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Actin quantum automata: Communication and computation in molecular networks

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ABSTRACT

Actin is filament-forming protein forming a communication and information processing cytoskeletal network of eukaryotic cells. Actin filaments play a key role in developing synaptic structure, memory and leaning of animals and humans; many psychiatric and neurological disorders are due to disfunction in the assembly of actin fibres. This is why it is important to develop abstractions of the information processing on the actin filaments. We model actin filaments as two chains of one-dimensional quantum automata arrays to describe hypothetical signalling events propagating along the chains. We study in detail several functions of automaton state transitions and compute examples of evolution to illustrate behaviour of the functions and a role of the superposition of the initial states. We uncover and analyse localisations, or particles, propagating along the actin chains. We demonstrate that logical gates can be realised in the result of the collisions. Using collisions between the travelling particles we implement binary adder.

1. Introduction

Two key components of a cytoskeleton—actin double helix (micro)filaments and tubule microtubule protofilaments. They are responsible for keeping a cell shape and implementing the cell's motility but also they play a role of the cell's nervous system: together with extracellular matrix [1] the intracellular networks of proteins process information and implement learning [2–10]. By modulating dendritic ion channel activity actin filaments determine rule of neural information processing and facilitate computational abilities of dendritic trees via facilitation of ionic condensation and ion cloud propagation [11]. Psychiatric and neurological disorders are caused by disfunctions in actin assembly or the actin association with other proteins and intracellular components [12–17].

Computational models tubule microtubules have been developed in 1990s and used to demonstrate that computation could be implemented in tubulin protofilaments by classical and quantum means [3,18–20]. Less attention was paid to actin double helix filaments, despite importance of the actin in learning and information pre-processing as might be hinted by pre-dominant presence of actin networks in synapses [21–24]. In our previous paper [25] we proposed a model of actin filaments as two chains of one-dimensional binary-state semi-totalistic automaton arrays to hypothetical signalling events. We analyse the complete rule space of actin automata using integral characteristics of space–time configurations generated by these rules and compute state transition rules that support travelling and mobile localisations. We found that some properties of actin automata rules may be predicted using Shannon entropy, activity and incoherence of excitation between the polymer chains. We also show that it is possible to infer whether a given rule supports travelling or stationary localisations by looking at ratios of excited neighbours that are essential for generation of the localisations. In the

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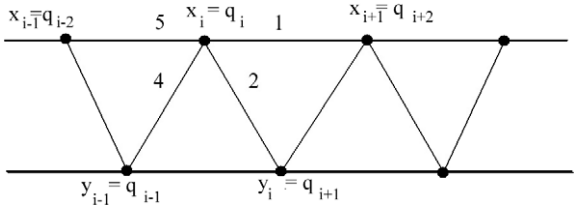

Fig. 1. A scheme of quantum actin automata.

present work we continue the line of investigation, using a quantum cellular automaton (QCA).

The actin double helix is an attractive candidate system for describing how data is processed and transmitted within a cell. Exact mechanisms for many of these processes have yet to be fully understood. We propose that a computation is implemented when localisations (defects, conformational changes, ionic clouds, solitons) representing data collide with each other and undergo state changes. Assuming that values of the computer variables are encoded in states of the localisations we come to the concept of collision-based computing [26–29]. The potential or ionic waves [30] or quantum protein transitions [20,31] might play roles of signal passing through the proteins and branches of the cytoskeletal network, colliding, changing their velocities or states, and thus performing Boolean logical operations [26].

Our aim is to show the computational power of the quantum automaton, without describing a detailed physical or chemical mechanism that could realise it in actin. Our basic hypothesis is that the 'hardware' is made of two layers of cells, whose internal state is influenced by four adjacent cells (Fig. 1). Although circuital models of actin have been proposed, where electrical pulses could be identified with signals [30], in the present work we will consider signals without making any specific hypotheses on their nature. We suppose that they can travel left to right and vice versa along each layer of the filament and between the two layers. Accordingly, we factor the state of each cell in five substates, one representing the specific excitation of the cell, the others the four pulses that can arrive from the neighbouring cells. The same model could be employed to deal with other systems, like e.g. kinks in zig-zag configurations of ion traps (see e.g. [32]).

