Is It the Right *Ansatz?*

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Abstract This article is a response to Rasmussen et al. [*Artificial Life, 7*, 329–350], in which the authors suggest that, within a particular simulation "framework," there is a tight correspondence between the complexity of the primitive objects and the emergence of dynamical hierarchies. As an example they report a two-dimensional artificial chemistry that supports the spontaneous emergence of micellar structures, which they classify as third-order structures. We report in this article that essentially comparable phenomena can be produced with relatively simpler primitive objects. We also question the order classification of the micellar structures.

1 Introduction

In this issue Rasmussen et al. [8] critique what they call the "complex systems dogma." As they correctly observe it has been a more-or-less explicitly stated principle in the field of complex systems research that simple rules are sufficient to give rise to complex dynamical structures. This widespread presumption among complexity scientists is mainly based upon numerous successful applications of simple agent-based models to produce or explain seemingly complex phenomena in many natural and man-made systems (see for examples [1, 3–7]). In this context the term "simple" means that the rules that govern the agents' actions and interactions are very elementary and can typically be formulated in a few sentences; that the environment in which the agents live is of little structure; and that the number of state variables that characterize an agent is low. The same thing is often expressed by saying that the microlevel of the model is simple.

Despite the simplicity of the microlevel, the collective behavior of the agents—often referred to as the macrobehavior—can be very complex, in the sense that it has very intricate statistical properties or closely resembles the behavior of some seemingly very complex natural systems; this can then be exploited to make simple models of complex phenomena. One might here think, for example, of Per Bak's self-organized criticality [3] as a paradigm case. The repeated successful use of microstructurally simple agent-based models for the modeling of complex natural systems has led many to suggest that complexity in nature can and *should* always be reduced to simple interactions at some microlevel. Rasmussen et al. call this conjecture the "complex systems dogma."

While accepting, in principle, that any (Turing computable) system behavior can be realized with a simple microlevel, Rasmussen et al. question the general explanatory power of such a modeling approach, particularly for the understanding of dynamical hierarchies. By contrast, for that case, they argue for the use of microstructurally complex models; and, indeed, for the progressive addition of complexity at the microstructural level to promote the emergence of greater hierarchical complexity.

In the context of agent-based models, microscopic complexity could manifest itself in basically three ways: through a high number of different types of primitive agents; through a high number of different modes of interaction of the primitive agents; and finally through more complicated functions/rules that define these interactions. Rasmussen et al. subsume this under the term object complexity.

Their notion of a dynamical hierarchy is closely connected to the definition of emergence and hyper-structure as proposed by Baas [2]. Assume the existence of primitive structures $S_1^1, S_2^1, \ldots, S_n^1$ each of which has certain observable properties; furthermore assume that these structures can engage in an interaction $I(S_i, S_k, \ldots, S_j)$. In an agent-based model the S_i^1 would be the primitive agents of the microlevel. The properties of a primitive structure can be detected by an observational mechanism O^1, which allows the detection of certain properties $O^1(S_i^1)$ of the structure. Which properties one detects depends on the nature of this (arbitrary) observational mechanism.

Interaction between the primitive structures potentially gives rise to compound structures or aggregations that could be regarded as second-order structures, $S_1^2, \ldots, S_m^2$; again each of those second-order structures will have certain properties $O^2(S_l^2)$ as observed by an appropriate mechanism O^2. Analogously one can define structures (or agents) and observational mechanisms of successively higher orders. According to Baas' definition a property P of a structure S_j^N is called emergent if it is observed on structures of order N or higher, but not lower; or to be more precise, P is emergent of order N if:

$$P \in O^N(S_j^N) \quad \text{but} \quad P \notin O^N(S_l^{N-1})$$

An S_j^N with this property is called a hyper-structure, if $N > 2$. Rasmussen et al. suggest that, within any particular dynamical systems "framework," additional object complexity will be necessary to produce such hyper-structures of higher orders in a dynamical hierarchy; but they leave open the possibility that there is a critical threshold of object complexity that can generate structures of arbitrary order.

