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Coarse-graining the Dynamics of Ideal Branched Polymers

Vincent Danos[a,1] Ricardo Honorato-Zimmer[b,2]
Sebastián Jaramillo-Riveri[c,3] Sandro Stucki[d,4]

[a] *School of Informatics*
University of Edinburgh
Edinburgh, United Kingdom

[b] *Informatics Life-Sciences Institute*
University of Edinburgh
Edinburgh, United Kingdom

[c] *SynthSys*
Edinburgh EH9 3JD, United Kingdom

[d] *PPS Laboratory*
Université Paris Diderot – Paris 7
Paris, France

Abstract

We define a class of local stochastic rewrite rules on directed site trees. We give a compact presentation of (often countably infinite) coarse-grained differential systems describing the dynamics of these rules in the deterministic limit, and study in a simple case finite approximations based on truncations to a certain size. We show an application to the modelling of the dynamics of sugar polymers.

Keywords: rule-based modelling, fragmentation, coarse-graining, ideal branched polymers

1 Introduction

There are well-understood limitations to using rate equations in the modelling of chemical and biochemical networks of reactions. Often, in realistic conditions, the number of molecules is small, stochastic effects become important and differential methods lose relevance. In this paper we will be concerned with another limitation induced by the *constructive complexity* of biochemical systems. To illustrate this idea

[1] Email: vdanos@inf.ed.ac.uk
[2] Email: s1066652@sms.ed.ac.uk
[3] Email: sjaramil@staffmail.ed.ac.uk
[4] Email: sandro.stucki@epfl.ch

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consider proteins that can bind together via specific domains [17,14] and create a number of different species which is so enormous that it calls for different methods, perhaps even different questions and perspectives on the protein world [10]. Enters *rule-based modelling*. The idea is that basic molecules are now described as sets of domains, and the various reactions in which they can take part are pooled together into reaction classes or *rules*. This gives means to describe highly constructive systems in a compact form and without having to enumerate a (possibly infinite) set of species. This idea has been captured, studied, and implemented in two languages which are essentially the same, namely Kappa and the BNG language [1]. Other formalisms, in the tradition of process algebras, use rules of less direct expressivity but broadly similar in their intentions, and have the same fundamental ability to cope with unbounded sets of species [2].

Let us make the idea of rules a bit more precise by considering a molecule (or agent) A with two domains x, y. We can write a generic rule $A(x), A(y) \to A(x^1), A(y^1)$ expressing the possibility of forming a bond between x and y (the bond is denoted by the shared superscript) provided they are both free. This rule will apply *regardless* of the larger context in which the two agents A are found. It follows that this single rule pools or subsumes countably many reactions. Indeed, the two agents of type A can themselves be part of two chains, perhaps formed by the repeated application of the same rule. Suppose now A has a third domain similar to x, say z, with a similar binding rule $A(z), A(y) \to A(z^1), A(y^1)$. Taken together these rules will lead to the formation of branched polymers. Note that in this paper, there is no attempt at representing the actual geometry of complexes or polymers. This corresponds in the vocabulary of polymer sciences to *ideal* or *spherical polymers*. Of course, not every polymer is like that. For polymers where geometry is important (as in some of the cell molecular machinery such as the proteasome [9]) other and richer methods are called for (e.g. see Ref. [5], same volume). Given the title of this paper, one might be tempted to conclude that we are interested in the macro structure of such polymers. This is not the case. Rather, we are interested in the fine details of the connectivity between monomers at the micro scale. At larger scales, other interesting phenomena occur such as those treated in Ref. [7].

What then, do we mean by coarse-graining? Due to the constructive complexity mentioned above, the old biochemical horizon of a few hundreds of species is broken. This is specially true for polymers, where the number of possible species generated by a single polymerisation rule is infinite. To deal with such systems, coarse-graining methods have been developed recently which can reduce considerably the number of variables to be considered. In the context of the present paper, we are interested in one of them, called *fragmentation*. This method is suited to rule-based models and allows one to extract a smaller dimensional, more efficient representation of the dynamics [11,12,3]. We will adopt the method presented in Ref. [12] and explore the implications of using it in a new setting. In this method, one starts with a set of observables S and the fragmentation will generate a differential equation that describes the evolution of each observable (or *fragment*) in S as a function of some other observables $T_1, \ldots, T_n$. One can apply the same treatment to these new