A SIMPLE MODEL OF THE BELOUSOV-ZHABOTINSKY REACTION FROM FIRST PRINCIPLES

Alasdair Turner

IMPLEMENTATION NOTE

A Simple Model of the Belousov-Zhabotinsky Reaction from First Principles

Alasdair Turner
Bartlett School of Graduate Studies, University College London, London
a.turner@ucl.ac.uk

19 March 2009

http://www.aac.bartlett.ucl.ac.uk/processing/samples/bzr.pdf

Abstract

The Belousov-Zhabotinsky (BZ) reaction is an example of a temporally oscillating chemical reaction. An unusual and interesting feature of the reaction is that as it progresses on a two-dimensional plate, self-organized spirals are formed. Many computer models have been constructed of the BZ reaction to simulate the evolution of these spirals. The models typically use cellular automata to allow progression of a wavefront through a notional substrate. Usually a single substrate is used with somewhat arbitrary transference rules. Here it is shown that cellular automata models of BZ spirals can be created by using a very simple set of equations based on a three substrate model with close connection to reaction-diffusion models, more closely resembling the actual BZ reaction. Source code for the model is given in the Processing language.

1 Introduction

Cellular automata (CA) models have frequently been used to model the Belousov-Zhabotinsky (BZ) reaction. Several popular implementations use a CA model due to Dewdney (1988), for example, the BZ reaction simulation included with sample chemical and physical models from NetLogo (Wilensky, 2003). Dewdney's 'hodgepodge' machine is a multiple state CA where the next state is a combination of other surrounding states and a factor to move forward a number of states. If the state reaches a maximum it is automatically reset, and the following step given a new initial state. The control parameters for the CA involve the initial state and the number of states to skip forward each step, g. In order to generate waves, g is set high, and this results in a rapid rotation of the states (as they reach the maximum value and are reset) before waves are established. Despite elegantly using a single parameter to model the BZ reaction, the actual working is somewhat haphazard and extremely sensitive to initial parameters.

A totalistic CA that responds with specific responses to each possible total count of states around it can also produce a wave-like pattern (Zammataro, 2008). Using Wolfram's (2002) formalism for enumerating CAs, Zammataro shows that CA number 1350851716507335422 generates spiral waves. Unfortunately, the spirals produced are slightly box-cornered, and, just as with Dewdney's CA, it is difficult to trace this back to an underlying model of the BZ reaction itself.

Therefore, here, an explicit reaction model is introduced to simulate the BZ reaction. Rather than use set states, the quantities of three chemical substrates will be represented with floating point values, although clearly quantized states could be used if preferred. The method ap-

proaches a reaction-diffusion model, although the diffusion of the process will be transferred in a traditional CA manner, using a summation of states surrounding a cell, taken at discrete time steps.

The approach taken here has some similarities to other continuous models, in particular to Barkley (1991). Barkley provides are more explicit wave model than used here. His model uses two parameters, one for the progression of a wavefront, and one for the current intensity of the wave. The dynamics of the wave movement are handled through equations that model the spatio-temporal dimension explicitly, rather than through discrete time steps, while maintaining a cell-like grid. A method such as Barkley's is clearly superior to model dynamic wave processes; however, it is hoped that the method here is intuitive, easy to understand, and reflects more closely the actual processes within the BZ reaction. In particular, no explicit assumption that waves will be generated is made, although the reaction is still very much idealized.

2 Method

Ball (1994) presents a simplified description of the BZ reaction as a series of chemical equations of the form[1]:

$$A + B \quad \rightarrow \quad 2A$$

In this equation, provided there is some quantity of B, the creation of A is autocatalyzed until the supply of B expires. A set of competing reactions can be formed by adding two similar chemical equations:

$$\begin{aligned} B + C \quad &\rightarrow \quad 2B \\ C + A \quad &\rightarrow \quad 2C \end{aligned}$$

With the addition of these equations, B can be created, but only if there is a quantity of C, and finally, C can be created, but only if there is a quantity of A, bringing the reaction full circle.

[1] The equations described here are not exactly as formulated by Ball, but the circularity introduced is useful to create a simple implementation.

These three equations will be used for the basis for the model here. With the reactions described, equations may be written for the quantity of A, B or C present as time progresses. The symbol a_t will be used to mean the quantity A at time t, similarly, b_t will denote the quantity of B at time t and c_t the quantity of C. In these symbols, the quantities of A, B and C at time $t+1$ can be written as:

$$\begin{aligned} a_{t+1} &= a_t + a_t(b_t - c_t) \\ b_{t+1} &= b_t + b_t(c_t - a_t) \\ c_{t+1} &= c_t + c_t(a_t - b_t) \end{aligned}$$

Note that a time $t+1$ each quantity is dependent on two competing processes. The quantity of A at $t+1$ is increased according to the amount of B present, but decreases due to the amount of C, as A is used up to create C. If desired, parameters can be added to change the reaction rates of the competing processes, but for the purposes of clarity at this stage, the parameters are not included.

These equations could be used to set up an oscillating reaction at a single location, but in order to create a two dimensional diffusion surface for the reaction, a cellular automata model will be used. In this model, in order to promote diffusion of the reaction, the amount of A, B and C is simply averaged for each cell and its neighbors before the reaction equations above are applied. That is, the values of a_t, b_t and c_t are simply summed for the 9 cells in the immediate vicinity (including the central cell), and divided through by 9. The new value for the cell at location x, y is then calculated by inserting the average values into the reaction equations above. This could clearly be enhanced to take into account the previous quantity of each substrate at the location, rather than its average, but it is satisfactory for this implementation.