2 The Model

Rasmussen et al. describe a (putatively) third-order structure in a two-dimensional, agent-based, artificial chemistry. The primitive agents of this system are "hydrophilic" and "hydrophobic" monomers together with vacuum/water particles. The monomers can, under some conditions, form bonds with each other: a hydrophilic monomer may bind to a hydrophobic monomer and a hydrophobic monomer may bind to an already bonded hydrophobic monomer. According to the authors, the data structure that is necessary to describe the state of the monomers in their model is of size seven. It describes the following variables:

1. Scheduling color

2. Type of particle (hydrophilic, hydrophobic monomer, water/vacuum)

3. Excluded volume particles

4. Incoming force particles

5. Current velocity

6. Bond information (coordinates of bonding partners)

7. Incoming binding force

For a detailed account of the function of all these data structures we refer the reader to the original article [8]; at this point it should be noted that the interparticle forces are mediated by virtual-force particles that are exchanged between the monomers. The updating process consists of five substeps for each of the two types of monomers.

1. Propagate information particles (incoming force, excluded volumes, incoming binding force particles).

2. Create new bonds.

3. Compute proper move direction.

4. Move molecules.

5. Clear lattice of information particles.

Starting from a random configuration and an approximately equal number of hydrophobic and hydrophilic monomers, Rasmussen et al. report that their model displays the formation of amphiphilic polymers: that is, chains of hydrophobic monomers with a hydrophilic head. These amphiphilic polymers then aggregate and form micelles by the following mechanism: The hydrophobic tails "hide" from the water and tend to remain in each others' neighborhood, thus forming clusters. Seeking the proximity of water, the hydrophilic heads of the polymers will stick out of these clusters, which creates the characteristic micellar structure. Rasmussen et al. claim that these micelles are an example of a third-order structure with third-order emergent properties. One example of such an emergent property is the separation between the inside and the outside. Given an observational mechanism, O^{io} which can detect the property $P^{io} = \{$presence of an inside and an outside$\}$ one finds that

$$P^{io} \in O^{io}(S_j^3) \quad \text{but} \quad P^{io} \notin O^{io}(S_k^2)$$

where the micelles are the third-order structure S_j^3 that resulted from the interactions of the second-order structures S_k^2, the polymers. Other third-order properties of micelles include a particular size distribution and a characteristic diffusion constant. Rasmussen et al. stress that the model's "ability to produce emergent structures is highly dependent on the degree of detail of the object models" [8, Section 5.3]. This encapsulates the core hypotheses of their article.

3   Is This Amount of Detail Necessary?

While the general intuition expressed by Rasmussen et al. about the relation between object complexity and the emergence of higher-order structures might be correct, we question whether the model they present adequately demonstrates or corroborates this claim. Especially we doubt that the degree of detail their model exhibits is necessary to produce the putatively third-order structures. We will demonstrate, by means of a simpler model, that the only features that are necessary to produce the micelles are the presence of water/vacuum particles and the hydrophobic/hydrophilic particles as well as their mobility and their ability to form the appropriate bonds. All other features of the Rasmussen et al. model are nonessential for the formation of micelles in a two-dimensional artificial chemistry; at the same time those nonessential features considerably add to the model's object complexity. The simplified model will compare in complexity with the simplest agent-based models.

Our model[1] consists of three types of particles, hydrophilic and hydrophobic mono-
mers as well as water/vacuum particles. The monomers can bond to each other in the
same way as the monomers in the Rasmussen et al. model. The monomers contain the
following state information:

- Type of particle

- Bonding information (coordinates of bonding partners)

There is no need for a scheduling color. At each time step each particle undergoes
the following simple rules:

- Attempt to form a new bond with a predetermined probability, or try to form a
  second bond with a predetermined probability (if applicable).

- Attempt a random movement with a predetermined probability. Retract this
  movement if constraints are violated.

The constraints come from the hydrophilic and hydrophobic properties of the mono-
mers and from the bond information:

- If a monomer A has an existing bond with another monomer B, then A may not
  move out of the neighborhood of B.

- If A is hydrophilic, then it may not move if it would have fewer water/vacuum
  neighbors after the movement.

