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COMPUTER SCIENCE COLLOQUIUM

The biochemist - the unknown creature

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Abstract:

Biological cells interact with their environment, respond to stimuli and stress and have to adapt their behavior to new situations. Due to that the cell's protein profile is changing constantly. This profile represents the status a cell is in and leads to insights about mechanisms of regulation, applicable in pharmacology, clinical diagnosis, etc. 2D gel electrophoresis is a conventional technique to identify protein profiles, where proteins are separated with respect to their charge and mass. 3D gel electrophoresis is an evolving technique for protein separation which allows a very efficient high throughput, where several protein samples are separated parallelly. The outcome of this experimental process is a image stack, where vertical sections represent the individual slab gels. Now, an image processing tool is needed to isolate the samples accurately and mimic conventional 2D gels for further quantitative protein analysis. This tool has to deal with computational, physical and biological concerns which have to be taken in account, e.g. amount of data, overlaps of sections, gaps in information, curves, etc.

Artificial Chemistries are computational models for chemical processes analogous to real chemical reactions. They are described by a set of molecules and a set of reaction rules, that stands for mechanisms for creating new molecules based on the existing ones. E.g. given an abstract cascading mechanism of chemical reactions (as an autocatalytic cycle), where molecules are not or only sparsely specified, the question arises if and how such a reaction mechanism can be implemented. One approach to artificial chemistries is to see molecules as graphs and reactions as graph transformations. Can we assign rules, such that there arises a feasible chemical process? And if not, can we use the information from this failure to extend the rule set, creating a new real life chemical process? But how much information about the structure of molecules is needed to assign the rules? And is it possible to generalize even more and use the strategy of assignment not only for molecules?