Dynamic modulation of boundary conditions

A new method for steering the self-organization of complex media

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Guided self-organization (GSO) is about manipulating the natural dynamics of a system so that it performs some desired function. Developing and investigating a GSO system involves two primary efforts. The first is to select the system that is to be guided. The second is to identify manipulations that can be applied to that system to cause it to perform in the desired way.

In the field of unconventional chemical computing, researchers have experimented with a variety biochemical systems, including enzyme reaction networks (Okamoto, 1992; Okamoto, Sakai, & Hayashi, 1987), gene-regulatory networks (Bradley, Buck, & Wang, 2016; Hasty, McMillen, & Collins, 2002; B. Wang, Kitney, Joly, & Buck, 2011), peptide-based computing (Ashkenasy, Dadon, Alesebi, Wagner, & Ashkenasy, 2011) and DNA-computing (Paun, Rozenberg, & Salomaa, 2005); and abiotic chemistry, including Belousov–Zhabotinsky oscillators (Dueñas-Díez & Pérez-Mercader, 2021; A. Wang et al., 2016), the bistable iodate–arsenous acid reaction (Laplante, Pemberton, Hjelmfelt, & Ross, 1995). The goal in this work is generally to identify manipulations of these chemical systems that cause them to perform logical operations such as OR, AND, NAND, etc.

A variety of techniques for guiding these systems have also been explored. These manipulations can generally be cast as 'boundary conditions,' i. e., artificial and fixed contexts in which the chemical medium operates. Boundary conditions affect the dynamics of chemical medium, and when the right boundary conditions are identified, the chemical medium performs in the desired way.

This use of boundary conditions is perhaps most clearly exemplified in work that uses spatial boundaries—i. e. the shape of the glass container in which the chemical medium sits—to sculpt the trajectories and shapes of waves that propagate through the excitable medium, and is done so in a way that causes the waves to interact in patterns of constructive and destructive interference that are analogous to logical operations—see e. g., (Lacy Costello, Adamatzky, Jahan, & Zhang, 2011).

Spatial boundary conditions are not the only kind. Other, non-spatial boundary conditions—e. g., temperature, pH, redox state, lighting level, electrical conditions, reactants present or absent, steadily added etc.—are equally influential and that can be leveraged as part of the steering process.

Now we come to a key point: the boundary conditions in these research projects and other efforts in guided self-organization are generally static. The glass containers in the example above do not change shape as the system evolves and other boundary conditions (acidity, temperature, etc.) similarly are generally kept fixed as the chemical computers perform their computations.

There are good reasons for keeping boundary conditions static. In particular, it simplifies the already very complicated systems that are being manipulated or studied, facilitating analysis and engineering. On the other hand, working only with static boundary conditions is limiting. A much wider range of manipulations (infinitely larger in fact!) becomes available when we consider the possibility that the boundary conditions can themselves be varied as a function of time.

In published work, we have demonstrated of the feasibility and power of employing dynamic boundary conditions. In this work, we use dynamic boundary conditions to transform the simulated cubic autocatalytic reaction diffusion system (Gray & Scott, 1985; Muñuzuri

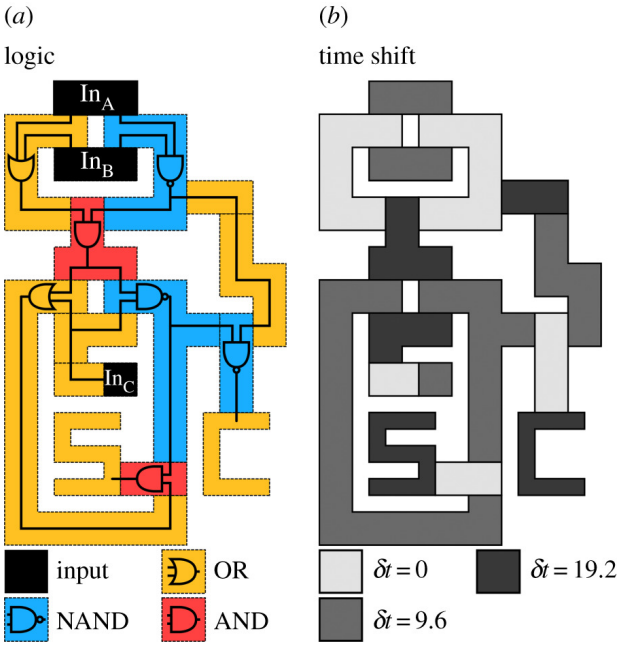

Figure 1: A contiguous and initially homogenous chemical medium is transformed by spatio-temporal modulation of boundary conditions into 7 logic-gates (plus connecting 'wires') that act as a full adder. Three binary inputs (black areas in left plot) are combined to produce the sum (S-shaped area) and carry (C-shaped area) values of their addition.

& Pérez-Mercader, 2022; Pearson, 1993; Sel'kov, 1968) into computational machinery.

This system involves an autocatalytic reaction, where autocatalyst V transforms a 'food' reactant, U into more of itself. This reaction is considered to be distributed in space and the reactants diffuse through this space. These processes are described by the following equations:

$$\frac{\partial U}{\partial t} = D_u \nabla^2 U - r_u U - \lambda U V^2 + F_u(x,t) \quad (1)$$

$$\frac{\partial V}{\partial t} = D_v \nabla^2 V - r_v V + \lambda U V^2 + F_v(x,t) \quad (2)$$

where the first term of each equation describes diffusion; the middle two terms describe the impact of the chemical reaction $U + 2V \rightarrow 3V$; and the final term describes the addition of the reactant, which varies as a function of position (x) and time (t) in ways that I shall describe in my talk.

In the first publication, we use the technique to transform a well-stirred chemical system into a single logic gate (Egbert, Gagnon, & Pérez-Mercader, 2018), and in the second (Egbert, Gagnon, & Pérez-Mercader, 2019) we use spatio-temporal modulation of boundary conditions to transform a contiguous and initially homogeneous simulated chemical system into a network of seven logic gates—a combination of OR, AND and NAND gates—that act, all together, as a full adder (i. e. they add together three binary digits—see Figure 1).

The way that the binary values 0 and 1 are represented is the same for the input as it is for the output, meaning that the method is, in theory, extensible to cause the reaction diffusion system to act as a computer of arbitrary complexity, though propagation of information through the system is limited by the rate of diffusion, and as the computer becomes more complex it will become slower. In any case, the goal of this work is not so much to produce a useful alternative computational device as much as to demonstrate the possibility of substantially altering the 'natural' dynamics of system by dynamically modulating the conditions in which that system operates.

It is also important to emphasize that our modulation of boundary conditions is independent of the input. Put another way: the computation is accomplished by the (manipulated) chemical medium and not by our manipulations of it. In my talk, I will explain what I mean by this. I will also provide details of the technique and how the solution that we identified operates. It is my hope that this will prompt discussion about (i) how these methods could be applied in other contexts, in ways that might cause other complex media to perform in other interesting ways; and (ii) how similar forms of (spatio-)temporal modulations of boundary conditions might be employed by biological systems, for example in morphogenesis or in the production of adaptive behaviour.

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