PH456 Complex Systems Essay: Belousov–Zhabotinsky Reactions

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1 Introduction

The Belousov-Zhabotinsky (BZ) reaction is an example of a oscillatory chemical reaction that exhibits self organised spirals on a 2D plane. This reaction usually entails an organic substrate and a catalyst-indicator, and through the mathematical model of the oregonator (and other models) a wide variety of chemicals can be used to create this experiment [1]. This experiment is usually carried out by adding energy into the system, either stirring or a flow of the chemicals entering the experiment, this can also be simulated computationally with random noise and starting conditions to keep it in the chaotic regime [2]. The behaviour of the BZ reaction, which is chaotic, can be described by the strange attractor in phase space and by an infinite number of unstable periodic oscillations if plotted against time. This means that the BZ reaction is extremely sensitive to initial conditions and also that the structure of the attractor are generally self similar. In an oregonator simulation, [3], the fractal dimension of the BZ reaction was calculated to be between 5.2 and 5.8, with the largest Lyapunov exponent being around $\lambda = 0.55$. This further suggests that the BZ reaction is a strange attractor and chaotic.

2 Theory

The BZ experiment is a class of experiments, but is usually given in the form of:

$$3CH_2(CO_2H)(aq) + 4BrO_3^-(aq) \rightarrow 4Br^-(aq) + 9CO_2(g) + 6H_2O(I) \qquad (1)$$

The reaction is a pair of auto-catalytic process's in which Bromine is an intermediary in the scheme, the Bromine will increase if there is enough reactants in the chemical solution and will produce bromide ions. Although this increases another reactant which depletes the Bromine, and after the Bromine is depleted the other reactant is depleted also leading it full circle [4]. The experiment also shows temporal and spatial changes in colour, clearly showing the oscillations and bifurcations. In experiments, i.e. not a simulation, the BZ reaction goes though three stages in the lifespan of the experiment; transitional period, induction period and main period. When a stage switches from the transitional period to the induction period there is a bifurcation from a monostable state to a bistable state. In relation to figures 4, 5 and 6, the bifurcation is the colour change in the 'chemicals' [1].

Figure 1: Image of a physical Belousov-Zhabotinsky reaction in a Petri dish.

2.1 Computational Model

The method being used to simulate the BZ reaction was presented by Ball(1994)[5], and it's described as a series of chemical equations [6]:

$$A + B \rightarrow 2A \tag{2}$$
$$B + C \rightarrow 2B \tag{3}$$
$$C + A \rightarrow 2C \tag{4}$$

This reaction is self referential as for an amount of A to exist there needs to be an amount of B, for B to exist there needs to be an amount of C, and finally for C to exist there needs to be an amount of A. These can be used to generate time dependant equations as such:

$$a_{t+1} = a_t + a_t(b_t - c_t) \tag{5}$$
$$b_{t+1} = b_t + b_t(c_t - a_t) \tag{6}$$
$$c_{t+1} = c_t + c_t(a_t - b_t) \tag{7}$$

Note that a_t is being used to denote the absolute amount of A at a specific time t, and similarly for b_t and c_t. Also a_{t+1} denotes the absolute amount of A at a specific time plus 1 time step.

For this Essay's visualisation of the BZ reaction a discretised grid (usually 300x300) was used to mimic the reaction that would usually take place on a Petri dish. Since the space is discretised the act of diffusion was averaged by a convolved 9x9 grid, that is to say the absolute amount of 'chemical' at any point on the grid was summed on the 9x9 grid and divided evenly at each point. Adjusting equations 5,6,7 the terms α, β, γ can be added to give control over the absolute amount of each 'chemical' at each time step:

$$a_{t+1} = a_t + a_t(\alpha b_t - \gamma c_t) \tag{8}$$

$$b_{t+1} = b_t + b_t(\beta c_t - \alpha a_t) \tag{9}$$

$$c_{t+1} = c_t + c_t(\gamma a_t - \beta b_t) \tag{10}$$

3 Results

The general trend that can be seen in figures 5,6 and 7 and can be seen in further detail if the animations are seen, shows that after a period of time the absolute amounts of each 'chemical' and therefor colour seem to stabilise into repeating waves. This is somewhat intuitive as chaotic attractors are locally unstable but globally stable once the graph has 'fallen' into the attractor, this behaviour can be seen in figures 2A and 3A. Another behaviour that can be observed from figures 2B and 3B is a recurrent non periodic behaviour as discussed in the notes.

