Swarm Chemistry

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Keywords
Artificial chemistry, swarm behavior, kinetic interaction, pattern formation, self-organization, interactive evolutionary method

Abstract We propose *swarm chemistry*, a new artificial chemistry framework that uses artificial swarm populations as chemical reactants. Reaction in swarm chemistry is not determined by predefined reaction rules as commonly assumed in typical artificial chemistry studies, but is spontaneously achieved by the emergence of a new spatiotemporal pattern of collective behavior through the kinetic interaction between multiple chemical species. We developed a prototype of an interactive simulation tool with which one can explore the dynamics of swarm chemistry using an interactive evolutionary method. Several preliminary results are reported to illustrate the characteristics and effectiveness of this framework, including spontaneous segregation of distinct chemical species, production and restriction of movements, and interactive design of complex biological-looking structures.

1 Introduction

Artificial chemistry is usually defined as a triplet (S, R, A), where S is the set of all possible molecules, R the set of reaction rules, and A the algorithm for simulating reaction processes using S and R [2]. A chemical reaction produces other molecules, which are also elements of S. The reaction rules and the simulation algorithm therefore collectively define a mapping network between the submultisets of the original set S.

While very powerful and useful as a generalized definition of theoretical chemical processes, the formal framework mentioned above gives us little insight into where those reaction rules come from, how the reactants' structures are transformed through the reaction, and so on. Several attempts have recently been made to draw a more detailed picture of artificial chemistry by constructing the entire chemical reaction processes from finer-scale virtual kinetic laws [7, 16, 8, 4].

Here we propose *swarm chemistry*, a new artificial chemistry framework that extends research on such artificial physico-chemical systems by combining them with the models of artificial swarm behaviors, another active area of investigation in artificial life and complex systems [12, 1, 18]. Each reactant in swarm chemistry is realized as a set of semi-autonomous agents that can move in a continuous space, sense other agents within their local perception range, and change their behavior as a response to perceived local conditions.

It is well understood that the local kinetic interaction among agents may give rise to the spontaneous formation of nontrivial dynamic patterns, as was originally modeled in Reynolds' *boids* [12], and more recently demonstrated physically through the attraction-repulsion interactions of small magnetized disks by Grzybowski et al. [6]. In swarm chemistry, however, the parameters that determine the ways of

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local interaction are assigned to each agent as its own attributes, so one can create two or more swarm populations with different parameter settings and experiment on how they *react* to each other if mixed together. This makes swarm chemistry distinct from other artificial chemistry models as well, in that the outcome of reaction is not directly given by a prescribed rule set but is spontaneously obtained as a new spatiotemporal pattern emerging through the kinetic interaction between populations.

We developed a prototype of an interactive simulation tool with which one can explore the dynamics of swarm chemistry using an interactive evolutionary method. In what follows, we report several preliminary results to illustrate the characteristics and effectiveness of this framework, including spontaneous segregation of distinct chemical species, production and restriction of movements, and interactive design of complex biological-looking structures.

2 Model

A swarm population in swarm chemistry consists of a number of simple, semi-autonomous agents. They can move in a two-dimensional continuous space, and each can perceive positions and velocities of other agents within its local perception range, and change its velocity in discrete time steps according to the following kinetic rules (adopted and modified from the rules in Reynolds' boids system [12]):

- If there are no local agents within its perception range, steer randomly (*straying*).
- Otherwise:
  - Steer to move toward the average position of local agents (*cohesion*).
  - Steer toward the average velocity of local agents (*alignment*).
  - Steer to avoid collision with local agents (*separation*).
  - Steer randomly with a given probability (*whim*).
- Approximate one's speed to one's own normal speed (*pacekeeping*).

These rules are implemented as shown in Table 1. Kinetic parameters used in this algorithm are listed and explained in Table 2.

