

Biomolecular Computation Based on Cell Communication

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ABSTRACT

In this paper, based on the signaling mechanism of phosphorylation and dephosphorylation, we have designed rewriting rules for graph automata by related pathways in kinase computing for 3-SAT problem solving in which linear complexity of control-space and time is derived to achieve efficiency in theory. This work is important for pathway design of autonomous kinase computation that has biological faithfulness.

Keywords: Bio-molecular computation; signaling pathways; automata

1. INTRODUCTION

In order to explore a new approach to autonomous kinase computing [1,2] in which cell-based computing processes are carried out by signaling pathways, graph rewriting for related automata is constructed by using interactions of term rewriting, string rewriting and hypergraphs, and the signaling pathways of phosphorylation and dephosphorylation regulated by kinases and phosphatases under the activation of Rho family GTPases are employed to design computing units.

2. RELATED WORK

In the field of cell-based computation, much progress has been reported, e.g., L. Landweber and L. Kari have proposed a molecular computing method based on a gene mechanism of evolution in a bacterium mechanism of ciliates and proved that it is capable of universal computation [3]. A. Ehrenfeucht et al. [4] have worked out a rigorous computation model of micronuclear genes in ciliate. R. Weiss and T. Knight have initiated amorphous computing [5]. G. Păun has originated a new branch of theoretical molecular computation that is called P-systems or “membrane computing” [6]. The work in [7] is an example of other types of cell-based computation. Furthermore, a Turing universal model based on chemical kinetics by M. O. Magansco is an important work on cell-based computing [8]. Another example is cell-based molecular systems [9], where cell-cell signaling mechanisms are used as key communication mechanisms. These successful works have shown the merits of cell-based computation on the adaptive

mechanism of inspired biologically information processing.

In this paper, we note that the signaling mechanism of cells is adaptive under the condition that related pathways are activated by certain functional enzymes. According to the adaptive regulation mechanism of signaling pathways in cells, we are studying proper control schemes in order to use engineered pathways of cells for the purpose of molecular computing.

3. DESIGNING GRAPH AUTOMATA BY INTERACTIONS OF PATHWAYS

Considering the constraint of a 3-SAT problem under the condition of $\{clause_1=[X_1 \vee X_2 \vee X_3], clause_2=[X_1 \vee X_2 \vee \neg X_4]\}$, the graph rewriting process of kinase computing for solving this problem can be constructed by graph automata represented in logic forms as shown in Fig. 1-3. In Fig. 1, **input-reactant [n]* refers to the initial state of n variables. At moment *t*, the input is *candidate-reactant [n × 1](t)* except for initial moment when it is **input-reactant [n]*. The index *l* is used for labeling status of molecular mixtures, *kinase [k × m]* refers to kinases, the index having a maximum of *k* is used for the kinases and the index having a maximum of *m* refers to the related clause. At moment $(t+1)$, the input is *candidate-reactant [n × 1](t+1)*. Figure 2 shows the operators for *clause₁* and *clause₂*. Fig. 3 shows the rewriting process for *clause₁* from initial state to the state at the next moment that gives out the candidate solution satisfying the condition “*x_l*” of *clause₁*. The molecule *L* refers to the labeling molecule. The straight line on the molecular mixture means that this molecular mixture cannot be produced by the related pathway. The left part away from the pathway in the graph is defined as the “activated” state, and the right part is the “operated” state. Signaling molecules such as *x₂**, *x₃**, *x₄** mean that they will take the true value or false value. The hypergraph, pathway structure and temporal updating of the states of the graph automata are integrated into an interacted architecture of parallel computing, systematically.

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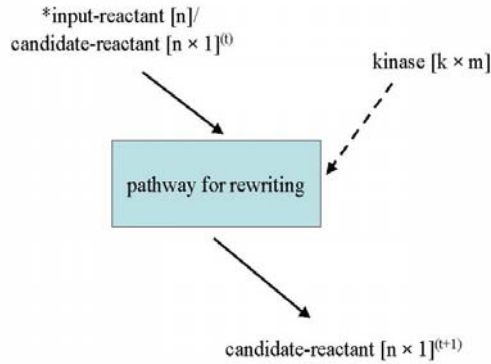


Fig. 1 A general form of rewriting in one step

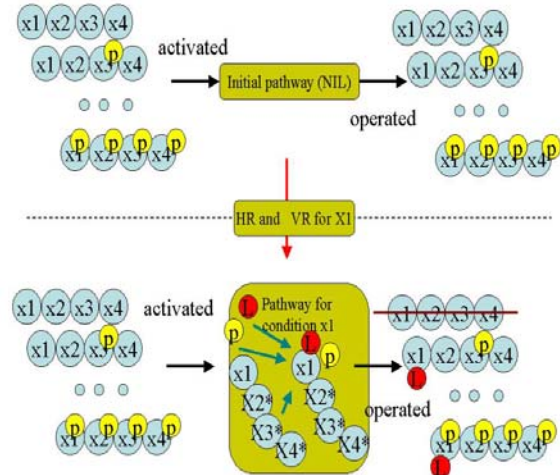


Fig. 3 Example of the rewriting process from the initial state to the state of running the pathway encoded for clause₁

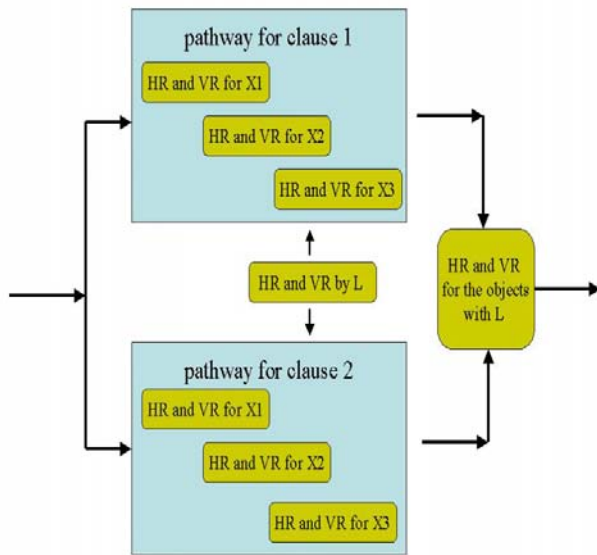


Fig. 2 Operators for pathways

4. CONCLUSION

Through the interactions of signaling pathways, we have designed the basic mechanism of kinase computing. The rewriting rules for graph automata in kinase computing systems are helpful for logic programming that is oriented toward building a scalable molecular computer using cells and developing its applications in bioinformatics and biomedical engineering.

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