As described in section 2 the amount of each chemical is dependant on relative amounts of the other chemicals in the experiment, this is analogous to the predator prey model. The predator prey model is governed by the Lotka-Volterra equations which denote the change in predator prey populations as such[7]:

$$\dot{x} = x(a - by) \tag{11}$$

$$\dot{y} = -y(c - dx) \tag{12}$$

In figure 10 it can be seen that for certain starting values of the particular predator prey model, for a period of time, follows the same pattern as figure 3. This growth and death of a population can particularly be seen in figure 10(b) and figure 3(B)(from $0 \rightarrow 300$ time steps)

4 Conclusion

In conclusion the Belousov-Zhabotinsky reaction is an example of a system that's in a thermodynamic non-equilibrium, this produces nonlinear chemical oscillations.

Due to this these reactions evolve chaotically under the condition of being perturbed slightly, whilst also being an attractor making this experiment a strange attractor. Also as mentioned in the notes if the sign of the Lyapunov exponent is positive, then the system is believed to be chaotic.

One draw back of using the computational method that was used is that the time steps are fixed, this produced plots that are more quantised rather than being continuous. The advantage is that it's simple to implement and runs relatively quickly, plus it uses pre made packages like scipy.signal.convolve2d which can easily deal with wrapping, so in effect the simulations showing the reaction are taking place on a torus.

References

[1] Gang Chen. A mathematical model for bifurcations in a belousov–zhabotinsky reaction. *Physica D: Nonlinear Phenomena*, 145(3-4):309–329, 2000.

[2] Valery Petrov, Vilmos Gaspar, Jonathan Masere, and Kenneth Showalter. Controlling chaos in the belousov—zhabotinsky reaction. *Nature*, 361(6409):240–243, 1993.

[3] D Mukesh. Modelling of belousov-zhabotinskii reaction on a surface. *Chaos, Solitons & Fractals*, 3(3):285–293, 1993.

[4] Ted Lister, Catherine O'Driscoll, and Neville Reed. *Classic chemistry demonstrations*. Royal Society of Chemistry, 1995.

[5] Philip Ball. *Designing the molecular world: Chemistry at the frontier*, volume 117. Princeton University Press, 1996.

[6] Alasdair Turner. A simple model of the belousov-zhabotinsky reaction from first principles. 2009.

[7] Shuichi Kinoshita. *Pattern formations and oscillatory phenomena*. Newnes, 2013.

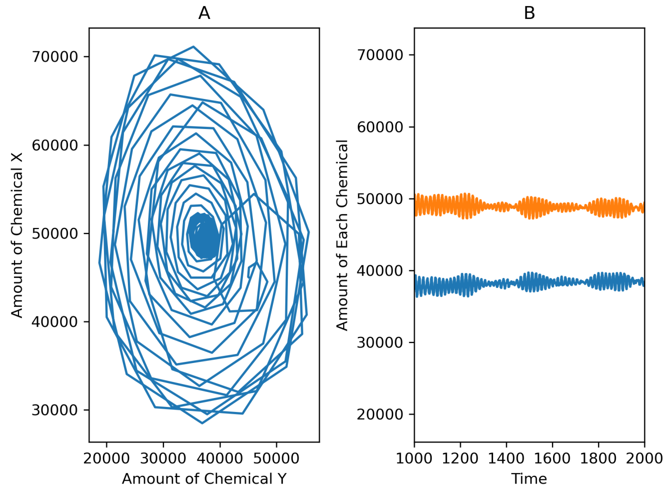

Figure 2: A) Plot showing the attractor nature of the system. B) Plot showing the unstable periodic oscillations over time. With $\alpha, \beta, \gamma = 1$.