2. Quantum cellular automata

In quantum cellular automata (QCA) cell states are represented by qubits or cubits, instead of classical bits. Several formal definitions have been proposed, see e.g. [33–35], and also methods to translate classical automata into quantum ones can be found in [36,37]. However, it is often difficult to check if a specific candidate system fulfils all the requirements to be a QCA; also the simulation of the evolution of a QCA is in general a complex task.

We start our discussion with two classical definitions of one dimensional QCA, 1QCA, due to Watrous [38,39,33].

Definition 1. A 1QCA $\mathcal{A} = \langle Q, \lambda, N, \delta \rangle$ is determined by a finite set Q of states, a *quiescent state* λ, a neighbourhood $N = \{n_1, \ldots, n_r\} \subseteq Z$, with $n_1 < n_2 < \cdots < n_r$ and a local transition function

$$\delta : Q^{r+1} \to C_{[0,1]} \tag{1}$$

satisfying the following three conditions:
(1) local probability: for any $(q_1, \ldots, q_r) \in Q^r$,

$$\sum_{q \in Q} |\delta(q_1, \ldots, q_r, q)|^2 = 1 \tag{2}$$

(2) stability of the quiescent state: if $q \in Q$, then

$$\delta(\lambda, \ldots, \lambda, q) = 1 \quad \text{if } q = \lambda, 0 \text{ otherwise.} \tag{3}$$

To state the third condition we have to introduce the automaton's mapping.

A configuration $c : Z \to Q$ is a mapping such that $c(i) \neq \lambda$ only for finitely many i. Let $C(\mathcal{A})$ denote the set of all configurations. Computation of $\mathcal{A}$ is done in the space $H_{\mathcal{A}} = l_2(C(\mathcal{A}))$ with the basis $\{|c\rangle \mid c \in C(\mathcal{A})\}$.

In one step, $\mathcal{A}$ transfers from one basis state $|c_1\rangle$ to another $|c_2\rangle$ with the amplitude

$$\alpha(c_1, c_2) = \prod_{i \in Z} \delta(c_1(i + n_1), \ldots, c_1(i + n_r), c_2(i)). \tag{4}$$

A state in $H_{\mathcal{A}}$, in general, has the form

$$|\phi\rangle = \sum_{c \in C(\mathcal{A})} \alpha_c |c\rangle \tag{5}$$

with normalised α_c. The evolution operator $E_{\mathcal{A}}$ of $\mathcal{A}$ maps any state $|\phi\rangle$ into $|\psi\rangle = E_{\mathcal{A}}|\phi\rangle$ such that

$$|\psi\rangle = E_{\mathcal{A}}|\phi\rangle = \sum_{c \in C(\mathcal{A})} \beta_c |c\rangle \tag{6}$$

where

$$\beta_c = \sum_{c' \in C(\mathcal{A})} \alpha_{c'} \alpha(c', c). \tag{7}$$

Now we can state the third condition:
(3) unitarity: the mapping $E_{\mathcal{A}}$ must be unitary.

In general, to decide whether the unitarity condition is satisfied is a nontrivial problem [40–42]. Partitioned quantum one-dimensional cellular automata, that are well suited to represent our cells and their states, are easier to deal with.

Definition 2. A partitioned quantum one-dimensional cellular automaton (P1QCA) is a 1QCA $\mathcal{A} = \langle Q, \lambda, N, \delta \rangle$ that satisfies the following conditions:

(1p) The set of states Q is the cartesian product $Q = Q_1 \times \cdots \times Q_r$ of $r = |N|$ nonempty sets.

(2p) The local transition function δ is the composition of two functions:

$$\delta_c : Q^r \to Q \quad \textit{a classical mapping} \tag{8}$$

$$\delta_q : Q \to C^Q \quad \textit{a quantum mapping} \tag{9}$$

where

$$\delta_c((q_{1,1}, \ldots, q_{1,r}), \ldots, (q_{r,1}, \ldots, q_{r,r})) = (q_{r,1}, q_{r-1,2} \ldots, q_{1,r}). \tag{10}$$

The function δ_q defines a 1QCA with operator

$$U_{\mathcal{A}_q}(q_2, q_1) = [\delta_q(q_1)](q_2). \tag{11}$$