Chemo-ethology of an Adaptive Protocell
Sensorless Sensitivity to Implicit Viability Conditions

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Abstract. The viability of a living system is a non-trivial concept, yet it is often highly simplified in models of adaptive behavior. What is lost in this abstraction? How do viability conditions appear in the first place? In order to address these questions we present a new model of an autopoietic or protocellular system simulated at the molecular level. We propose a measurement for the viability of the system and analyze the 'viability condition' that becomes evident when using this measurement. We observe how the system behaves in relation to this condition, generating instances of chemotaxis, behavioural preferences and simple (yet not trivial) examples of action selection. The model permits the formulation of a number of conclusions regarding the nature of viability conditions and adaptive behaviour modulated by metabolic processes.

1 Connecting Biological Organization and Adaptivity

Conceptualizing adaptivity (the capacity of a system to cope flexibly with its environment in order to survive and reproduce) is far from trivial. The widespread strategy is to model adaptivity as the optimization of certain parameters (captured by the notion of fitness) or as the maintenance of certain variables (often called essential variables—[1]) within viability limits. As a consequence, models of adaptive behavior generally fall under one of two categories (or a combination of both). *Externalist*: Optimization techniques are used to constrain the behavior of a system to achieve the desired adaptive coupling with its environment in relation to a set of parameters or "fitness" criteria. This category includes different types of supervised learning algorithms for NN, simulated annealing or artificial evolution techniques to design control architectures (as used in Evolutionary Robotics, [2]) or, simply, hand design. *Internalist*: Models belonging to this class incorporate a set of internal variables often interpreted as energy sensors, pain or pleasure indicators, etc. These "value modules" are then coupled to other control mechanisms in order to tune the behavior of the system (as in reinforcement learning) or to choose between competing possibilities for action (acting as an action selector [3,4]).

In both cases the parameters or functions to be optimized are explicitly represented either as an external fitness function or as an internal value module, abstractly measuring how well adapted/adapting the system is. There is

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generally no reference or feedback to the processes from which these criteria emerge. How those boundaries of viability or optimal values come to be there in the first place is rarely addressed and modelled. As Randall Beer recognizes, "this explicit separation between an animal's behavioral dynamics and its viability constraints is fundamentally somewhat artificial. (...) However (...) we can assume that its viability constraint is given a priori, and focus instead on the behavioral dynamics necessary to maintain that existence. [5, p.265]".

At first sight, and for many cases, this abstraction seems reasonable. For instance it is obvious that above a certain temperature value an organism will die or that without a certain quantity of resources it would cease to exist. However, these conditions (or value functions) are often variable and difficult to determine, they show temporal variability and subtle interactions with other processes (e.g. you can survive at a low temperature for some time but not for "too long" and this in turn might depend on your diet, etc.). Critically, the behavior of organisms might be sensitive to these conditions in many and sophisticated ways that are lost when a priori abstractions are made. For instance, organisms might display a complex dynamic interplay between internal and behavioral adaptive modulations where mechanisms of self-repair, growth, digestion and maintenance are integrated with behavior generating mechanisms in many subtle ways [6].

What happens when we remove this somewhat artificial and explicit "separation between an animal's behavioral dynamics and its viability constraints"? To address this question requires reference to more fundamental aspects of biological organization such as the the modelling of energy consumption processes, metabolic organization, generation of movement, etc. However, on this side of the relationship between behavioral adaptivity and living organization (dealing with the emergence of viability conditions) life is usually modelled without including behavioral adaptivity. These models emulate the biochemical processes that make viability conditions and value functions be there in the first place. They describe life as a networked set of chemical reactions (metabolism) continuously re-producing the conditions required for their existence. Standing in far-from-thermodynamic-equilibrium conditions and, therefore, in a continuous need for matter and energy for their maintenance, minimal protocells [7] (or autopoietic systems [8]) come to capture the fundamental root of adaptivity: the need to actively compensate for a decaying or precarious existence that also defines the fragile limits (viability conditions) of their otherwise dissipating organization. However, these types of models tend to place the system in environments which do not require any system-level regulation of interactions with the environment (behavior) to maintain themselves (e.g. [9]). A few recent models (see [10,11]) have begun incorporating mechanisms of system level behavior, e.g. motion, upon which the autopoietic processes depend. Yet, many aspects of the interplay between behavior and metabolism are still to be explored.

