq \hat{v}_{\text{max}} \), where \( \hat{v}_{\text{min}} \) is the value of \( \hat{u} \) at the resting state, i.e., the stable solution of \( g(\hat{u}, \hat{v}) = 0 \) and \( f(\hat{u}, \hat{v}) = 0 \). Likewise, \( \hat{v}_{\text{max}} \) is the value of \( \hat{v} \) at which \( h_0(\hat{v}) = h_+(\hat{v}) \). At this value of \( \hat{v} \), \( h_+(\hat{v}) \) is not stable. At \( \hat{v} = \hat{v}_{\text{max}} \), a waveback occurs as a jump from \( \hat{u} = h_+(\hat{v}) \) to \( \hat{u} = h_-(\hat{v}) \).

To convert a PDE of this sort into a cellular automaton, I introduce two new variables

\[
u = \begin{cases}
  0 & \text{if } \hat{u} = h_-(\hat{v}), \\
  1 & \text{if } \hat{u} = h_+(\hat{v}),
\end{cases}
\]

(recovering state)

(excited state)

and

\[
u = L(\hat{v}) := \frac{\hat{v} - \hat{v}_{\text{min}}}{\hat{v}_{\text{max}} - \hat{v}_{\text{min}}} v_{\text{max aut}}.
\]

In the automaton, I shall convert \( \nu \) into an integer.

Diffusion of the variable \( u \) and the excitation jump at the wavefront are simulated by using a big mask (Fig. 17) to count the number of excited cells in the neighborhood and applying a threshold function to the resulting (weighted) count, \( \text{Sum} \). This threshold function is selected such that the correct wave speed is obtained for all values of \( \hat{v} \). To construct this threshold function, first I calculate from the PDE the planar wave speed \( c = c_2(\hat{v}) \) of an isolated front propagating into medium with recovery value \( \hat{v} \). Then, from simulations of wave propagation using the mask with threshold \( k \), I determine the function \( c_1(k) \), the planar wave speed as a function of the threshold (averaged over all directions).
These two speeds should be equal (in their respective time and space scales) for all values of \( \dot{u} \). Therefore

\[
(15) \quad k(v) = c_1^{-1}(\alpha c_2 (L^{-1}(v))).
\]

Here \( L^{-1} \) is an affine transformation from the automaton variable \( v \) into the PDE variable \( \dot{u} \) and \( \alpha \) transforms the units of measurement for wave speeds.

So a rule for updating \( u \) in the automaton is:

\[
\text{Sum} := M \ast \text{Sign} \ast u^t;
\]

\[
\text{if } \text{Sum} > k(v) \text{ then } u^{t+1} = 1
\]

\[
\text{else } u^{t+1} = 0;
\]

where the superscript refers to the time step \( t \) and \( '\ast' \) denotes convolution.

9. Time and space scales

In this section the space and time scales of the excitable medium, the PDE model, and the cellular automaton are compared. I use the units \( \text{cm} \) and \( s \) (centimeter and second) for the excitable medium, \( su \) and \( tu \) (space unit and time unit) for the PDE model and \( \Delta x \) and \( \Delta t \) for the cellular automaton.

To determine time and space scales, I use the strategy introduced by Gerhardt at al. [7, 8]. The first equation to relate these scales describes the diffusion coefficient in the excitable medium \( (D) \), the PDE model \( (\varepsilon) \), and the cellular automaton \( (D_m \text{ as determined by } (7)) \):

\[
(16) \quad D \frac{cm^2}{s} = \frac{su^2}{tu} = D_m \frac{\Delta x^2}{\Delta t}.
\]
A second relation comes from equating the speeds of a solitary plane wave (that is a plane wave propagating into resting medium):

\[
V \frac{cm}{\varepsilon} = c_{2\text{max}} \frac{su}{tu} = c_1(k_{\text{min}}) \frac{\Delta x}{\Delta t}
\]

(17)

Here, \(c_{2\text{max}} = c_2(\bar{v}_{\text{min}})\) in the PDE is independent of \(\varepsilon\) as long as \(\varepsilon\) is small. In the CA, \(k_{\text{min}}\) is the minimum possible threshold, and \(k_{\text{min}} = k(0)\). This minimum threshold should be large enough so that the effective diffusion coefficient is approximately constant (see Section 5).