- If A is hydrophobic, then it may not move if it would have more water/vacuum
  neighbors after the movement.

Note that these constraints are only applicable if the particle moves actively; in
particular, a hydrophobic monomer might move into the neighborhood of a hydrophilic
monomer and thus decrease the number of vacuum/water particles in the neighborhood
of the latter.

Our model thus consists of just three types of agents, each with only a small num-
ber of state variables, interacting according to relatively simple rules. The model's
complexity is, we claim, comparable to the simplest (nontrivial) agent-based models.

In our simulations we used a two-dimensional lattice of size 150×150, with a trian-
gular neighborhood. Initially we placed an equal number of monomers (1,500 of each
sort) at random positions. At each time step neighboring free monomers formed bonds
with a probability of 0.999; and each available hydrophobic monomer was added to
an already existing polymer with a probability of 0.001. This setting ensured that most
monomers were bonded after only a few time steps (see Figure 1). During the early
stages of the simulation, the short, but relatively mobile, polymers aggregated around
longer, rather immobile, polymers; those longer chains thus functioned as "crystalliza-
tion" points. Similar mechanisms were reported by Rasmussen et al. After a transitional
period we observed the formation of micellar structures qualitatively similar to those
of Rasmussen et al. (compare Figure 2 and Figure 2 in [8]).

The results obtained from this relatively simple model support our claim that many of
the features of the Rasmussen et al. two-dimensional model were actually not essential
to the emergence of higher-order structures. It would probably make little sense to

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1 The model has been implemented using the Swarm simulation platform; full source code is available at: http://www.eeng.dcu.ie/
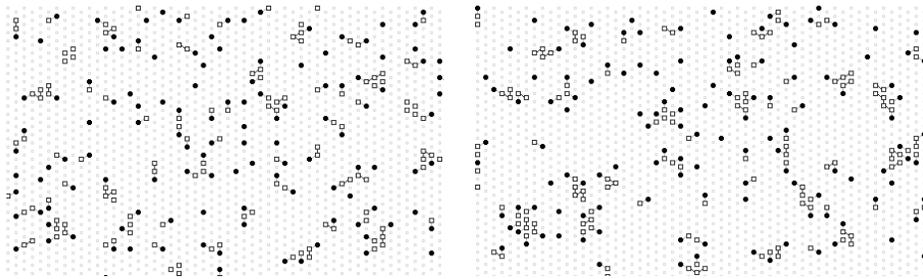   alife/src/s-micelle/.

Figure 1. The left side is the configuration of our model after 70 time steps. To the right we see approximately the same region at time step 292. There are hardly any free monomers left. The solid round objects are the hydrophilic monomers and the squares represent the hydrophobic monomers.
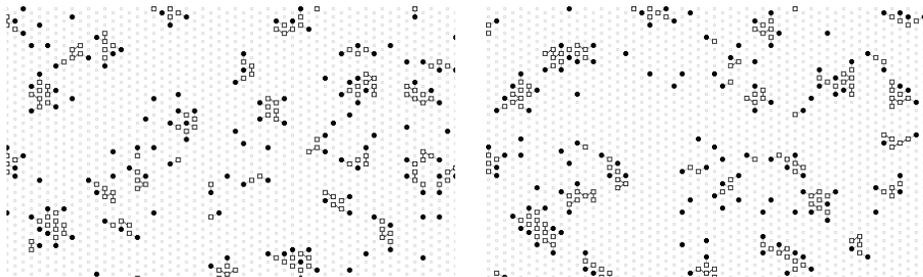

Figure 2. A screenshot from our model. We see the time steps 1,517 and 3,429 to the left and right, respectively. We clearly discern the micellar structures.

attempt to give a precise comparison between the object complexity of our model and that of Rasmussen et al. However, in our model the monomers only have information about their type and their bonding partners; whereas the monomers in the Rasmussen et al. model require seven state variables (see above). Excluded volumes and interparticle communications, which are realized by special force-particles in the Rasmussen et al. model, are here implicit in simple rules, very much in the spirit of the "complex systems dogma." Even if one fails to accept that the Rasmussen et al. model is significantly more complex than our version, then it still seems difficult to deny that our model is of complexity comparable to the simplest agent-based models in the literature. It was precisely the simplicity of such models that gave rise to the "complex systems dogma."