In this paper we present a model of minimal metabolism and motility in a protocellular system simulated at the molecular level. The model is rather minimal yet capable of raising conceptual issues around the nature of viability conditions, temporal aspects of adaptive processes and the mutual dependence

between metabolism and behavior. Section 2 presents details of the model. Section 3 presents a set of experiments with the protocell behaving adaptively by performing chemotaxis and showing emergent forms of action selection without explicit sensors. Finally we conclude with section 4 addressing some theoretical implications and future extensions of the present model.

2 A Chemo-ethological Model of an Adaptive Protocell

We take a chemo-ethological approach in our explorations: a combination of aspects of artificial chemistry and forms of behavioral modelling and analysis. Our model is a modified version of a model presented in [11] and can be thought of as a highly simplified model of a protocell[7]. It takes place in a two-dimensional arena 256 units square. The model is simulated at the molecular level. It comprises three types of interactants: metabolites, resources and a membrane that encapsulates the reaction network. The interactants are governed by a set of chemical reactions giving rise to a self-maintaining metabolic network. Interactions between the metabolites and the membrane endow the system with an ability to move around the environment which contains generators of the necessary resources.

Metabolites. A metabolite is specified by five attributes, x, y, s, d and T. x and y represent the metabolite's spatial position and s represents the size of the metabolite, which affects its rate of thermal motion (more below). The type of a metabolite, T, indicates which chemical reactions the metabolite can participate in. The final metabolite parameter, d, represents the stability of the metabolite. Each iteration, there is a chance ($p = 5d \times 10^{-3}$) that the metabolite disintegrates. As one would expect, metabolites of the same type have the same s and d values. The metabolites are simulated as if in Brownian motion using the following equations: $x_{t+\delta t} = x_t + \delta t(g_x + 0.75v_x)$, $y_{t+\delta t} = y_t + \delta t(g_y + 0.75v_y)$. Here v_x and v_y represent the 2D velocity of the membrane. g_x and g_y represent displacement due to thermal motion and are selected each iteration from a Gaussian distribution (mean 0, std. $0.1/s$) where s represents the size of the metabolite and indirectly its rate of thermal motion.

Reactions. Metabolites are governed by the reactions shown in Table 1. Each reaction has a rate (ρ) which determines the likelihood of the reaction occurring. Reactions are simulated by picking 2 metabolites within the simulation N times (where N is proportional to the number of metabolites in the simulation) and performing their reaction if they are within 2 units of distance from each other. Metabolites never exist outside of a cell membrane as they are created inside the cell and can not move through the membrane.

Resources. There are three types of resource (R_0, R_1, and R_2) that react with the metabolites (see Table 1). Resources are represented by a 64×64 lattice of squares of width 4.0 units, the nodes of which are updated according to the following differential equation which simulates diffusion. $d\phi(\boldsymbol{r}, t)/dt = D\nabla^2\phi(\boldsymbol{r}, t) + q(r)$. Where $\phi(\boldsymbol{r}, t) \in [0, 3]$ represents the concentration of the resource at location $\boldsymbol{r}$ at time t, and $q(r)$ represents the addition of resources

Table 1. Metabolite Types & Chemical Reactions. ρ_f and ρ_b represent the rate of chemical reactions in the forward and backward directions respectively.

Metabolite Types

Name	Size	Stability	ΔPhosph.	Δvel.
X	0.8	0.005	0.00	0.0
Y	0.8	0.005	0.00	0.0
Z	0.5	0.001	0.15	0.1

Reactions

#	$R_1+R_2 \leftrightarrow P_1+P_2$	ρ_f	ρ_b	κ
0:	$Z + R_0 \leftrightarrow Z + Z$	1×10^{-2}	0	0.7
1:	$X + R_1 \leftrightarrow X + Y$	1×10^{-2}	0	0.7
2:	$Y + R_2 \leftrightarrow Y + X$	1×10^{-2}	0	0.7
3:	$X + Y \leftrightarrow Z + Z$	5×10^{-3}	1×10^{-3}	n/a

to the environment at resource *generators* which are placed in different areas depending on the experimental scenario. The local concentration of resource is increased by a fixed amount every iteration. Resources can act as one of the reactants in a chemical reaction. The parameter κ indicates the quantity of resource consumed by the reaction.

