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蛋白質配列のメカニズムによる並列計算プロトタイプ

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あらまし

分子計算において，新しい代数学的な表現方法を提案し，並列計算の問題に対して一定的な優れた性能を示す。

キーワード：分子計算，分子工学，分子エレクトロニクス

Extending Proteomic Computing to a Parallel Prototype

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Abstract -- This paper proposes a novel approach to proteomic computing based on algebraic representation. And simulation and discussion are made to show its performance in a parallel framework.
Keywords: Molecular Computing, Moleware Engineering, Molecular Electronics.

1. Proteomic Computing

Artificial chemistry [1,2] and signal transduction in cell biology [3] have given us enough enlightenment for constructing the robustness mechanism in "proteomic computing". These merits make it possible for us to explore an available way to build fault-tolerant prototypes for molecular computation. The proteomic computing can be represented as the following five major forms:

(1) ODE and analog algorithmic chemistry as described in [4].

(2) Non-linear dynamics (procedural model):

$$\dot{X} = f\ (X, t)$$

where X is defined as the state vector that corresponds to the set of dynamically updated variables (i.e. the chemical materials). Notice that here it is made by stochastic calculus (Ito-Calculus).

(3) "ALife"/cybernetics algorithms:

The population is defined as the set of X and selection rules are exerted on it.

(4) Abstract machine (from words to "robust" codes):

For alphabet $A = \{x_0, x_1, .. x_n\}$, the word set W is made through the graph rewriting system with representation by L_1 and L_2, where corresponding language sets L_1 and L_2 represent the context-sensitive and context-free, respectively.

(5) Graph rewriting system and sub-classes related to context-free languages.

Notice that modeling and errors-reduction are necessary in the processes concerned.

2. Parallel-Composition for Kinase Computing Systems

For a parallel structure, we limit our discussion within the domain of "kinase computing" [4], which is defined as the adaptively self-adjusting (e.g. self-catalysis) mechanism for pathways embedded in the interactions of biochemical reactions within the inter/intra cell communication, where metabolism is carried out in the processes mentioned above. The kinase computational units consist of the following parts:

(1) Interactions of dynamical pathways by graph rewriting systems.

(2) Operation by rewriting with morphisms.

(3) Inferring by context-free sets.

(4) The feasible of encoding schemes.

Briefly speaking, a prototype [4] is made for a parallel structure where different sets reflect corresponding (different) classes of PE and "autonomous" controlling procedures assigned for them.

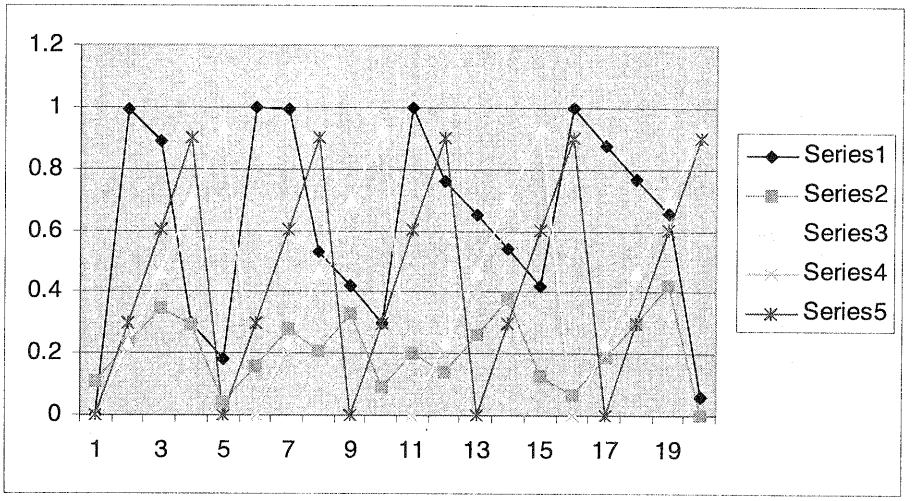

Fig. 1 (a) Activity vs. time

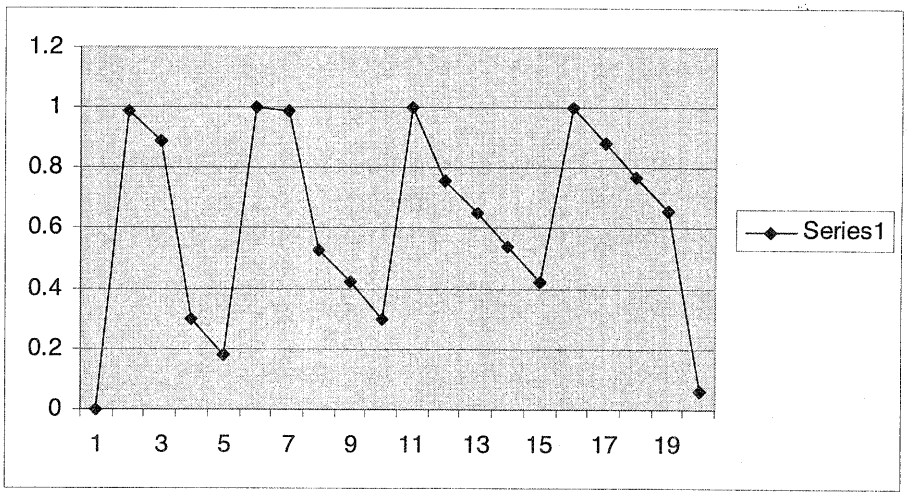

Fig.1 (b) Activity vs. time

3. Discussion

Fig. 1 (a) and (b) show the simulation results. Series 1 represents the normal curve. Series 2~5 represent those in the abnormal situation, but the units concerned have been kept "living" in the meaning of artificial life.

About our efforts toward a systematic theory of molecular computation, open problems remained as follows:

(1) The interactions in kinase computing cause some processes that are undecidable.

(2) The upper bound of the computability of kinase computing if they are provable.

(3) A systematic representation for formalization of the high-dimensional pathways in kinase computing.

Our future (further) works are concentrated on exploring the formal language theory for molecular computing based on the following direction:

genomic information -> words -> codes -> languages and automata
-> robust codes -> ...

we hope that this will lead us to a deeply-and-concentrated understanding of molecular computation through algebraic theory.

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References

[1] Peter Dittrich, Artificial Chemistries, Tutorial held at ECAL'99 (European Conference on Artificial Life, 13-17 September1999,Lausanne,CH), http://ls11-www.informatik.unidortmund.de/achem/tutorialAChemECAL99-normal.ps.gz.

[2] Peter Dittrich, Personal Communication, September, 2000.

[3] K. Kaibuchi, S. Kuroda and M. Amano, Regulation of the cytoskeleton and cell adhesion by the Rho family CTPases in mammalian cells, Annu.Rev.Biochem. 68, 1999; 459-486.

[4]Jian-Qin Liu and Katsunori Shimohara, Proteomic Computing: Theory and Practice, ATR Technical Report, 2001.