Report on IWRS 2018

First International Workshop on Reaction Systems

Paolo Bottoni
Dept. of Computer Science, Sapienza University of Rome, Italy
Dirk Janssens
Dept. of Math. and Computer Science, University of Antwerp, Belgium

The First International Workshop on Reaction Systems was held in Milan, within the facilities of the Bicocca University, from 11 to 15 June. The workshop gathered researchers, mostly European, but also with participants from Japan and USA.

Reaction systems were introduced some 10 years ago by A. Ehrenfeucht and G. Rozenberg as a computation model inspired by the functioning of the living cell. It is a simple, elegant model where states represent sets of species and biochemical reactions interact in two ways: facilitation and inhibition. A striking characteristic of the approach is that (motivated by the bioenergetics of the living cell) there is no implicit preservation of entities not produced by some reaction: hence, something can be present in a successor state only if it is a product of some internal reaction using entities (reactants) present in the current state, or if it has been contributed by the external environment (the context of the system). Also, assuming the principle of the threshold nature of resources (motivated by the level of abstraction of this model), there is no counting in the model: something is either present (and in that case it participates in all the reactions in which it acts as reactant and it can forbid any reaction in which it acts as an inhibitor), or it is not. Moreover, motivated by the fact that the living cell is an open system, the dynamic processes of reaction systems are influenced by their environment. Consequently, reaction systems are a model of interactive computation.

The workshop was chaired by G. Mauri and G. Rozenberg and perfectly organised by L. Manzoni, D. Besozzi, A. Dennunzio, and C. Zandron, all from Universitá degli Studi di Milano-Bicocca. It is the first issue of what is intended to be a series: next year it will be organized by M. Koutny in Newcastle, UK. With 37 registered participants from 11 countries, it was quite successful in bringing together the small but growing group of researchers who are actively working on the topic, while also attracting people that are becoming interested in it. Noteworthy was also the fact that about one third of participants were female, a welcome departure from the usual situation in computer science.

The workshop program was a balance of established results and original research, illustrating the main tendencies in the field. Three broad lines of work can be identified:

1. exploration of the expressive power of the classical model of reaction systems;

2. extensions of the standard definition in order to model specific features;

3. comparisons with other models.

In the first day of the workshop, after a recapitulation of the standard model by G. Rozenberg, the creator of reaction systems (together with A. Ehrenfeucht), L. Manzoni and A.E. Porreca ("State Sequences of Interactive Processes of Reaction Systems") recalled basic properties of processes of reaction systems. Among others, they discussed the expressive power of minimal reaction systems and the role of the environment in limiting non-determinism. The second topic was hinted at in the reflection by R. Brijder ("Chemical Reaction Networks and Reaction Systems") on relationships with networks of chemical reactions, while M. Koutny ("Reaction Systems, Transition Systems, and Equivalences", joint work with J. Kleijn, L. Mikulski and G. Rozenberg) introduced several notions of equivalence for reaction systems and discussed forms of encoding of reaction systems into transition systems, thus opening the way to the comparison with standard notions of equivalence and bisimulation developed in the field of concurrency. The afternoon session was completed with the presentation by S. Azimi ("Open Repository for Research on Reaction Systems") of a repository of material (papers, slides, tutorials, etc,) concerning reaction systems, also intended as a platform for discussion and promotion of joint research. It can be found at `https://github.com/RS-Repo/library/issues`.

All three talks of the morning session on Tuesday were devoted to the second general topic mentioned: the relationship between reaction systems and other, more established models of biological processes. Firstly, D. Besozzi ("Biological Aspects of Reaction Systems") discussed the main biological aspects underlying the reaction system model, to then give a systematic overview of other modeling approaches, while highlighting the differences with reaction systems and finally touching upon several emergent phenomena (robustness, adaptability, redundancy) that should be visible in a successful model. Subsequently S. Azimi ("From Quantitative Models to Reaction Systems", joint work with E. Czeizler, C. Gratie, B. Iancu, S. Ivanov, C. Panchal and I. Petre) explained how her group succeeded in building in a systematic way reaction system models for biological phenomena such as the formation of intermediate filaments and the heat shock response. In the last talk, P. Milazzo ("Modeling Gene Regulatory Networks with Reaction Systems', joint work with R. Barbuti, P. Bove, R. Gori and F. Levi) proceeded by modeling gene regulatory networks in terms of Boolean networks, which can then in turn be translated into reaction systems.