4   Conditional Conclusion 1

If micelles are third-order emergent structures, then third-order structures can spontaneously emerge from models in which the microstructures are not significantly more complex than those of the simplest agent-based models; this would appear to corroborate the "complex systems dogma."

   This does not mean that it is not worthwhile to make complex models, such as that of Rasmussen et al.; but rather only that this additional agent complexity is not *necessarily* required for the emergence of third-order structures.

   Having said this, we acknowledge that there are significant difficulties in making comparisons between different simulation models. In particular, it may be argued that the model we present above represents a completely different simulation "framework," rather than (as we have implied) a model in essentially the same "framework" but with

reduced object complexity. Rasmussen et al. explicitly raise this potential difficulty of changing "framework." It might be fruitful to pursue a more precise formulation of this concept that would provide criteria (either theoretical or pragmatic) for deciding when "frameworks" are the same or different.

5   But Are Micelles Third-Order Structures?

Conditional conclusion 1 rests on the presumption that the micellar structures that are described by Rasmussen et al. are indeed of third order. On the contrary, in this section we will argue that the micelles should, in fact, be properly regarded as being of only second order.

To do so, let us first clarify the definition of an Nth-order structure. There are at least two possible interpretations.

One possibility is that we call an object A an Nth-order structure if it consists of several other objects of which at least one is a structure of order $N - 1$. According to this definition the micelles described by Rasmussen et al. are certainly third-order structures, because they need to include polymers, which are second-order structures.

However, the problem with this interpretation is that it allows for trivial higher-order structures. Consider the example of a pile of sand. We can (arbitrarily) partition this sand pile into pairs of adjacent grains and designate these pairs as second-order structures. We can then similarly designate pairs of pairs of grains of sand as third-order structures. Iterating this procedure allows the definition of successively higher-order structures and imposes a correspondingly complex hierarchical structure on the sand pile. Obviously this is not what we mean when we talk about hierarchy. It therefore seems that this interpretation of higher-order structure is not a very useful one.

A possible objection to this argument is that pairs of grains of sand do not really constitute a second-order structure, and that there is no justification to consider them as anything other than two separate objects. While this is intuitively true, it is also a fact that a pair of grains of sand fulfills the above proposed definition of a second-order structure as it consists of several (in this case two) objects of which at least one (in this case both) is a first-order structure. This first interpretation corresponds to Baas' definition of hyper-structures where "no action," that is, $I(S_i, \ldots) = \{\}$, is an admissible interaction between structures.

A different but perhaps more sensible and intuitively correct interpretation of an Nth-order structure is to demand that it necessarily involves the interaction of $(N-1)$th-order structures either during its formation or later (or both); this interpretation would correspond to Baas' definition of a hyper-structure where "no-action" is not considered as a valid interaction.

We will argue that micelles are not third-order structures according to this second, substantive interpretation, because polymer interaction is essential neither for the ontogeny nor for the continuing existence of micelles. Rasmussen et al. mention in their article that the micelles are "stable" once they have formed, which means that these structures are immobile and lack any interesting dynamic properties (see caption to Figure 2 in [8]). This suggests that any kind of self-maintenance, reproduction, or dynamic behavior is not essential for micellar-ness. Consequently, any kind of polymer–polymer or polymer–monomer interactions that might be observable are only accidental features. We thus conclude that micelles, once formed, do not necessarily include interactions of second-order structures. This leaves us with the possibility that interaction of second-order structures must be essential during micelle formation. We suggest that this is actually not the case and conclude that the micelles of the type described in [8] are in fact not third-order structures.

We demonstrate that micelles can be produced, by direct interaction of primitive structures only, by means of the same relatively simple model that we have described above.