Membrane and Motion. The membrane is specified by three attributes: x, y, and p. It is circular and centered at x and y with the parameter p representing the number of phospholipids in the membrane which is directly proportional to the circumference, relating the radius of the membrane to the number of phospholipids thus: $r = 20p/2\pi$. The number of phospholipids in a membrane decays exponentially according to the equation $dp/dt = -5p \times 10^{-4}$.

Upon contact with the membrane, metabolite Z both imparts an outward radial velocity to the membrane and becomes part of the membrane as a quantity of phospholipids. The other metabolites simply bounces off the membrane, being returned to a position slightly closer to the center of the cell. Each iteration the membrane's location is updated according to its velocity which is reduced each iteration by a fixed drag constant.

3 Exploring the Dynamics of the Protocell

Measuring Viability Conditions. The first, simplest scenario that we examine with our model is one in which the environment contains a fixed quantity of homogeneously distributed R_0. Inside this environment there is one protocell containing a number of Z metabolites. Z is auto-catalytic in the presence of R_0 (see Table 1). Also note that Z contributes phospholipids to the membrane and that this contribution is the only process that counteracts the continual degradation of the membrane. It follows that if R_0 is sufficiently high, the autocatalysis of Z will be sufficient to completely compensate for the degradation of the membrane. If not, the membrane will shrink until the cell dies[1]. Therefore, a good candidate for a viability condition across different environmental situations is

[1] The relationship between resource availability and membrane size is not as simple as it might first appear. A smaller membrane requires less Z-production to maintain its size, but also has non-linear effects upon the levels of resource that are available to the protocell.

the rate of production of Z in relation to the rate at which the membrane degrades, $\Delta V \equiv d(Z/\mathrm{p})/dt$ (where Z is the number of Z metabolites and p is the number of phospholipids in the membrane). Furthermore, $\Delta V = 0$ is an interesting reference as protocells that maintain a negative ΔV for an extended period of time will die, unlike those that maintain a ΔV of 0 or greater.

This can be seen in Figure 1 which depicts values of ΔV for agents in the fixed resource environment[2]. Thinner trajectories plotted in grey tended to die. Note the 'viability boundary' located at $\Delta V = 0$, dividing those trajectories that tend to live from those that tend to die. The viability measure, ΔV can be thought of as a measure of what would happen should the protocell remain in its current situation for a long time. Negative values indicated a propensity towards death and positive values indicate the opposite. Note that this viability condition of the system is not explicitly encoded (unlike classical approaches) but is rather a statistical measure of spatially distributed molecular processes.

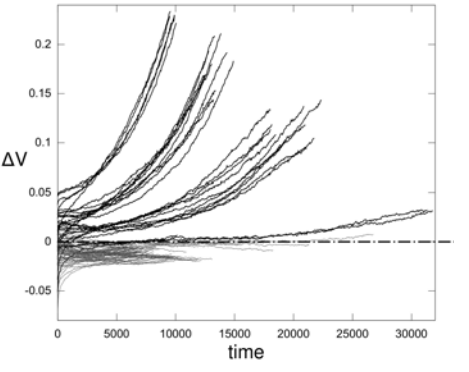

Fig. 1. System Viability

Experiment 1: Chemotaxis and its effect on viability. For the first experiment we move into a more complex scenario where rather than having a fixed homogeneous concentration of R_0, we utilize a R_0 generator which rotates through four different locations, moving every 5000 iterations. Figure 2 (left) shows the behavior of the protocell, which performs chemotaxis towards the generator. This motion is the result of the asymmetrical distribution of R_0 within the protocell. The portion of the protocell that has a higher concentration of R_0 will produce more Z. Accordingly, more Z particles will collide with the membrane in this area of the protocell, inducing an overall up-gradient motion.