The afternoon session was devoted to extensions of the basic model. In the first talk A. Labella ("Networks of Reaction Systems', joint work with P. Bottoni and G. Rozenberg), started an exploration on a possible form of structuring context, by viewing it as composed of reaction systems, organised into a graph structure. In this model, observations on a designated node show a behaviour richer than that of context-independent systems, but the overall behaviour of the network is totally determined by the initial configuration. In the second talk, J. Kleijn ("Evolving Reaction Systems", joint work with A. Ehrenfeucht, M. Koutny, and G. Rozenberg) considered reaction systems where the set of reactions may evolve at each step, a generalization that is again motivated by biological considerations, e.g., related to the theory of punctuated equilibria. In particular, she presented the notion of "Invisible changes': under certain sequences of events the behaviour of the system is indistinguishable from that of the original system, until a certain context can reveal it. The session was concluded by a discussion, led by S. Azimi and D. Besozzi, reflecting on topics such as the position of reaction systems w.r.t. quantitative and qualitative models in biology, the possibility to synthesize a reaction system from a specification of a biological system and the role of transition systems in such specifications. During the discussion, seeds were also sown for establishing more stable collaboration among groups working in the area.

We concluded Tuesday with a nice dinner in restaurant "El Brellin', enjoying typical Milanese cuisine near the Naviglio Grande canal, a lively area of the town.

Wednesday morning session consisted of two talks. The first by R. Gori ("Dynamic Causalities in Reaction Systems and their Applications", joint work with P. Milazzo, R. Barbuti and F. Levi) focused on the possibility of predicting causalities between entities (e.g., molecules) taking place in interactive processes in reaction systems. In particular, the question arises of identifying the set of entities that is needed from the environment for a certain set of entities to appear in the result set at a given step of a process. The problem is modelled by defining a logical formula synthesising the dependencies between entities as defined by the set of reactions (positive dependencies connect reactants to products, while negative dependencies connect inhibitors to products). Logical formulas are also used by C. Formenti ("Reaction Systems, Complexity and Bits of Category Theory", joint work with A. Dennunzio, L. Manzoni, and A.E. Porreca) to encode the result function of a reaction system, so that methods developed in general for discrete dynamical systems can be applied to establish the complexity of deciding some properties of reaction systems. It turns out that many interesting problems are computationally hard and even complete for some complexity class. After a lunch offered by the Rector of the Bicocca University, which celebrated its 20th anniversary exactly in the week of the workshop, the afternoon session saw two presentations from the USA participants. In the first, N. Jonoska ("Graph Isomorphism and Equivalence of Reaction Systems", joint work with H.J. Hoogeboom

and D. Genova) mastered a real blackboard to illustrate concepts of equivalence, companionship, and skeletons on graphs, summarising the possible dynamics of reaction systems with arbitrary context. The equivalence of such dynamics can be established as the isomorphism of the corresponding graphs. D. Genova, instead, provided a presentation of forbidding-enforcing systems, defined on linear words over an alphabet, drawing their similarities and dissimilarities with reaction systems ("Forbidding-Enforcing Systems, a Precursor of Reaction Systems", based on work with N. Jonoska and H.J. Hoogeboom). In this case, the mechanisms of facilitation and inhibition central to reaction systems are hinted at by two collections of constraints, negative ones stating that some words must not exist in some language (or some subword in some sentence) and positive ones, stating that if some word (subword) exists in a language, then also some other word (subword) must be present.

