Chemical computation in arrays of relaxation oscillators coupled via mutual inhibition

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It is well known that computational simulations can provide insight into, and are in turn constrained by, physical principles that underlie the laws of nature. This synergetic relationship is especially salient in the context of dynamical systems, wherein the processes in question can essentially be thought of as computations that iteratively transform input to output states. Thus, the generation of spatiotemporal patterns in such systems can in principle be related to computational processes [1]. Most notable in this regard are cellular automata which evolve in discrete space and time, facilitating an intuitive connection with existing abstract models of computation. A property of certain classes of cellular automata that has been connected with their capability for universal computation is the existence of coherent propagating structures, such as "gliders" [2]. Intriguingly, similar structures have been reported in spatially extended arrays of diffusively coupled relaxation oscillators [3], including propagating phase discontinuities (or "defects") that are visually analogous to gliders. This suggests the possibility that interactions between defects could be used for computation.

In this work, we introduce two paradigms for implementing computation using local perturbations on the collective dynamics of a model system of coupled relaxation oscillators. As the model system under consideration has close connections to the experimental setup for microfluidic chemical oscillators, the principles we have presented here could potentially be used for constructing chemical logic gates [5]. The approach presented here differs from previous attempts at using chemical systems for computation (see for example [6, 7]) in that oscillations in the active species plays a fundamental role in enabling computation.

To describe the collective dynamics of the oscillatory chemical system, we consider a ring of N oscillators coupled diffusively coupled through their inhibitory components. Following [3] the local dynamics of individual oscillators are all identical, and described by the generic FitzHugh-Nagumo (FHN) model - a phenomenological representation of the mechanism underlying periodic activity in many chemical and biological systems [4]. This model comprises dynamical variables u_i and v_i that respectively correspond to the fast activation and slow inactivation process in node i, and which evolve as

$$\begin{aligned} \partial u_i/\partial t &= u_i(1-u_i)(u_i-\alpha) - v_i \,, \\ \partial v_i/\partial t &= \epsilon\,(ku_i - v_i - b) + D_v(v_{i+1} + v_{i-1} - 2v_i) \,, \end{aligned}$$

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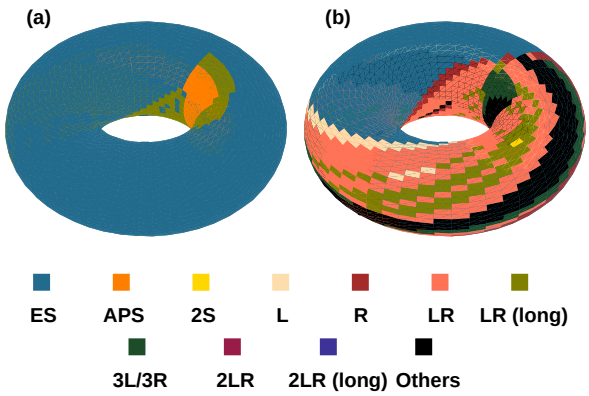

Figure 1: Perturbation response ($\phi_i - \phi_p$) diagrams (represented on a 2-D torus) for a ring of $N = 20$ oscillators, initially in an ES state, diffusively coupled to their nearest neighbors via the inactivation variable v. As indicated in the color scheme shown below the panels, a wide range of defect patterns arise. The phases ϕ_i and ϕ_p correspond to the two axes of the toroid. The perturbation schemes used to represent these figures are (a) $1010\ldots$ and (b) $101111\ldots$. In these simulations each oscillator is assumed to be identical, and is described by the parameter values $\epsilon = 0.001$, $k = 0.6$, $b = 0.1$ and $\alpha = 0.139$. Adjacent oscillators are coupled diffusively with strength $D_v = 1.13 \times 10^3$.

where $\alpha = 0.139$, $k = 0.6$ describe the kinetics, $\epsilon = 0.001$ characterizes the recovery rate, b modulates the asymmetry of the oscillator and the diffusion coefficient D_v represents the strength of coupling between the v components of adjacent nodes.

This system exhibits a wide range of complex spatiotemporal patterns including "phase defects" characterized by one or more discontinuities of phase moving against a background of synchronized oscillations, and Spatially Patterned Oscillator Death (SPOD) where the oscillators are arrested in different stationary states. We first utilize the phase defect pattern to implement a form of computation. Specifically, this involves resetting the initial phase (ϕ_i) of selected oscillators in a ring of exactly synchronized (ES) nodes to another phase (ϕ_p). The choice of nodes to perturb can be thought of as a binary string that acts as the input for computation. Depending on the choices of ϕ_i, ϕ_p and input string, a wide range of defect patterns can be obtained for a given choice of b and D_v.

Using this phenomenology, a possible principle for

computation can be realized by applying perturbations to selected oscillators. In particular, we investigate the implementation of a two-input logic gate by perturbing a pair of elements that are initially in phase ϕ_i to phases ϕ_{p1} and ϕ_{p2}, respectively. Interpreting low and high values of ϕ_{p1} and ϕ_{p2} as 0 and 1, respectively, any combination of two binary inputs can be implemented. If we consider the output to represent 1 if the state of the system after perturbation is different from ES, and 0 if it remains ES, we observe that certain schemes correspond to NAND logic. That is, only the case where both ϕ_{p1} and ϕ_{p2} are in a high state result in a low state of the output (analogous to a NAND gate which only gives an output of 0 if both inputs are 1).

Our results suggest the intriguing possibility that spatiotemporal patterns in relaxation oscillators could be used for implementing computation. As NAND gates are considered to be universal gates, our demonstration of NAND logic is of particular interest. However, as this implementation implicitly involves phase detection, it is preferable to have a scheme that requires minimal information overhead.

To this end, we present a potential technique for chemical computation that involves perturbations to the SPOD state seen at high diffusion. Here, a perturbation is provided for a brief duration to a chosen set of oscillators in a 1-D array that are initially in the SPOD state. As the input state is temporally invariant it can, for a suitable threshold, be represented as a binary string (where 0 and 1 correspond to the low and high states), and similarly each perturbed oscillator could be assigned a binary value. Furthermore, as the resultant state is also a SPOD for high enough D_v, the output can also be thought of as a binary string. Hence, a perturbation to this system can be interpreted as an implementation of a specific logic gate or a combination of gates in the neighborhood of the stimulated oscillators.

While NAND logic is yet to be demonstrated in the latter scheme, this framework is a potentially rich theoretical testbed for exploring how chemical oscillators can be utilized to develop logic gates. Indeed, the generic nature of our model implies that both schemes could be tested experimentally, for instance using light-sensitive chemical systems [8]. It is particularly notable that the above may provide an intriguing link between the two enduring legacies of Alan M. Turing, namely pattern formation in reaction-diffusion systems and universal computation.

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