From equations (16) and (17) one finds that the correlation between PDE and CA is

\[
\Delta x = \frac{c_1(k_{\text{min}})}{c_{2\text{max}}} \frac{\varepsilon}{D_m} su
\]

(18)

\[
\Delta t = \left( \frac{c_1(k_{\text{min}})}{c_{2\text{max}}} \right)^2 \frac{\varepsilon}{D_m} tu,
\]

the correlation between PDE and excitable medium is

\[
su = \frac{c_{2\text{max}} D}{V} \frac{\varepsilon}{cm}
\]

(19)

\[
tu = \left( \frac{c_{2\text{max}}}{V} \right)^2 \frac{D}{\varepsilon} s,
\]

and the correlation between CA and excitable medium is

\[
\Delta x = \frac{c_1(k_{\text{min}})}{V} \frac{D}{D_m} cm
\]

(20)

\[
\Delta t = \left( \frac{c_1(k_{\text{min}})}{V} \right)^2 \frac{D}{D_m} s.
\]

We also need \(\alpha\), the conversion factor for wave speeds:

\[
\alpha = \frac{c_1(k_{\text{min}})(\frac{\Delta x}{\Delta t})}{c_{2\text{max}}(\frac{su}{tu})}.
\]

(21)
10. Update $v$

The update function for $v$ is obtained directly from the PDE for $\hat{v}$:

$$\frac{\partial \hat{v}}{\partial t} = \begin{cases} g(h_+(\hat{v}), \hat{v}) & \text{if } u = 1; \\ g(h_-(\hat{v}), \hat{v}) & \text{if } u = 0. \end{cases}$$

$g(h_+(\hat{v}), \hat{v}) \geq 0$ and $g(h_-(\hat{v}), \hat{v}) \leq 0$ and in the typical PDE model.

The rule for updating $v$ in the automaton is:

if $v^t = v_{\maxaut}$ then

$$u^{t+1} = 0$$

$$v^{t+1} = v^t$$

else if $u^t = 0$ then

$$v^{t+1} = \max\{0, v^t + [L' g_-(v) \Delta t]\}$$

else if $u^t = 1$ then

$$v^{t+1} = \min\{v_{\maxaut}, v^t + [L' g_+(v) \Delta t]\},$$

where $L' = dL/d\hat{v} = v_{\maxaut}/(\hat{v}_{\max} - \hat{v}_{\min})$, $g_\pm = g(h_\pm(\hat{v}), \hat{v})$ with $\hat{v} = L^{-1}(v)$, and $\Delta t$ is the length of one CA time step measured in PDE time units: $\Delta t = \alpha^2\epsilon/D_m$.

If $v_{\maxaut}$ is big, the error introduced by the discretization of $\hat{v}$ (the $\lfloor \rfloor$ and $\lceil \rceil$ operations) is small.

Another rounding error is introduced by the $\min\{\cdots\}$ function. Recognizing that the jump from $u = 1$ to $u = 0$ occurs as soon as $v$ reaches $v_{\maxaut}$, one can determine the time of the jump within the current timestep. After the jump, $v$ is decreased according to the rules for $u = 0$. Assuming that the increase in $v$, $[L' g_+(v) \Delta t]$ is distributed linearly over the time step, an improved rule is
if \( u^t = 0 \) then
\[
v^{t+1} = \max \left\{ 0, v^t + [L' g_-(v) \Delta t] \right\}
\]

else if \( u^t = 1 \) then
\[
v_d := [L' g_+(v) \Delta t];
\]
if \( v^t + v_d \leq v_{\text{maxaut}} \) then
\[
v^{t+1} = v^t + v_d
\]
else
\[
u^{t+1} = 0;
\]
\[
v^{t+1} = v_{\text{maxaut}} + \left( 1 - \frac{v_{\text{maxaut}} - v^t}{v_d} \right) [L' g_-(\hat{u}_{\text{max}}) \Delta t].
\]

If we want \( \hat{v} \) to be a diffusive variable (\( \delta \neq 0 \) in Eq. (2)), then the time step is completed by averaging \( v \) with a square mask of an appropriate size to give the desired value of \( \delta \). Typically, I use a square mask of radius 3, so that \( v \) diffuses with \( D_m = 2 \), i.e., \( \delta = 0.5 \).

