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Hearing the shape of a chemical reactor with a deep network of swarms

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Abstract: Biological swarms - from the simplest bacteria to large populations - compute the solution of geometrical problems for their growth and survival. In order to engineer synthetic swarms, it is of interest to understand how biological swarms relate space and time to sense their geometry. Here we propose a swarm architecture that senses the shape of its environment, using agents that form Turing patterns as "sonar", and neural-like layers to process those Turing patterns and find the shape of reactor that generate them.

Keywords: Biochemical-micro-robots, Swarm robotics, Reaction-diffusion, Turing pattern, Pattern recognition

1. INTRODUCTION

Many swarms in biology - ranging from social insects and multicellular organisms to films of bacteria and biomolecules- have evolved to solve problems of computational geometry. Termites build nests with elaborate 3D structures, and ants find the shortest route to a food source (foraging) [1]. Bacteria films estimate their density with quorum sensing [2]. During the development of a multicellular organism from a single cell (morphogenesis), cells decide on a spatial reference and form a fully differentiated organism [3]. And at the molecular scale, the population of biomolecules that makes up a cell collectively interact to find the center and poles of the cell - a prerequesite to ensure its even division [8].

Shape sensing by swarm raises an interesting fundamental challenge: How can a swarm estimate geometric features that are vastly larger than the size of its agents ? In the above cases, the passing of chemical messengers between the agents of the swarm was shown to be crucial. Ants lay down pheromones that build up along the best trail [1]. And bacteria broadcast chemical signals - autoinducers - to measure their fluctuation of density [2].

Many of these problems have been framed with reaction-diffusion PDEs, starting with the pioneering work of Turing on morphogenesis [4]. In reaction-diffusion PDEs, a chemical reaction term interacts with a diffusion term, the Laplacian. The chemical reaction term encodes local and direct interactions between agents, while the Laplacian operator encodes global and indirect interactions through diffusion by Brownian motion. Alan Turing suggested a simple model with two chemical species (one activator and one inhibitor) to capture the essence of morphogenesis. He showed that -surprisingly - this reaction-diffusion system supports steady states that are spatially inhomogenous, typically consisting of stripes or spots. His model has since been refined and studied extensively in mathematical biology to explain the formation of biological patterns. Turing patterns have also inspired swarm engineering [5].

The existence and nature of the Turing patterns is closely related to the boundary conditions - and thus the shape of the reactor - through the eigenvalues and eigenmodes of the Laplacian. In the textbook derivation, one checks the stability of the homogeneous state by considering a small perturbation, which is decomposed into the eigenmodes of the Laplacian. Eigenmodes whose eigenvalues fall within a given range (which depends on the chemical constants and diffusion coefficient, but not the geometry of the reactors) are amplified, while other eigenmodes decay. Since the spectrum of the Laplacian forms a discrete set, it may or may not contain eigenvalue whose eigenmodes are amplified. We turn this observation upside down: by looking at the existence of Turing

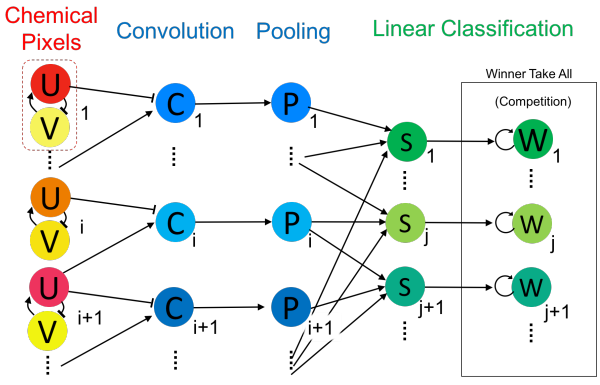


Fig. 1 Illustration of the general architecture of the swarm. The first layer contains "chemical pixels", which are pairs of agents forming a Turing pattern. The convolution layer acts as an "edge detector", picking up differences between chemical pixels. Lastly the pooling layer averages concentration at the scale of the reactor, and the last layer classifies the resulting signatures to recognize the shape of the reactor.

† Nicolas Lobato-Dauzier is the presenter of this paper.

patterns for a given set of chemical and diffusion parameters, one infers the existence of an eigenvalue in the aforementioned range. By repeating this test for many different parameters, one gleans information about the whole spectrum of eigenvalues, from which in principle we can (approximately) reconstruct the shape of the reactor.

Based on this, we propose a swarm that senses the shape of its reactor, with agents that form Turing patterns as "sonar", and information-processing layers to recognize the shape that generates these Turing patterns.

At the bottom of the network sits a Turing layer (Fig. 1). It comprises pairs of agents (the Turing nodes) obeying the same Schnakenberg kinetics [6] (except for the scaling of their chemical term) and forming Turing patterns at steady state. The Turing nodes act as chemical pixels which individually capture information on the geometry of the reactor at a given length scale. The next layer is a convolution filter that performs the equivalent of chemical edge detection: it pairwise compares the concentrations of species from two pairs in the Turing layer and produces an output species if their concentrations differ noticeably. The layer produces an activation map that detects sudden bifurcation in the Turing pattern with respect to the chemical strength.