To demonstrate our claim we adjust two of its parameters. The idea is as follows: We start with an initial state identical to the one we used in the first experiment. If the monomers do not form bonds to each other initially, then (as Rasmussen et al. have acknowledged) the free hydrophobic monomers will quickly form clusters, "hiding" themselves from the surrounding water. Once formed these structures will be relatively stable; at this stage most monomers in the system will still be without bonds. Hydrophilic monomers that come into the neighborhood of the clusters can form bonds with the outermost monomers. Finally, over time, further monomers can form bonds to already existing polymers inside the clusters. This will produce patterns that are virtually indistinguishable from micelles, but their generation only involved the interaction of monomers. Obviously the initial clustering is nothing but a collective effect of hydrophobic monomers and thus comprises interactions between first-order structures only; similarly the subsequent polymerization process is an interaction between two monomers, that is, again an interaction between first-order structures. The micelles are thus second-order structures.

In this second experiment the micellar structures also show the property P^{io} of having and inside and an outside. Only this time we find

$$P^{io} \in O^{io}(S_b^2)$$

The P^{io} belongs to a second-order structure, which contradicts Rasmussen et al.'s above result. Also note that the extension of the polymers involves the interaction between a second- and a first-order structure, but in this case this is a logical necessity and not essential to the formation of the pattern in question. It would seem that similar arguments can be formulated for other third-order properties of micelles that Rasmussen et al. mention.

To realize the scenario in our model, we set the probability for bonding so low that initially only very few polymers form, which guarantees that there are enough free hydrophobic monomers available for the aggregation process; since this process happens quickly, it is sufficient to set the monomer–monomer bonding probability to 0.0995 (thus a bond will only be formed at roughly every 10th encounter of suitable monomers). By the time the hydrophobic monomers have aggregated most hydrophilic monomers are still unbound (see Figure 3). So no second-order interaction is responsible for the formation of the clusters. Once the clustering process is finished there are only very few hydrophobic monomers outside clusters. This in connection with the low bonding probability means that the probability of polymer formation outside clusters is very low (see Figure 4). Consequently, the only way for polymers to come into existence is that hydrophilic monomers form bonds to the outermost monomers in the clusters—again an interaction between primitive structures. This process takes some time, but takes place eventually. Once the bonds between monomers are formed, we observe the extension of the polymers, which happens with a probability of 0.005. We have run our model for a little bit longer than 50,000 time steps. As Figure 5 shows, at this time there are clearly visible micellar structures in the model, all of which are essentially a result of interactions between first-order structures. We have thus demonstrated that micelles can be formed by interaction of primitive structures only.