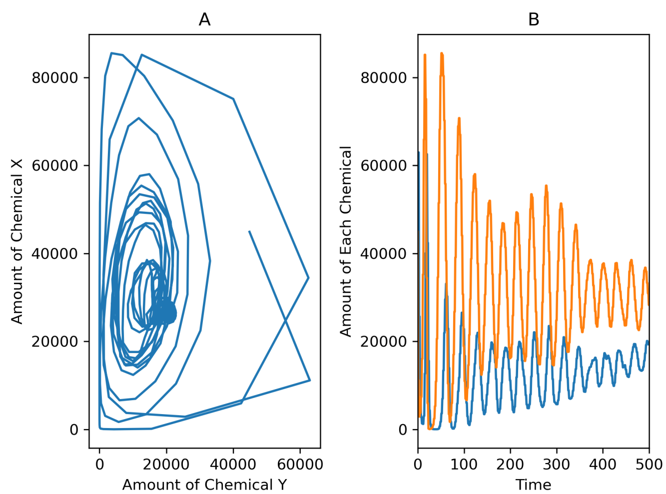

Figure 3: A) Plot showing the attractor nature of the system resembling the Brusselator in a stable regime. B) Plot showing the unstable periodic oscillations over time .With $\alpha = 1.7, \beta, \gamma = 1$.

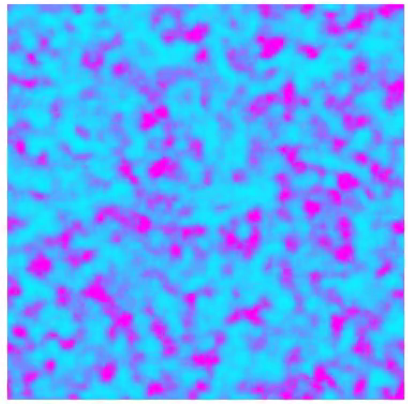

Figure 4: Image of reaction at time step 0 with $\alpha, \beta, \gamma = 1$, can be seen with no pattern yet apart from initial random noise entered into the system.

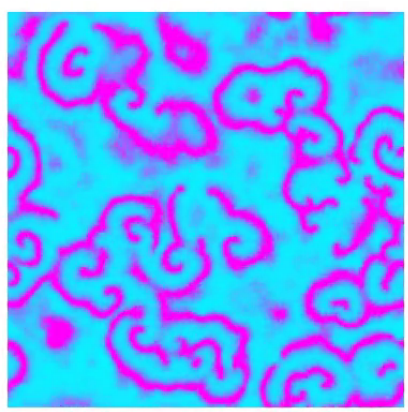

Figure 5: Image of reaction at time step ≈ 300 with $\alpha, \beta, \gamma = 1$, can be seen exhibiting wave fronts characteristic of the BZ reaction.

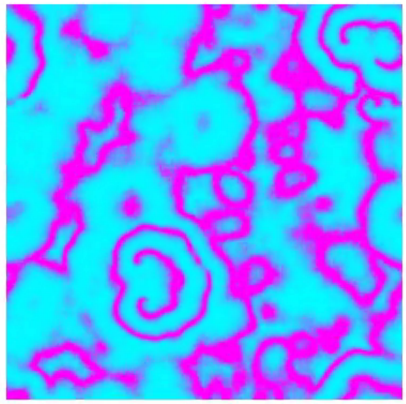

Figure 6: Image of reaction at time step ≈ 300 with $\alpha = 1.2, \beta, \gamma = 1$

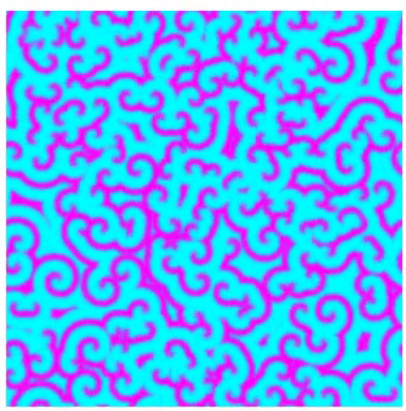

Figure 7: Image of reaction at time step ≈ 300 with $\alpha = 3, \beta, \gamma = 1$