11. Simulating the Oregonator

To complete the description of a CA model, the functions \( f(\hat{u}, \hat{v}) \) and \( g(\hat{u}, \hat{v}) \) in (1) must be specified. The Oregonator model [28] is chosen:
\[
f(\hat{u}, \hat{v}) = \hat{u}(1 - \hat{u}) - \hat{\nu} \frac{\hat{u} - q}{\hat{u} + q},
\]
\[
g(\hat{u}, \hat{v}) = \hat{u} - \hat{v},
\]
with \( q = 0.002 \). In all calculations, I take \( \epsilon = 0.01 \).

As a compromise between roundoff error and computational complexity, \( v_{\text{maxaut}} = 1000 \) is used. For \( \hat{f} = 3 \) the intersection of \( f(\hat{u}, \hat{v}) = 0 \) and \( g(\hat{u}, \hat{v}) = 0 \) is \( \hat{v}_{\text{min}} = 0.00399 \) and

34
Figure 18: Speed as a function of recovery variable $\check{\nu}$ ($c_2(\check{\nu})$).

The intersection of $h_0(\check{\nu})$ and $h_+(\check{\nu})$ is $v_{\text{max}} = 0.084$. The function $c_2(\check{\nu})$ is calculated as the solution of the nonlinear eigenvalue problem [30]

$$x'' + c_2(\check{\nu})x' + x(1-x) - \hat{f}\check{\nu}\frac{x-q}{x+q} = 0,$$

$$x(-\infty) = h_-(\check{\nu}), \quad x(+\infty) = h_+(\check{\nu}).$$

The result for $\hat{f} = 3$ is shown in Fig. 18. The speed vs. threshold function $c_1(k)$ is shown in Fig. 10. In order to calculate $k(v)$ (from (15)), $\alpha$ needs to be known. There are two possibilities: (a) fix $k_{\text{min}}$ and calculate $\alpha$ from (21) or (b) fix $\alpha$ and calculate $k_{\text{min}} = c_1^{-1}(\alpha c_{2\text{max}})$. I use the second possibility and choose $\alpha \approx D_m$, for the following reasons. The thickness of a wavefront is $O(\epsilon)$ in the PDE models of excitable media [30], but it is less than one cell length in the CA model. In order that the space scale not be too small compared to the thickness of the wave front, we should require $\Delta x > \epsilon$, which implies $\alpha > D_m$. However, $\alpha$ cannot be chosen too large, because it is also desired that $k_{\text{min}} > 50$, see Fig. 9a. Choosing $\alpha$ too small does not affect $u$, since only the speed of wave propagation is modeled correctly for $u$. However, the update rules for $v$ assume that the jumps in $u$ at wavefronts are instantaneous, so some errors are introduced into the $v$ dynamics if $\alpha$ is too small. As a compromise, in my examples, where $D_m = 4$ and
$c_{2\text{max}} = 1.533$, I use $\alpha := 3$, so that $c_1(k_{\text{min}}) = 4.599$ and $k_{\text{min}} = 68$. The resulting function $k(v)$ is shown in Fig. 19.

The updating rule for $v$ is shown in Fig. 20, where $dv = v^{t+1} - v^t$ is shown for both $u^t = 0$ and $u^t = 1$. The sharp change in $dv$ for $u = 1$ marks the point where the jump from front to back occurs within the current time step. At $v^t \approx 1000$, the jump occurs at the beginning of the time step, therefore the behavior is essentially the same as for $u^t = 0$.