A possible objection to our second experiment might be that our interpretation of the role of the polymers outside the clusters is incorrect and that they actually play an essential role in the formation of the micelles by drifting in the neighborhood of a cluster where they will get caught. This process would take considerably more time
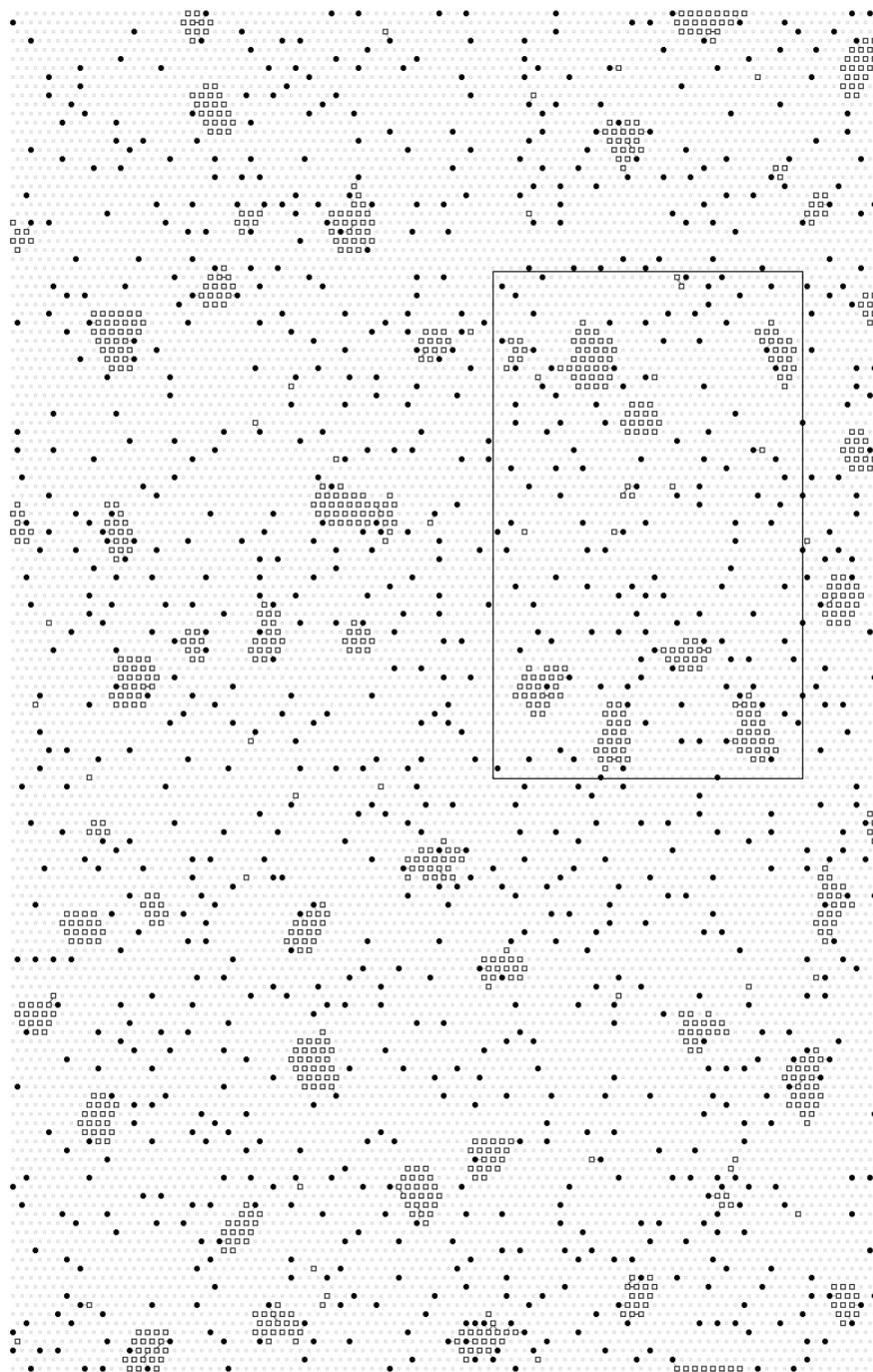
Figure 3. The second experiment at time step 6,572. There are only very few polymers, but the clustering process is already well advanced. Comparison to the screenshots of the first experiment show that the polymerization process is now much slower than the clustering process. Thus first we get the clusters of the hydrophobic monomers and then polymers form. The region inside the black rectangle is roughly the region of the following screenshots.
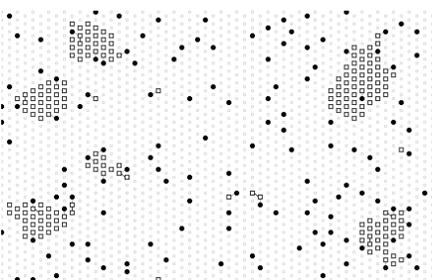
Figure 4. Here we see a screenshot from the second experiment at time step 11,339. The formation of the clusters is fast compared to the bonding between monomers. This ensures that little second-order interaction occurs before the clustering process is effectively finished. In this picture we clearly see that there are only very few polymers outside the clusters.
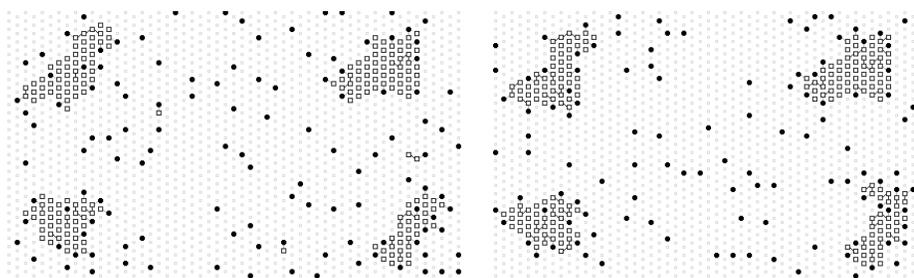