Figure 2 (right) shows how ΔV oscillates above and below ($\Delta V = 0$). This plot indicates how the system is behaving adaptively; not in relation to an a priori and somewhat artificial parameter, but in relation to the very conditions upon which the system's ongoing survival depends. When the generator disappears, the ΔV becomes increasingly negative. This tendency is inverted by the system as it approaches the next generator. The protocell compensates for the negative tendency of ΔV by *behaving* (i.e. changing the conditions such that the ΔV becomes positive again).

Experiment 2: Oscillatory behavior between two generators. In our second experiment, we designed an environment in which even if resources are

[2] To generate this plot, the simulation was initialized with protocells with different starting conditions ($\#Z = \{50, 100, 150\}$, p= $\{8, 10, 12\}$, $\mathrm{R}_0 = \{0.3, 0.4..0.8\}$) and we plotted the mean trajectory of 25 runs in ΔV over time (data was also smoothed using a 250 iteration running-mean low-pass-filter).

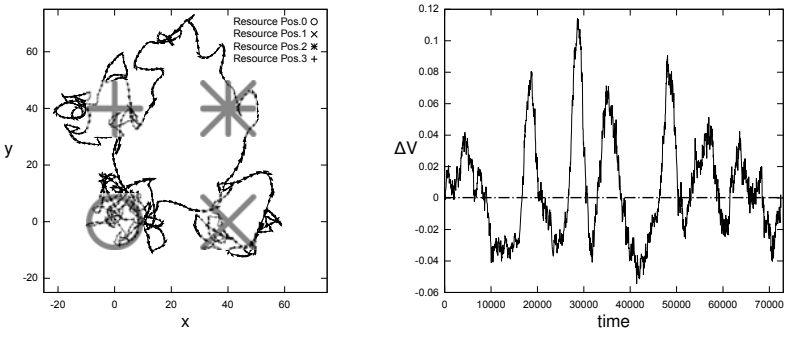

Fig. 2. Experiment 1, the protocell's response to a moving resource generator

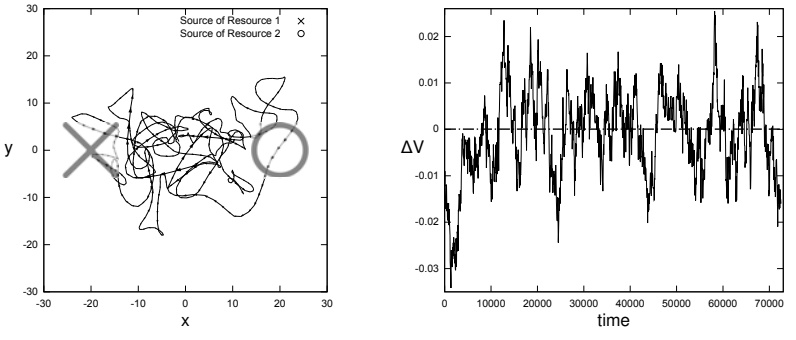

Fig. 3. Experiment 2, Dependence upon two different resources

fixed, the protocell can not survive without behaving – thereby forcing the system into a continuous transient of viability. We accomplished this by introducing two stationary resource generators; one of R_1 and one of R_2. The protocell oscillates back and forth between both generators (see Figure 3 left). Again the motion towards the relevant resource-source is produced primarily by the asymmetry within the cell of the production of Z. In this scenario, Z is only produced by an interaction between X and Y[3]. It is accordingly produced more in areas of the cell that are high in both X and Y than areas that have low concentrations of one of these metabolites. If the cell is located at e.g. the generator of R_0, there tends to be lots of Y throughout the cell and the concentration of X is the limiting factor in the production of Z. Thus more Z is produced in areas of the cell where there is more X. As before, the asymmetrical concentration of Z induces a motion towards the area that results in the production of the most Z. As the

[3] In the absence of R_0 metabolite Z is the product of only one reaction, X + Y → Z + Z. Thus, if Z is to be produced we will require some of both X and Y. Metabolites X and Y are reflexively autocatalytic, i.e. X catalyzes the production of R_0 → Y and Y catalyzes the production of R_1 → X (see reactions 1 and 2 in Table 1). As generators of R_0 and R_1 are separated spatially, it is necessary for the cell to move back and forth between the two resources if it is to maintain non-zero populations of X and Y.