The next layer, the pooling layer, smooths the concentrations of the convolution layers to produce spatially-uniform species. In other words, the smoothing layer compresses spatial information into a finite-dimensional vector - a signature of the geometry in which the swarm evolves. The last layer performs pattern recognition and classifies the shape of the reactor. In this paper, we have not implemented the pooling and classification layer, although we are confident that classification schemes issued from DNA computing might prove useful [7].

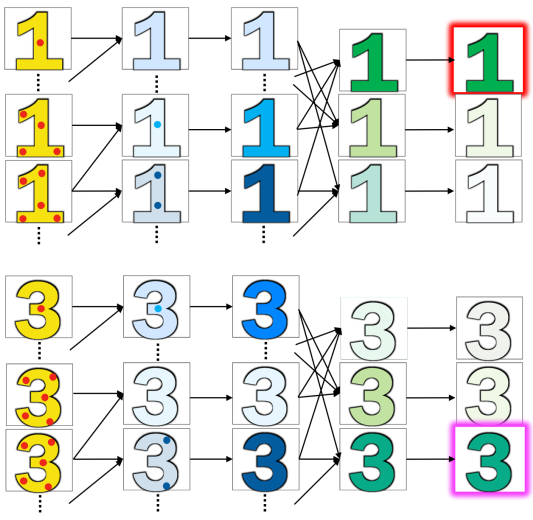


Fig. 2 Schematics of the recognition process for two geometries of reactor

2. MODELLING

We consider a swarm whose agents emulate chemical reactions and diffusion. We work in the limit of continuous space and time, treating the agents as molecules that randomly diffuse, collide and react, or bounce off the walls of the reactor Ω. The goal is to prescribe rules to the swarm so that at the steady state, emerges a species in the swarm that classifies the shape of the reactor.

Agents in layer at the bottom, the Turing layer, adopt one of three following states: reserve state (noted R), activator state (U_i), and inhibitor state (V_i). We assume that the number of agents in the reserve state is so large that it effectively acts as a reservoir for the swarm. We denote by $u_i(x,t)$ the density of U_i states at point $x \in \Omega$ and time t (and similarly for $v_i(x,t)$ and V_i).

The rules of the Turing layer are described in Figure 3. Briefly, agents in the U_i and V_i states are produced at a constant rate from the reservoir. Agents in the V_i state also decay to the reservoir at a constant rate. Lastly, when two U_i agents and one V_i agent are close to each other, the V_i agent is switched to a U_i agent. A pair u_i and v_i in the Turing layer is modelled with a Schnakenberg reaction-diffusion PDE, with no flux on the boundary (Neumann condition):

$$\begin{array}{rcl} \frac{\partial u_i}{\partial t} & = & \gamma_i(a - u_i + u_i^2 v_i) + d_u \Delta u_i, \\ \frac{\partial v_i}{\partial t} & = & \gamma_i(b - u_i^2 v_i) + d_v \Delta v_i, \\ \frac{\partial u_i}{\partial \mathbf{n}} & = & 0, \text{on } \partial\Omega \\ \frac{\partial v_i}{\partial \mathbf{n}} & = & 0, \text{on } \partial\Omega \end{array} \qquad (1)$$

where γ_i is a scaling parameter setting the strength of the chemistry for the node i, a and b are constants setting the conversion rate of agents from the reservoir to U_i or V_i. The diffusion coefficients of U_i and V_i are d_u and d_v respectively.We note that the existence of Turing patterns famously requires that $d_v >> d_u$.

Each γ_i gives rise to a specific steady state for u_i(a Turing pattern), typically consisting of a number of discrete spots of similar sizes that repel each other. As γ increases, the number of spot grows discretely, starting with no spot for $\gamma = 0$ (pure diffusion), and incrementing for specific values of $\gamma = 0$ that depend on the precise

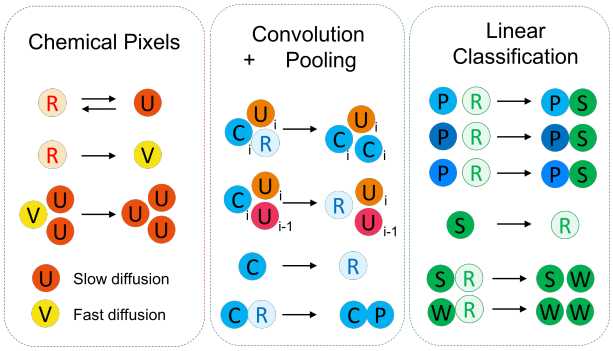


Fig. 3 Chemical reactivity rules. In this paper, we implement the chemical pixels and the convolution layer.

geometry of the reactor Ω. This set forms a signature of the reactor Ω which we will use to infer its shape.