Figure 5. We see the same region as in Figure 4, but at the time steps 29,400 and 53,840. There are still many free monomers available, but after more than 50,000 time steps the micellar structures are clearly visible.

than the direct attachment of hydrophilic monomers (because of the higher diffusion constant of polymers) but the second experiment probably provided enough time. While it cannot be denied that second-order interaction sometimes takes place in the second experiment, we claim that it is not essential. To demonstrate this we performed a control experiment where we increased the speed of the micelle formation, which excludes the possibility that the slow higher-order interactions played a significant role in the micelle formation.

In this third experiment we "grew" clusters of hydrophobic monomers from the same initial state as in the previous two experiments while bonding was disallowed. Once the clusters formed we halted the simulations and changed the parameters such that hydrophilic monomers attempt to form a bond to the hydrophobic monomers with a probability of 0.999 and the extension of an existing polymer is attempted with the probability of 0.001. After restarting the simulation we observed that the hydrophilic monomers quickly attached to the outermost hydrophobic monomers in the clusters. Compared to the second experiment this process happened considerably faster; thus the few "free" polymers have enough time to travel and attach to the clusters in significant numbers. Less than 3,000 time steps after we changed the parameters the clusters have effectively transformed into micelles. We show the development of one such cluster in Figure 6.

Of course, these empirical results refer only to our relatively simplified model, rather than the original model of Rasmussen et al. They thus do not definitely show that the micellar structures in that original model are of only second order; it is conceivable that, in the simplification process, some significant polymer–polymer interactions have been lost, which were in fact essential to micelle formation (in that model/framework).
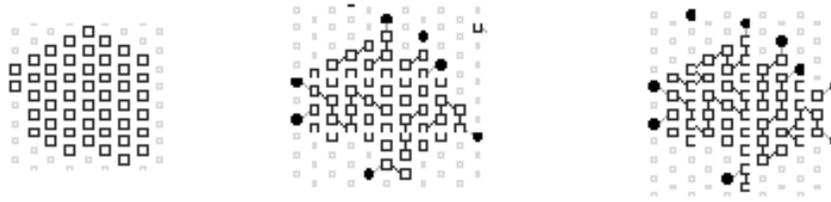
Figure 6. One of the clusters at different time steps in the simulation. To the left we see it at the time of the change of parameters; the next two are the same cluster 1,365 and 2,920 time steps after that. Note that the number of hydrophobic monomers in the cluster increases by only one in this interval; this contradicts the assumption that micelles are produced by attachment of short polymers and thus supports our claim that micelles are second-order structures.

However, at the very least, these results suggest that the practical classification of order in dynamical hierarchies is still a nontrivial problem.

6 Conditional Conclusion 2

In general, the formation of a micellar structure does not *necessarily* involve the inter-action of nonprimitive structures, and a number of its properties may, in fact, be only second-order emergent and not third-order emergent. This suggests that the claimed hierarchical structure in the two-dimensional experiment of Rasmussen et al. may be less intricate than it might seem at a first glance.

7 Final Conclusion

Although the general critique of the "complex systems dogma" presented by Rasmussen et al. *might* be correct, it is not clear to what extent their specific computer simulations have demonstrated this. Certainly, micellar structures can be reproduced by a model with complexity comparable to the simplest agent-based models; but the significance of this depends on the order classification of these micellar structures. Ironically, this may save (at least partly) the main argument of Rasmussen et al. We have only shown that micellar structures—not third-order structures in general—can spontaneously emerge in simpler agent-based models. If these micelles are indeed only second-order structures, then nothing of substance has been determined. Nonetheless, in any case, we conclude that the methodological value of the "complex systems dogma" is still very much open for discussion.

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