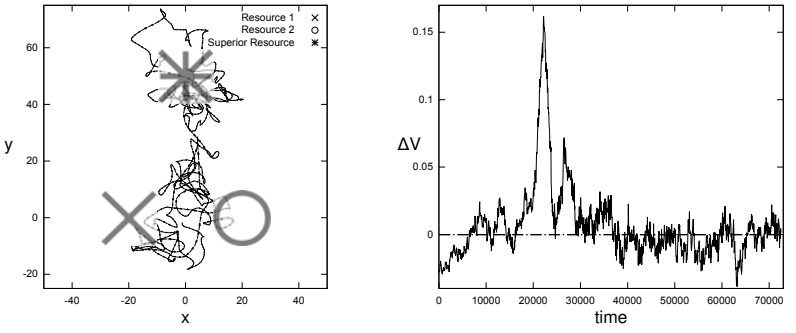

Fig. 4. Experiment 3, the protocell moves to utilize the most profitable resources, maximizing its viability

cell moves up the R_1 gradient to its generator, the concentration of Y decreases and becomes the limiting factor in the production of Z. A symmetrical process causes the cell to move back towards the original resource generator. These two process result in the oscillation of the cell between resource generators. We can again observe how the system behaves adaptively in relation to viability (Figure 3 right): when the ΔV starts to decay behavioral shifting towards the other generator inverts the tendency.

Experiment 3: Preference behavior towards better generator. First, two generators (R_1 and R_2) are presented, like in experiment 2, (see Figure 4 left) and at iteration 5000 a generator of R_0 is added at location $0, 50$. Soon after the protocell moves towards the new resource. However, as the original two resources R_1 and R_2 start to grow, they become a better quality resource and the protocell returns to them. We could interpret this behavior as an instance of action selection sensitive to viability.

4 Conclusions

We were able to observe how our model protocell behaves in relation to the conditions of long-term viability, generating instances of chemotaxis and simple (yet not trivial) examples of action selection without explicit sensors or motor and without an explicit encoding of viability conditions (as previous models of adaptive behavior assumed necessary). The adaptive nature of the behavior is shown not only in that ΔV tendencies were inverted through behavior but also because the behavior was not purely reactive nor stimulus driven. Going one step farther, the system could be interpreted as actually evaluating the value of its interactions with the environment with respect to their effect upon viability.

The model highlights the temporal aspects of the notion of viability which should be associated with tendencies of the entire situation (metabolic and environmental) rather than with regions of prohibited states. We have described the conditions under which the protocell is non-viable in the long term, and yet we see it move into those conditions and out of them in transients that are

brief enough to keep the protocell alive. This theoretical possibility (which would probably be less obvious otherwise) is highlighted by allowing a self-sustaining metabolism to move in its environment in a metabolically-regulated action. Behavior can adaptively invert the negative tendencies becoming a necessary condition for the maintenance of the system. In experiment 2, where the protocell requires two resources that are spatially separate, the long-term tendency of an unmoving cell at any point in space is certain death – no location presents a sufficient level of combined resources. However, in this environment, the cell can survive if it moves. Thus, adaptive behavior, typically conceived as something added on top of metabolism and that confers certain advantages to an already stable self-sustaining entity, turns out in this case to be an essential ingredient for the very conditions that keep the system alive. We conclude that we should remain open to seeing *agency as implicated in metabolism and metabolism as implicated in agency.*

Several measures of long-term viability could be tested instead of the one we have used here and this is a matter for further exploration, as is also the possibility of more complex behaviors enabled by more sophisticated metabolic networks and by the possibility of different forms of environmental couplings. For instance, it may be possible to explore conditions where the cell is able to perform delayed satisfaction "decisions" and other memory-related tasks, such as habituation to noxious stimuli. Such experiments may help us elucidate further the notion of viability as a temporally extended concept once the system is allowed to behave plastically.

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