The convolution layer locally compares the density of u_i and u_{i+1}, detecting appearance of spots between the Turing patterns for γ_i and γ_{i+1}. The dynamic of the convolution layer is modelled by the following PDE

$$\begin{array}{rcl} \frac{\partial c_i}{\partial t} & = & c_i u_{i+1}/(K_m + u_i + c_i) - c_i + d_c \Delta c_i \\ \frac{\partial c_i}{\partial \mathbf{n}} & = & 0, \text{on } \partial\Omega \end{array} \quad (2)$$

The first term is a first-order Michaelis-Menten production rate, stating that c_i is an auto-catalyst promoted by u_{i+1} and repressed by u_i. To see how this layer performs a comparison, let us temporarily omit diffusion and solve the steady state for c_i (since the layers are feed-forward, the steady states of u_{i+1} and u_i are independent of that of c_i):

$$u_{i+1}/(K_m + u_i + c_i) = 1 \quad (3)$$

which is solved by

$$c_i = max(u_{i+1} - u_i - K_m, 0) \quad (4)$$

The positive part ensures that the concentration is not negative. If the Turing pattern u_i associated with γ_i, and the Turing pattern u_{i+1} associated with γ_{i+1} are similar to each other, ($u_i \approx u_{i+1}$, no new spot has appeared), then c_i decays to 0. On the other side, if a new spot does appear when going from γ_i to γ_{i+1}, then this region becomes a local source of c_i because locally $u_{i+1} > u_i$, resulting in non-null steady state.

3. RESULTS

As a proof of principle, we investigate a simple network comprising only two Turing nodes and a convolution node. As a geometrical benchmark, we use digit-shaped reactors, (handwritten digits were historically the first images on which neural networks were trained).

We solve the PDE with an in-house FEM solver written in Mathematica. Briefly we discretize equations 1 and 2, turning the system into a matrix differential equation, which we solve with an explicit Euler method. The swarm is initially confined in a small square area at the top of the reactor, and allowed to evolve at time $t = 0$.

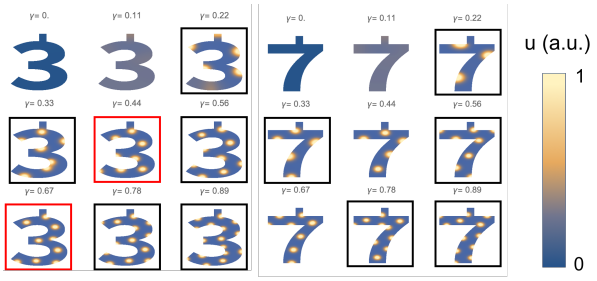


Fig. 4 FEM simulations of the Turing for two geometries and various chemical strength γ patterns.Color bars are in arbitrary units of density

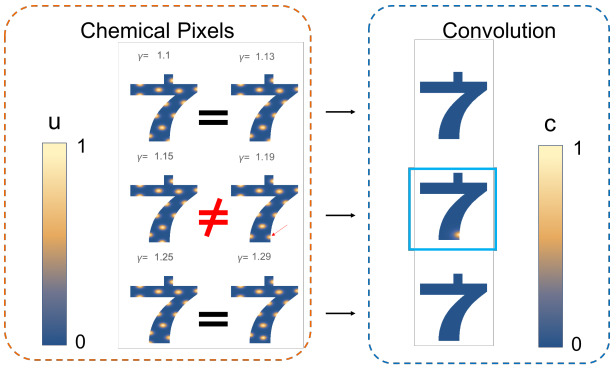


Fig. 5 FEM simulations of steady states for pairs of Turing nodes with close chemical strength γ (plotting u in each Turing node) and the corresponding convolution layer. Color bars are in arbitrary units of density

We first sought to visualize the dependence of the Turing patterns on the geometry of the reactor. Figure 2 shows for two geometries the steady state of u for a Turing node whose chemical strength γ varies from 0 to 0.89. The number of spots, and the chemical strength for which they appear, depend intimately on the geometry of the reactor.

We next verified that the convolution layer can detect local changes in steady state of u_{i+1} and u_i. Figure 5 shows the steady state of u for pairs of chemical pixels with similar γ. As expected, the convolution node is non-null only when the Turing pattern changes suddenly (bifurcates) with the chemical strength, (here with γ going from 1.15 to 1.19).

4. CONCLUSION

We proposed a swarm architecture for sensing the geometry of an environment based on Turing patterns. Preliminary PDE simulations of the first two layers indicate that distinct geometries can be sensed. But further work is be needed to explore and concretize this idea. First, full networks comprising the full typology of layers (chemical pixels layer, convolution layer, pooling layer and classification) should be simulated, with a larger variety of geometries. In order to address the heavy computational load of these simulations, parallel computing approaches based on GPUs should be considered. Secondly, we approximated the swarm in the continuum limits, using PDE inspired from chemical reaction-diffusion and essentially considering the agent as point-like. More realistic simulations modelling swarm as discrete and solid agents will be needed to assess the relevance in real world situations.

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