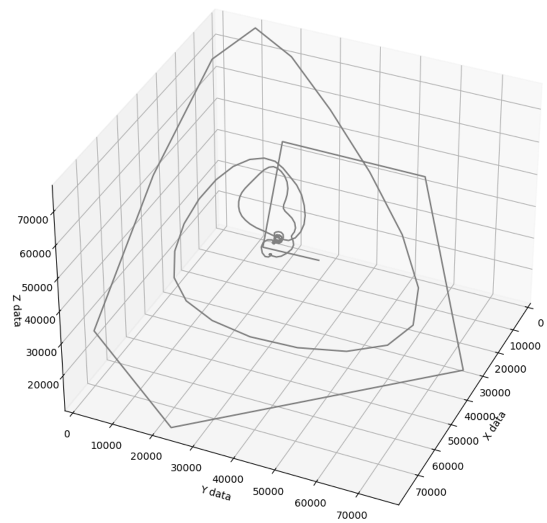

Figure 8: 3D plots of absolute amount of a_t, b_t, c_t with $\alpha, \beta, \gamma = 1$

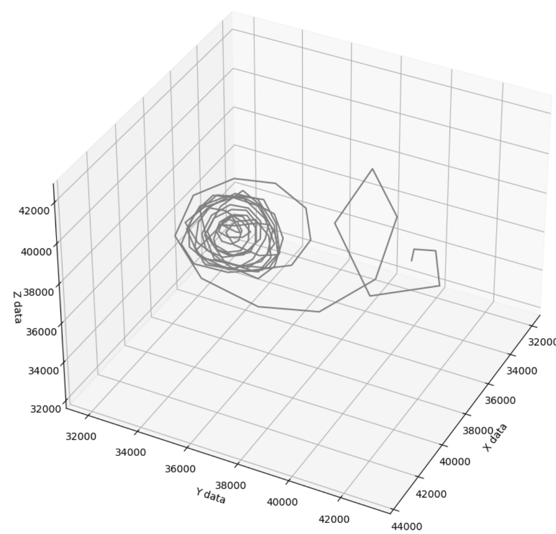

Figure 9: 3D plots of absolute amount of a_t, b_t, c_t with $\alpha = 1.2, \beta, \gamma = 1$

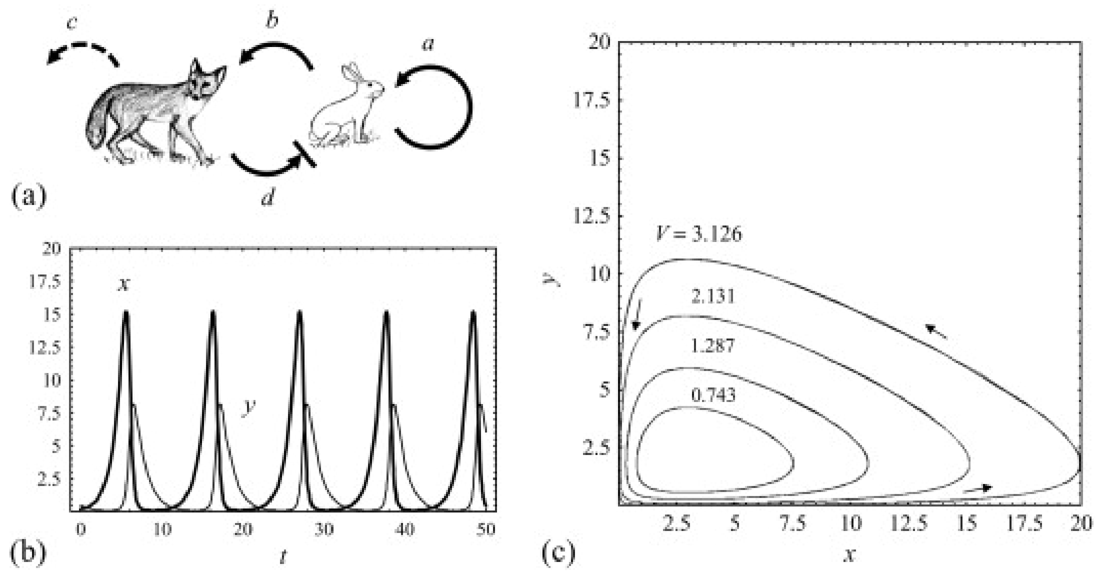

Figure 10: Lotka–Volterra system taken from Pattern formations and oscillatory phenomena[7]