

# Dynamical Systems Analysis of a Protocell

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## Introduction

We design a novel dynamical system of a protocell (PC) that exhibits metabolism-based behavior, based on a previous model developed by Egbert et al. (2009).

The original model was instantiated in an environment of artificial chemistry, and was used to explore how a system could modulate its behaviour in response to the implicit viability that arose from the system itself. It was simulated on a particulate level; i.e. with the simulation of spatially embedded particles in a two-dimensional environment, undergoing Brownian motion. The PC consisted of a membrane enclosing various metabolites, and would demonstrate metabolism-based behavior that would maintain its viability.

We recreate this model using ordinary differential equations (ODEs), which leads to some simplifications. The concentrations of various metabolites, as well as the spatial location, become functions of time. We study the various behaviors that emerge from the interaction of the PC with two food sources, both necessary to produce and sustain motility, so another aspect of the simplification results in us using only one spatial dimension. However, having the model as a set of ODEs allows us to use the rich tools of dynamical systems analysis to see how various behaviours vary with the alteration of parameters.

Further, we investigate the health of these behaviors using the concept of a virtual gradient.

## Our Model

We use a steady state solution to the diffusion equation, with source and decay to model the distribution of two different foods  $A$  and  $B$ . Conceptually, this serves to capture a system where we have a steady inflow of the food at a given location with steady consumption occurring.

$$h(x) = \begin{cases} \frac{M}{2\sqrt{DK}} \cdot \exp\left(-\sqrt{\frac{K}{D}} \cdot x\right) & x > 0 \\ \frac{M}{2\sqrt{DK}} & x = 0 \\ \frac{M}{2\sqrt{DK}} \cdot \exp\left(\sqrt{\frac{K}{D}} \cdot x\right) & x < 0 \end{cases}$$

Where  $M$  is the rate of input of the chemical (food),  $K$  is the rate of decay,  $D$  is the rate of diffusion, and  $x$  is a spatial

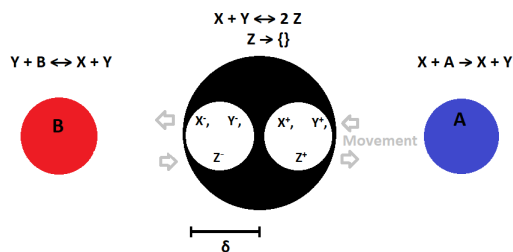


Figure 1: Protocell (black, with the two compartments), and the food sources (red, blue).

coordinate, with the source being at  $x = 0$ .

The PC contains three metabolites:  $X$ ,  $Y$ , and  $Z$  and a fixed amount of a ‘catalyst’ molecule,  $C$ . The following reactions occur within the PC:

Reaction	Fwd Rate	Bkwd Rate
$B + Y + C \rightarrow X + Y + C$	$f_x$	-
$A + X + C \rightarrow Y + X + C$	$f_y$	-
$X + Y \leftrightarrow 2Z$	$f_z$	$b_z$
$Z \rightarrow \emptyset$	$f_e$	-

These equations are slight variations of the ones used in Egbert et al. (2009). The first two are the transformations of the foods into the PC’s constituent metabolites, the third is the reaction producing the metabolite responsible for movement and (in the original model) health, while the fourth is the degradation of the components.

In the original model,  $Z$  would be absorbed into the membrane, increasing its size and triggering motion. Thus the PC would move in the direction determined by where more  $Z$  was being produced in any given moment. To model this, our PC is divided into two compartments, each representing the left/right side (Figure 1). At the locations of these compartments, the absorption of the foods happens, and these then react with the metabolites. The PC is propelled in the direction where there is more  $Z$ , thus modelling the mechanism of movement in the original model.

The resulting model is described by the following ODEs:

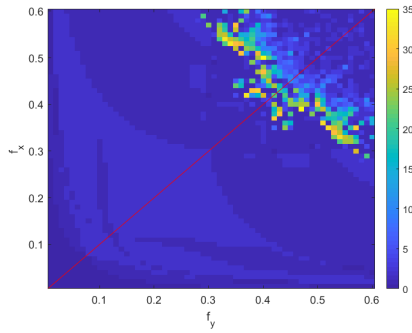


Figure 2: Parameter space  $f_x$  vs  $f_y$ . The color of each region represents the number of distinct POs.

