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Abstract

This paper summarizes some of the problems associated with the generation of higher order emergent structures in formal dynamical systems as well as some of the formal properties of dynamical systems capable of generating higher order structures.

1 Molecular Self-Assembly

In biological systems, higher order hyperstructures occur both in an intuitive and a formal sense: monomers, polymers, membranes, organelles, cells, tissues, organs, etc. constitute an observable hierarchy, apparently generated by the underlying biomolecular process. However, in models and simulations of these systems, it has turned out to be quite difficult to produce higher order emergent structures from first principles.

The first problem is to agree on what a higher order structure is. An emergent structure can be defined through an introduction of an *observational function* [1]. If a property can be observed in the dynamics, but not at the level of the fundamental first order interacting structures, we define it to be *emergent.* It is well known that second order structures occur relatively easy in simulation, so the problem is how to proceed to third and higher order without external interference [3]. A third order structure is defined through the interaction of second order structures forming a new observable not found at the lower levels.

We can discuss these problems in the light of a Lattice Gas Automata [5] style discrete field automata, a Lattice Polymer - or Molecular - Automata (LPM, LMA) [9, 6] for molecular self-assembly where we can demonstrate the generation of higher order structures from first principles [3]. These formal systems are interesting in their own right, since this level of description allows the generation of entropic and enthalpic flows in a microcanonical, molecular ensemble bringing insight to entropy-driven processes in molecular many-particle systems. Structural features of a polar solvent can be generated together with cluster-formation of hydrophobic monomers and polymers in a polar environment. Polymerization processes, and the self-assembly of micelle-like structures of lipid polymers can also be followed. Membrane stability, microtubule assembly/disassembly and cytoskeletal re-organization can also be generated. However, the central issue here is dynamics and not molecular self-assembly. For a detailed discussion of the physico-chemical properties of these self-organizing processes we refer to [6]. For an alternative approach to the dynamics of self-organization we refer to [4, 8]. See also [2].

The cellular automata we use to describe the dynamics of these simple molecular self-assembly systems can be formulated as interacting objects of the form

$$S_i(x_i, y_i, z_i, f_{ij}, t) \tag{1}$$

where S_i is the ith molecule, x_i its position on a 2-D lattice, y_i its current state: velocity, kind of molecule, and bond directions; z_i its neighborhood, incoming force particles from neighboring molecules j; and f_{ij}, the object-object interaction rules

$$f_{ij}(x_i(t), y_i(t), z_i(t)) \rightarrow (x_i(t+1), y_i(t+1)), \tag{2}$$

which change the location and the internal state of current object depending on the way the object updates are scheduled (which e.g. can be random or parallel).

For a detailed description of the rules in (1) and (2), their assumptions, and the LMA dynamics, we refer to [9, 6, 3]. For an alternative cellular automata approach we refer to [7].

If we define monomers to be first order structures, then polymers will constitute second order structures. Third order structures will then be given by micelles. Polymers carry second order emergent properties such as elasticity; micelles and membranes carry third order emergent properties such as permeability - and an inside and an outside. Defining a dynamical system as an LMA, it becomes possible to generate higher order emergent structures from first principles as can be seen in figure 1. It should be noted that this particular process is chosen, because of its *conceptual clarity* and not because it models any particular biomolecular process.

It is clear from the observations we have made of the dynamics of the discrete field automata systems, that their ability to produce emergent structures is highly dependent on the degree of detail - or fidelity - of the objects in (1). As more and more interactions (f_{ij}) - and more and more different molecules and molecular states (y_i) - are taken into account, the more complex emergent structures the lattice automata systems are able to produce.

For example allowing only a simple molecule-molecule interaction without any excluded volume, enables us to define Lattice Gases [5] which can generate a variety of macroscopic fluid dynamics phenomena. By defining an excluded volume for the monomers together with binding and scheduling information to each of the molecules, it becomes possible to generate polymer dynamics. These are examples of second order emergent phenomena, as we have mentioned earlier. If binding information is present and the initial configuration is a random configuration of polymers with hydrophilic heads and hydrophobic tails the formation of micelle-like aggregates becomes possible. However, in a direct way the polymers can be generated by the dynamics if we allow an interaction which is specific for a polymerization process. If bond information together with polymerization interactions as well as hydrophobic/hydrophilic molecules all are defined, it becomes possible to generate micelle-like polymer aggregates from an initial condition of random monomers as seen in figure 1. Intermediate configurations of the dynamics will then be dominated by the newly polymerized hydrophobic/hydrophilic polymers. Thus, it is possible to produce third order structures from first order structures.

Another way of saying this, is that a more detailed description of the Physics is necessary to allow the formal system to produce higher order structures [1]. Weaker effects also have to be taken into consideration if more complex structures have to be explained.

Since the very beginning of the study of Complex Systems the dogma described in figure 2 has been dominating.