For the parameter $\hat{f}$, several values are tested. An example of a snapshot of a spiral is shown in Figure 21. Here $\hat{f} = 3$ and the diffusion coefficient for $v$ is 2 (compared to a
diffusion coefficient of 4 for $u$) and therefore $\delta = 0.5$. The grey levels indicate the value of the recovery variable $v$. This CA simulation of the spiral wave shows many features that appear in simulations of the Oregonator PDEs by standard numerical methods [13,14].

The Oregonator is a model of the Belousov-Zhabotinskii reaction [5,28]. In this case, equations (16) and (17), which determine time and space scales, are

$$1.5 \times 10^{-5} \frac{cm^2}{s} = 0.01 \frac{su^2}{tu} = 4 \frac{\Delta x^2}{\Delta t},$$

and

$$0.013 \frac{cm}{s} = 1.53 \frac{su}{tu} = 4.59 \frac{\Delta x}{\Delta t}.$$

Thus,

$$\Delta x = 0.0075 su = 0.0013 cm,$$

$$\Delta t = 0.0225 \ tu = 0.47s.$$

12. Comparison to the “second generation” automaton of GST

The “second generation” automaton developed by Gerhardt, Schuster and Tyson (GST) [7,8,9] was also intended to model the BZ-reaction. To compare my automaton with theirs, I reconstructed the threshold function, using a square mask of radius 6 (as in [9]). Figure 22 compares this new threshold function, for $\alpha = 4.5$, with the piecewise linear function from [7].

For updating $v$, Gerhardt et al. used constant rates $v^{t+1} = v^t + g$ with $g = 20$ (when $u = 1$) and $g = -5$ (when $u = 0$). Taking into account that $v_{\text{max}} = 100$ in [9] and 1000 here, these values are not far from the $v$-updating rules in Fig. 20. The major difference is that, during the recovery phase, $v$ decreases by a constant amount in each time interval in
Figure 21: Spiral wave (recovery variable v) for $\hat{f} = 3$ on a 686 x 960 cell domain

(5.1 x 7.2 Oregonator space units, or 0.91 x 1.27 cm).
Figure 22: Threshold $k(v)$ for the new automaton (dots) and the GST automaton (lines). In the gap from $v = 71 \cdots 85$, the GST automaton disallows changes in $u$.

[9], whereas it decreases exponentially in the model presented here. Furthermore, in [9] the values $+20$ and $-5$ were chosen empirically, i.e., to get a good fit of the automaton to the observed period of rotation of spiral waves in the BZ reaction. On the other hand, in my approach, the $v$-dynamics is derived directly from the PDE for $v$. A final difference is that $v$ is nondiffusive in [9], but allowed to diffuse in the present model.

13. Comparison of cellular automaton simulations to PDE simulations

An interesting feature of solutions to the Oregonator PDEs is the meandering of the tip of a spiral for certain parameter values. A study of the meandering for different values of $\dot{f}$ and $\epsilon$ in the Oregonator model was undertaken by Jahnke and Winfree [14]. They used explicit numerical methods to solve the PDEs.

Using the automaton I study the behavior of the tip for different values of $\dot{f}$. Sections of tip traces are shown in Fig. 23. Comparing Fig. 23 to Fig. 3 of [14], we can observe that the tip traces from the automaton are comparable to the PDE solutions for $\epsilon = 0.01$. Another value to compare is the period of rotation for spirals and the wavelength far from
Table 4: Periods and wavelengths for some spirals compared to results from Jahnke and Winfree (J+W) (all in cellular automaton units).

<table>
<thead>
<tr>
<th>f</th>
<th>λ</th>
<th>J+W λ₀</th>
<th>τ</th>
<th>J+W τ₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>116</td>
<td>144</td>
<td>58</td>
<td>70</td>
</tr>
<tr>
<td>2</td>
<td>147</td>
<td>170</td>
<td>65</td>
<td>76</td>
</tr>
<tr>
<td>3</td>
<td>220</td>
<td>228</td>
<td>75</td>
<td>90</td>
</tr>
<tr>
<td>4</td>
<td>245</td>
<td>270</td>
<td>87</td>
<td>101</td>
</tr>
<tr>
<td>6</td>
<td>320</td>
<td>354</td>
<td>122</td>
<td>124</td>
</tr>
</tbody>
</table>

the tip of the spiral. For meandering spirals, an average over many rotations is taken. These values are listed in Table 4 and compared to the values determined by Jahnke and Winfree. Note that the scaling used by Jahnke and Winfree differs by a factor of \( \sqrt{c} \) in the space scale.