$$\begin{aligned}
 [\dot{X}]^+ &= f_x[Y]^+ ([B](r+\delta)+[C]) - f_z[X]^+[Y]^+ + b_z([Z]^+)^2 \\
 [\dot{Y}]^+ &= f_y[X]^+ ([A](r+\delta)+[C]) - f_z[X]^+[Y]^+ + b_z([Z]^+)^2 \\
 [\dot{Z}]^+ &= f_z[X]^+[Y]^+ - b_z([Z]^+)^2 - f_e[Z]^+ \\
 [\dot{X}]^- &= f_x[Y]^- ([B](r-\delta)+[C]) - f_z[X]^-[Y]^- + b_z([Z]^-)^2 \\
 [\dot{Y}]^- &= f_y[X]^- ([A](r-\delta)+[C]) - f_z[X]^-[Y]^- + b_z([Z]^-)^2 \\
 [\dot{Z}]^- &= f_z[X]^-[Y]^- - b_z([Z]^-)^2 - f_e[Z]^- \\
 \dot{r} &= \frac{[Z]^+ - [Z]^-}{2\delta}
 \end{aligned}$$

Superscript + and -, and the square brackets, respectively describe the right and left concentrations of metabolites  $X$ ,  $Y$ , and  $Z$ .  $r \in \mathbb{R}$  is the location of the center of the PC with the parameter  $\delta$  being its radius.  $[A]$  and  $[B]$  are concentrations of the food sources at given locations instantiated using the function  $h$  described above, while  $[C]$  is a constant representing the concentration of the catalyst. The rest of the parameters correspond to the reaction rates discussed above.

## Dynamical Systems Analysis

For our initial dynamical systems analysis we explore the parameter space of  $f_x$  and  $f_y$  (which model the conversion of  $A$ ,  $B$  into  $X$ ,  $Y$ ). We see a surprising amount of complexity here, finding a large variety of periodic orbits (POs) (Figure 2). Some dynamics observed included the PC going back and forth between the two food sources, going around one food source a specific number of times before travelling to the other, and more, all related to specific choices of parameters.

## Health and the Virtual Gradient

Following from the original model, we take the indicator of health of the PC to be the concentration of  $Z$ . We now consider its behavior, and the connection between the two. The

relation can be discussed via the notion of ‘virtual gradient’. We use this to shed light onto some of the mechanisms at play.

First, we construct the virtual gradient of  $Z$ . Given a PC at a particular location, we take the average concentrations of each metabolite, call this  $m \in \mathbb{R}^3$ , and consider the function  $g(r, m, n) \mapsto z$  s.t.  $z$  is the concentration of  $Z$  in a PC at time  $n$ , stationed at location  $r$ , with initial concentrations  $m$ . Then, the virtual gradient of order  $n$  w.r.t. the given PC is the gradient of  $g$  over  $r$ , namely, given fixed  $m$  and  $n$ :

$$\nabla g(r) = \frac{dg(r, m, n)}{dr}$$

For small  $n$ , the PC effectively travels up this gradient (Figure 3 (a), (b)), demonstrating its ability to evaluate the local environment and act accordingly; for instance it would favor approaching the local optima as opposed to the global optima.

With respect to larger  $n$ , however, this is not the case. As  $n$  becomes large,  $g$  becomes invariant under  $m$ , and maps to relatively large concentrations of  $Z$  at the locations of the food sources (Figure 3 (c)), thus showing that the optimum behavior would be to move to one of these and stay there. Such behavior would yield higher concentrations of  $Z$  than are found in any given PO. This demonstrates that the given POs all prove to be sub-optimal, when considering all possible behaviors. Hence, this becomes an interesting example where metabolism-based behavior that arises from the evaluation of the local environment is sub-optimal.

What is also interesting, is that the disparity in health between such optimum behavior as remaining at a food source, and the PO behaviors, decreases when the parameter  $f_e$  is increased, which determines the deterioration rate of degradation of  $Z$ . One way to conceptually understand this, as the overall system becomes more precarious (with the increase of  $f_e$ ), the type of behavior becomes more efficient. We are currently investigating these phenomena, in order to

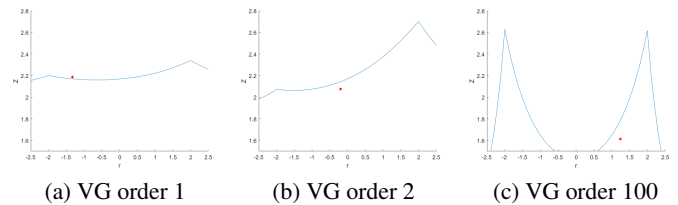


Figure 3: Three examples of the PC and the VG. PC is represented by the red triangle. (a) PC is moving left towards the local optima (left), (b) PC moving right towards the global optima (right), (c) PC is moving left, its behavior doesn't correlate with the gradient.

better understand the mechanisms responsible for the sub-optimality of such metabolism-based behavior.

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