[1] We use Physics to denote principles of Nature independent of our description or knowledge of it. We use physics to denote our formal understanding and models of these principles.

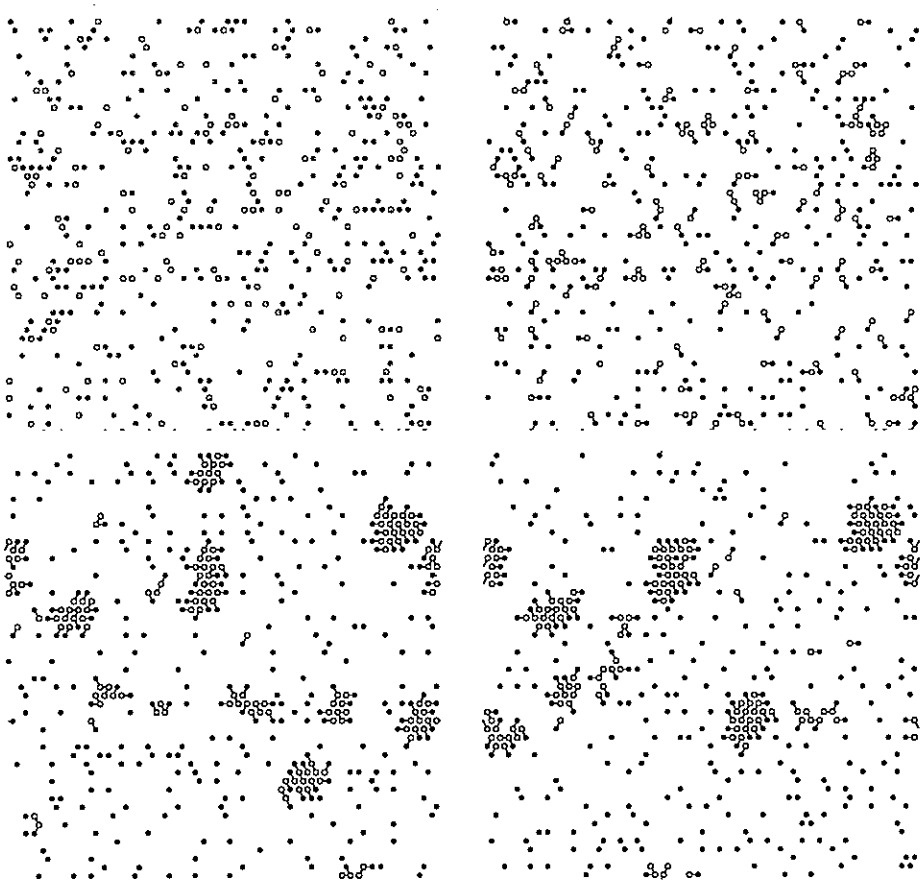

Figure 1: *Generation of third level structures in the lattice automata system. (monomers at time t = 0) → (polymers at time t = 20) → (micelle-like aggregates at time t = 20000 and t = 60000). Initially there is a 7 to 3 ratio of hydrophobic (black) to hydrophilic (white) monomers. The polymerization occurs such that a hydrophobic monomer (which is the nucleation center) can form a bond to a hydrophilic monomer which in turn can polymerize another hydrophobic monomer etc. At time t = 20 almost all free hydrophilic monomers are polymerized. Note that many of the hydrophilic monomers are not able to polymerize due to the relatively low concentration of hydrophobic monomers. The formed micelle-like clusters are quite dynamic for these initial conditions and parameters which can be see by comparing the aggregates at time t = 20000 and 60000. For a higher initial concentration of hydrophobic monomers, longer polymers (with less mobility) on average are formed and thus more stable aggregates emerges.*

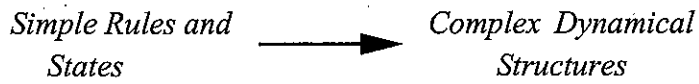

Figure 2: *Complex Systems Dogma.*

Is this really true? Could our "complex" hyperstructures have been created only starting with very simple object states and interaction rules without any external interaction with the system? [2] We doubt it. We do not doubt that complex structures in formal systems do arise from rule and state descriptions simpler than the structures. However, we question a stronger version of the dogma that essentially holds that a common minimal simplicity underlies all emergent structures. The notion of a *critical object complexity* is presumably important for the generation of dynamical hierarchies up to a given level. Whether more explicit internal object complexity always will be necessary to obtain yet higher order emergent structures - and whether there is an object complexity limit above which any functional property can be produced, we do not know. We would at least like to believe that the latter is true. See also [3].