In the first talk on Thursday M. Koutny reported on efforts to provide a Petri net semantics for reaction systems ("Petri Nets and Reaction Systems", joint work with L. Mikulski, J. Kleijn and G. Rozenberg). This leads to a new variant of Petri nets, called Set Nets, where tokens in common input places are shared between transitions, rather than leading to a conflict as in the more traditional approach. The hope is evidently that useful concepts and methods, such as process semantics, can be transferred from Petri nets to reaction systems. Then W. Penczek ("Model Checking for Reaction Systems', joint work with M. Koutny, A. Męski and G. Rozenberg) presented work on Parameterized Model Checking for reaction systems: the idea is that one considers LTL formulae for desired behavior of reaction systems where information is missing; this missing information is represented by the parameters. One can then synthesize these parameters from "experiments" or simulations where the entities of the environment are given, thus filling in the missing information in a reaction system that is only partially defined (the tools are available at `http://reactionsystems.org`). The last talk of the session was by F. Okubo ("Reaction Automata', joint work with T. Yokomori). Reaction automata are language acceptors with a multiset rewriting mechanism controlled by reactants, inhibitors and products akin to those of reaction systems. They can operate in various modes, e.g., maximally parallel or sequential, and one may also look at subclasses such as the one obtained by omitting the inhibitors. This leads to a number of results concerning Turing universality and space-boundedness, in line with the approach from traditional language theory.

The afternoon session consisted of two presentations. In the first one E. Csuhaj-Varjú presented anther bio-inspired variant of the model ("Networks of Bio-inspired Language Processors", joint work with A. Alhazov, R. Feund, K.A. Lázár, C. Martin-Vide, V. Mitrana, A. Salomaa, Gy. Vaszil and S. Verlan). She considered networks where each node is associated with a set of strings (its state) and a language processing mechanism, in particular a Lindenmayer system or

an evolutionary processor. Even with restricted size these networks are Turing equivalent. Subsequently we returned to the study of reaction systems proper: L. Manzoni ("Complexity of Interactive Processes of Reaction Systems', joint work with A. Dennunzio, E. Formenti and A.E. Porreca) reported on a number of complexity results concerning certain aspects of the dynamic behavior of reaction systems. They concentrated on the occurrence of fixpoints and attractors. Most of the resulting decision problems turn out to be intractable in general.

The last talk was however not the last activity of the day: that was a visit to the exhibition of modern art in the nearby Pirelli Hangar Bicocca, with works by Eva Kot'átková and Matt Mullican as well as Anselm Kiefer's impressive "Seven Heavenly Palaces".

Since reaction systems are an idealized mathematical model abstracting from complex physical systems, where only incomplete information is available, one needs a framework to deal with such incomplete information, in order to acquire the data needed for the model. For that reason the first speaker on Friday, A. Skowron, proposed to link reaction systems with the idea of rough sets, where situations of the physical word are perceived via a set of attributes ("Linking Reaction Systems with Rough Sets", joint work with S. Dutta, A. Jankowski and G. Rozenberg). The talk consisted mainly in a somewhat broader reflection about the relationship between mathematical models and physical reality. In the second talk, by Luca Manzoni ("Cellular Automata and Reaction Systems', joint work with A. Dennunzio, E. Formenti and A.E. Porreca), another older bio-inspired model, cellular automata, was considered. Cellular automata share a number of characteristics with reaction systems, such as their definition in terms of simple rules that together generate complex behaviour. The complexity of various simulations between cellular automata, reaction systems, and Boolean networks was discussed, e.g., the fact that reaction systems can efficiently simulate cellular automata, but not the other way around.

In the last talk of the workshop, G. Rozenberg ("Reaction Systems and Graph Transformation", joint work with H.J. Kreowski) recalled the main notions of zoom structures, which he developed in cooperation with A. Ehrenfeucht, and demonstrated how their combination with reaction systems provides an elegant general framework for exploring a discipline of knowledge. Finally he pointed out how a novel approach to graph transformation is obtained by replacing the set of entities over which a reaction system is defined by a universe graph, hence adding structure: the dynamic behaviour of the obtained system can be seen as "surfing" on the universe graph, moving between its subgraphs.

Afterwards there was nothing left for us to do but to close the workshop with a warm "thank you' for L. Manzoni and the other organizers, as well as for G. Mauri.