

Metabolic algorithms and signal transduction dynamical networks

Luca Bianco, Vincenzo Manca

University of Verona
Department of Computer Science
strada Le Grazie, 15
37134 Verona, Italy
E-mail: {bianco@sci., vincenzo.manca@}univr.it

Abstract

The *Group for Models of Natural Computing* (MNC group) in Verona developed *Psim*, a simulator of P systems. It's based on the implementation of the *metabolic algorithm* which is developed in Java and proves to be a cross platform application. In the first part of the talk we describe the algorithm and some details of the java simulation engine.

Then we focus our attention on the importance of *reactivity coefficients* as means to regulate the policy of rules' application and give an example of the algorithm application to the famous Belousov-Zhabotinsky reaction.

The crucial importance of reactivity coefficients in the metabolic algorithm lead us to the formulation of the *inverse oscillation problem* and we propose a strategy of resolution of this problem, based on cycling dynamics.

We conclude the discussion by outlining one of the problems we are actually facing: the simulation of *signal transduction networks*. This kind of networks describe protein-protein interactions, whose importance is crucial in the understanding of all regulating mechanisms of living cells (and in general of living organisms). From a mathematical viewpoint they turn out to be representable as graphs. Every node contains a certain amount of one actor of the regulating network (e.g. proteins, substrates, protein complexes). Arcs represent the possible set of interactions between contiguous nodes (e.g. activation, inhibition, production, degradation).

Two main kinds of investigations could be carried out on signal transduction networks: a *statical* one, whose aim is to measure some topological parameters of the network; a *dynamical* one, whose purpose is to calculate the behaviour of the system as time elapses, according to some initial conditions.

Due to the very high number of nodes and arcs constituting those networks, the development of reliable simulation tools for the investigation of their dynamic is very important (networks composed by thousands of nodes and arcs are frequent in biological interesting mechanisms).