The code presented at the end of this note is slightly complicated by two factors. The first is the placement onto a von Neumann or toroidal grid. The edges are wrapped around using the modulo operator, so what was `a[i][j]` becomes `a[(i+width)%width][(j+height%height)]`. This formalism simply means that if `i` is `-1` it is set to `width-1` and if `i` is `width` it is set to `0`. The second factor is that the values, having being calculated, are constrained to the range 0 to 1. This is only included so that the values stay in range for the color display. The equations as stated maintain a equal amount of substrate overall, although individual cells might overstep the level. The algorithm alternates the values of `p` and `q` as the current time step and the next

time step so that values do not have to be explicitly transfered from step $t+1$ to step t.

Once new values for the level of each substrate have been updated, the only remaining line is to set the color of each pixel according to the level of the substrate. Emulation of an 'indicator' is chosen, so that the amount of color is dependent on the amount of substrate A at any one location. This could be made more colorful by adapting it so that it works of hue rather than brightness.

3 Results

The algorithm as stated, and shown at the end of this note, starts to produce spiral patterns after about 70-80 frames and stabilizes to constant generation of spirals. Figure 1(a) shows the self-organization of wave formations as they stand at about 100 frames.

The wavefront established can be varied by adjusting the relative rates of the reactions. The rate of each reaction may be adjusted by adding parameters to the standard three reaction equations as follows:

$$\begin{aligned} a_{t+1} &= a_t + a_t(\alpha b_t - \gamma c_t) \\ b_{t+1} &= b_t + b_t(\beta c_t - \alpha a_t) \\ c_{t+1} &= c_t + c_t(\gamma a_t - \beta b_t) \end{aligned}$$

In this format, the amount of one substrate produced and another consumed can be increased by altering the parameters. So, for example, increasing α will increase production of A, but only at the expense of also consuming B more rapidly. Figure 1(b) and figure 1(c) show the effect this has on the waves. In these figures, α is set to 1.2, while β and γ are left at 1.0. The spirals now take an increased amount of time to form, and when they do, the wavefronts are considerably longer.

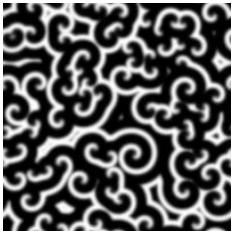
(a)  (b)  (c) 

Figure 1: (a) State after approximately 100 frames using the standard algorithm. (b) State after approximately 100 frames with $\alpha = 1.2$. (c) State after approximately 400 frames with $\alpha = 1.2$

4 Conclusion

This note has presented the algorithmic implementation of an idealized Belousov-Zhabotinsky (BZ) reaction. It has shown that spiral waves as seen in the actual reaction may be recreated by using a three substrate system of reaction equations with a cellular automata model to diffuse the substrate across a grid surface. The implementation provides more predictable generation of spiral waves and more intuitive grounding for the model than typical CA approaches.

Acknowledgements

Thanks to Philip Ball for an inspirational lecture that prompted me to have a go at coding the BZ reaction, and Jaap Bax for excellent and clear descriptions of various oscillatory mechanisms at `http://www.metafysica.nl/`.

References

Ball, P. 1994 *Designing the molecular world: Chemistry at the frontier*. Princeton, NJ: Princeton University Press.

Barkley, D. 1991 A model for fast computer simulation of waves in excitable media. *Phyisca D*, **49**(1–2), 61–70.

Dewdney, A. K. 1988 The hodgepodge machine makes waves. *Scientific American*, **259**(2), 104–107.

Wilensky, U. 2003 NetLogo B-Z reaction model. NetLogo library, Northwestern University, Evanston, IL.

Wolfram, S. 2002 *A new kind of science*. Champaign, IL: Wolfram Media.

Zammataro, L. 2008 Idealized Belousov-Zhabotinsky reaction. Online contribution, The Wolfram Demonstrations Project.

Processing Source Code

```
// Idealised Belousov-Zhabotinsky reaction
float [][][] a;
float [][][] b;
float [][][] c;

int p = 0, q = 1;

void setup()
{
  size(400,400);
  colorMode(HSB,1.0);
  a = new float [width][height][2];
  b = new float [width][height][2];
  c = new float [width][height][2];
  for (int x = 0; x < width; x++) {
    for (int y = 0; y < height; y++) {
      a[x][y][p] = random(0.0,1.0);
      b[x][y][p] = random(0.0,1.0);
      c[x][y][p] = random(0.0,1.0);
    }
  }
}

void draw()
{
  for (int x = 0; x < width; x++) {
    for (int y = 0; y < height; y++) {
      float c_a = 0.0;
      float c_b = 0.0;
      float c_c = 0.0;
      for (int i = x - 1; i <= x+1; i++) {
        for (int j = y - 1; j <= y+1; j++) {
          c_a += a[(i+width)%width][(j+height)%height][p];
          c_b += b[(i+width)%width][(j+height)%height][p];
          c_c += c[(i+width)%width][(j+height)%height][p];
        }
      }
      c_a /= 9.0;
      c_b /= 9.0;
      c_c /= 9.0;
      a[x][y][q] = constrain(c_a + c_a * (c_b - c_c), 0, 1);
      b[x][y][q] = constrain(c_b + c_b * (c_c - c_a), 0, 1);
      c[x][y][q] = constrain(c_c + c_c * (c_a - c_b), 0, 1);
      set(x,y,color(0.5,0.7,a[x][y][q]));
    }
  }
  if (p == 0) {
    p = 1; q = 0;
  }
  else {
    p = 0; q = 1;
  }
}
```