One can of course also question our current approach. In addition to the minimal rules related to properties that define monomer-monomer interactions in bulk solution, we include two different kinds of monomers as well as water, which are all crucial in the resulting polymer-polymer interactions and the resulting formation of the polymer aggregates. Considerable care is required in defining such additional rules or they may simply "script" the outcome of the dynamics. However, the rules presented here do not do that and their rationale is well-formed. A rule inside a monomer object that references other monomers is obviously a second order predicate where first order predicates reference monomer properties within itself. However, all explicit predicates are self-referential and local; they all reference monomers in the neighborhood. They do not "cross" the levels and reference polymers or polymer aggregates. Thus, the interactions these rules describe are non-trivial relative to the production of higher order structures. The question of minimal description therefore relates directly to this issue: What are the minimal rules and states, from the perspective of a monomer, that can induce these higher order structures?

Thus, in this study, we investigate a (close to) minimal description of monomers that can entail polymer and micelle-like structures. We have picked a level of analysis and model at that level and investigate the entailed properties of object interactions at that level. Every scientific investigation establish such a working level. Our level is the level of monomers and water. Not lower (atoms, elementary particles, etc), and not higher (polymers, membranes, etc.).

[2] Note that we are considering fixed objects with no self-programming or "mutations" in the explicit rules and variables. Our objects do not learn, which seems reasonable, since they model simple invariant molecules.

2 Simulations as Formal Dynamical Systems

What are the formal requirements for systems that are able to generate dynamical hierarchies? By extracting some of the formal principles involved in the generating higher order (hyper-) structures in molecular self-assembly systems and relating them to dynamical systems, one of the central issues becomes the notion of a *simulation* as a synthetic mathematical method. We may define a simulation as a dynamical system that formally is constituted by an ensemble of objects

$$S_i = S_i(f_{ij}, s_i, \tau_i), \tag{3}$$

$i = 1, \ldots, n$, where S_i is an object with internal state s_i, object-object interaction function f_{ij} (which typically will have its own state s_i as an argument together with the state(s) of the object(s) that it is interacting with $s_j, j = i, 1, 2 \ldots$.), and local time τ_i. To generate dynamics these object-object interactions have to be scheduled by an *update functional* U (e.g. parallel, random, discrete event, etc). If we for simplicity assume that the update is times stepped (as in the above LMA systems), which means that all objects always have the same local (= global) time t, the dynamics of the interacting objects in (3) is given by

$$\{S_i(t+1)\} = U\{S_i(t)\}, \tag{4}$$

$i = 1, \ldots, n$. Note that in general no *explicit*, closed form function $F : \mathbf{X} \rightarrow \mathbf{X}$ exists that takes the current global state

$$X(t) = (s_1(t), \ldots, s_n(t)) \in \mathbf{X} \tag{5}$$

and maps it into some other state in the state space $\mathbf{X}$

$$F(X(t)) = X(t+1). \tag{6}$$

Such a function is only *implicitly* given through (4). Systems which can be expressed explicitly in the closed form (6) we may call *models*. Obviously, the classical dynamical systems which can be explicitly written in the form (6) are special cases of the form given in (3) and (4). This is true, because a system that explicitly can be written in the form (6) can be viewed as a *single* object S_1 from (3) which is iterated by f_{11}. Since there is no scheduling with only a single object, the update functional U, becomes the identity.

One of the mathematical consequences of having the dynamics of the form (3) and (4), is that (4) may not be updatable due to conflicts between the f_{ij}'s and U. Thus, a notion of *simulatability* can be defined [10]. The connection between the notion of simulatability and the notion of computability can now be studied, and indeed the concepts are different, since computability is defined through

$$\{S_i(t+T)\} = U\{S_i(t)\}, \quad T \rightarrow \infty \tag{7}$$

and simulatability is defined through

$$\{S_i(t+T)\} = U\{S_i(t)\}, \quad T = 1. \tag{8}$$

Thus, we can have simulatable systems with non-computable properties generated by the dynamics. In addition a mathematical machine, *a universal simulator* (US), can be defined, which in a finite number of steps determines whether a system is simulatable or not by describing the conditions under which a system of the form (3) and (4) can distribute update functions over system objects [10]. Further, it can give an appropriate order of updating for the objects, if it is simulatable, and detect where the problems are if the system is non-simulatable. Thus, the *scheduling problem* naturally lives in the US. Because each operation done by the US can be interpreted as having a computational cost, the *load balancing problem* also naturally lives in this mathematical machine. For a more detailed discussion of some of the mathematical consequences of the above we refer to [10].

Thus, by defining dynamical systems of the form (3) and (4) an alternative and more general avenue is open. We are not limited to closed form models which only keep track of the *number, or concentration,* of particular objects and where novel relations and objects cannot in a natural way be generated as a function of the dynamics (as e.g. in differential equations). Since the objects in (3) and (4) are explicitly represented, so are their *functional properties,* thus the molecular aggregates and their formation rates discussed above all come out as observable, emergent properties generated by the dynamical system. Therefore with this approach there is no need for *explicitly* taking all conceivable interactions and new possible products into account together with postulates about their formation rates. By defining the objects, the update functional, and the observational functions appropriately, everything of interest will be generated by the dynamics. Thus, we may view a simulation as an *emergence engine.*

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