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Artificial Biochemistry

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Abstract

Chemical and biochemical systems are presented as collectives of interacting stochastic automata: each automaton represents a molecule that undergoes state transitions. This framework constitutes an *artificial biochemistry*, where automata interact by the equivalent of the law of mass action. We analyze several example systems and networks, both by stochastic simulation and by ordinary differential equations.

1 Stochastic Automata Collectives

This paper is an empirical investigation of an *artificial biochemistry* obtained by the interactions of stochastic automata. The study of such artificial frameworks has been advocated before [2]; we explore a modern version based on a theory of concurrent processes that obeys the equivalent of the law of mass action. Foundations for this work have been investigated elsewhere [1]; here we aim to give a self-contained and accessible presentation of the framework, and to explore by means of examples the richness of "emergent" and unexpected behavior that can be represented by combinations of simple building blocks.

By a *collective* we mean a *large set* of *interacting*, *finite state* automata. This is not quite the situation we have in classical automata theory, because we are interested in the behavior of a large set of automata acting together. It is also not quite the situation with cellular automata, because our automata are interacting, but not necessarily on a regular grid. It is also not quite the situation in process algebra, because again we are interested in the behavior of collectives, not of individuals. Similar frameworks have been investigated under the headings of collectives [12], sometimes including stochasticity [6].

By *stochastic* we mean that automata interactions have rates. Stochastic rates induce a quantitative semantics for the behavior of collectives. Collective behavior cannot be considered quite discrete, because it can be the result of hundreds or thousands individual contributions. But it is not quite continuous either, because of the possibility of non-trivial stochastic effects. And it is also not hybrid: there is no switching between discrete and continuous regimes.

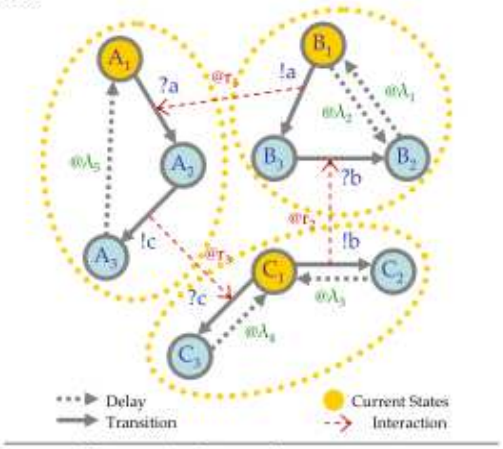

Figure 1 Interacting automata

Stochastic collectives are inspired by biochemical systems, which are large sets of interacting molecules/proteins, whose stochasticity ultimately derives from Brownian motion. An underlying as-

sumption, here, is that proteins can be regarded as *finite state* components that are subject to automata-like *transitions* between well-defined states. While certainly not accurate at the atomic level, this assumption is corroborated by the fact that much of the knowledge being accumulated in Systems Biology is described as state transition diagrams [5].

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