14. Parallel implementation

Parallel implementation on a ring-connected multicomputer is straightforward: for \( p \) processors, the simulation domain is split into \( p \) strips of equal width. Each processor stores this strip plus two overlap areas each with a width equal to the radius of the mask. At the end of each cellular automaton step, which is carried out exactly as in the sequential implementation, the information in the overlap areas is updated by messages between neighboring processors. This scheme is efficient as long as the width of each strip is larger than the size of the mask used. Some speed examples on the Intel iPSC860 hypercube with 128 processors are listed in Table 5. Here \( N_{\text{int}} \) refers to the number of cells in the \( x \)-direction assigned to each processor. In the \( y \)-direction there are 700 cells. Thus the total amount of work is proportional to the number of processors. These measurements are taken without control over the load of the host processor, which is the bottleneck for small \( N_{\text{int}} \). Also, each reported run time is the result of averaging 3 or 4 runs with 200 steps each. Factors
Figure 23: Tip traces for different values of $\dot{f}$. The position of the tip is the point of largest cross product of the gradients of $u$ and $v$. Space scale: the length of the ruler on top is 133 cells or 1 Oregonator space unit.
Table 5: Simulation speed on the iPSC/860 hypercube. Times in μsec for one cell-update on each processor.

<table>
<thead>
<tr>
<th>processors</th>
<th>$N_{int} = 15$</th>
<th>$N_{int} = 25$</th>
<th>$N_{int} = 100$</th>
<th>$N_{int} = 400$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>14.33</td>
<td>11.95</td>
<td>6.56</td>
<td>7.83</td>
</tr>
<tr>
<td>4</td>
<td>12.39</td>
<td>8.76</td>
<td>6.85</td>
<td>7.83</td>
</tr>
<tr>
<td>16</td>
<td>12.14</td>
<td>9.33</td>
<td>6.85</td>
<td>7.83</td>
</tr>
<tr>
<td>64</td>
<td>12.33</td>
<td>9.62</td>
<td>6.85</td>
<td>7.83</td>
</tr>
<tr>
<td>128</td>
<td>12.75</td>
<td>9.91</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Influencing the performance are (i) the speed of the host and (ii) the cache hit ratio on the i860 processors. It can be seen that the overhead for higher degrees of parallelism is negligible (the execution time is independent of the number of processors if the problem size is proportional to the number of processors as in the columns of Table 5). In other words, this application belongs to the applications ideally suited even for distributed memory parallel machines.

15. Conclusion

I have shown how to calculate the effective diffusion coefficient of several different masks that are used in cellular automata simulations of excitable media. Experimental investigation shows that the linear curvature relationship $N = c - D K$ holds reasonably well for most masks and thresholds considered. However, I find that the apparent diffusion coefficient ($D$) is not independent of the threshold, as it should ideally be. The best masks in this respect are the combinations of square and diamond masks, for which the apparent diffusion coefficient varies little with threshold and is (when averaged over all thresholds) very close to the effective diffusion coefficient predicted by theoretical considerations. These masks are also computationally efficient. Therefore these masks are considered the best candidates for the development of cellular automata that mimic the reaction-diffusion equations of excitable media.
Such an automaton is constructed based on singular perturbation analysis of the partial differential equation models for excitable media. The construction shows the close relationship between the cellular automaton and the PDEs. It is not necessary to use the simulation results for tuning parameters, since all aspects of the automaton rule are derived from the PDE model. This approach is applicable to all PDE models that can be expressed in the form of (14), with a small parameter $0 < \epsilon \ll 1$. Since simulations of this automaton are computationally inexpensive compared to standard numerical methods for solving the PDE, three-dimensional calculations become more feasible.
16. References


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**PUBLICATIONS**


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