Each agent is assigned its own kinetic parameter settings. We call a collection of identical agents that share the same kinetic parameter settings a *chemical species* (or just *species* for short). *Reaction* is defined as a process in which swarms of two or more species or their compounds are blended together and a new spatiotemporal pattern emerges through the kinetic interaction between different chemical species (Figure 1).

Note that individual agents remain exactly the same during this reaction process; only higher-order properties of the population as a whole (shapes, movement, etc.) may change. Such a nature of reactions in swarm chemistry may be a reasonable analogue, at least conceptually, of what is going on in real chemistry, where the observed changes of chemical properties are due to the rearrangements of the participating elements and not due to the changes of the elements themselves. It should also be noted, however, that the kinetic interaction rules assumed in swarm chemistry have nothing to do with atomic or molecular interactions in real chemistry. The terminology is borrowed from chemistry just for the purpose of making intuitive analogy.

3 Simulator

To explore the possible dynamics of swarm chemistry, we developed a prototype of the interactive simulator for it, using Java 2 SDK Standard Edition 1.5.0. It runs as either a standalone Java application or an online Java applet on any computer platform equipped with Java 2 Runtime Environ-

Table 1. The algorithm used to simulate the behavior of agents. $\overrightarrow{x_i}$, $\overrightarrow{v_i}$, and $\overrightarrow{v_i'}$ are the location, the current velocity, and the next velocity of the ith agent, respectively. $\overrightarrow{a}$ is a local variable temporarily used to represent an acceleration. r and $r_{\pm p}$ represent random numbers taken from $[0, 1]$ and $[-p, +p]$, respectively.

for all $i \in$ agents **do**

$N \leftarrow \{j \neq i$ that satisfies $|\overrightarrow{x_j} - \overrightarrow{x_i}| < R^i\}$

// Finding other agents within its local perception range

if $|N| = 0$ **then**

$\overrightarrow{a} \leftarrow (r_{\pm.5}, r_{\pm.5})$ // Straying

else

$\langle\overrightarrow{x}\rangle \leftarrow \Sigma_{j\in N}\, \overrightarrow{x_j}/|N|$ // Calculating the average position of local agents

$\langle\overrightarrow{v}\rangle \leftarrow \Sigma_{j\in N}\, \overrightarrow{v_j}/|N|$ // Calculating the average velocity of local agents

$\overrightarrow{a} \leftarrow c_1^i\,(\langle\overrightarrow{x}\rangle - \overrightarrow{x_i}) + c_2^i\,(\langle\overrightarrow{v}\rangle - \overrightarrow{v_i}) + c_3^i \Sigma_{j\in N}\,(\overrightarrow{x_i} - \overrightarrow{x_j})/|\overrightarrow{x_i} - \overrightarrow{x_j}|^2$

// Cohesion, alignment, and separation

if $r < c_4^i$ **then**

$\overrightarrow{a} \leftarrow \overrightarrow{a} + (r_{\pm 5}, r_{\pm 5})$ // Whim

end if

end if

$\overrightarrow{v_i'} \leftarrow \overrightarrow{v_i} + \overrightarrow{a}$ // Acceleration

$\overrightarrow{v_i'} \leftarrow \min(V_m^i/|\overrightarrow{v_i'}|, 1) \cdot \overrightarrow{v_i'}$ // Prohibiting overspeed

$\overrightarrow{v_i'} \leftarrow c_5^i\,(V_n^i/|\overrightarrow{v_i'}| \cdot \overrightarrow{v_i'}) + (1 - c_5^i)\,\overrightarrow{v_i'}$ // Pacekeeping

end for

for all $i \in$ agents **do**

$\overrightarrow{v_i} \leftarrow \overrightarrow{v_i'}$ // Updating velocity

$\overrightarrow{x_i} \leftarrow \overrightarrow{x_i} + \overrightarrow{v_i}$ // Updating location

end for

ment. Its applet demonstrations, source codes, and compiled class files are freely available from the author's Web site.[1]

We adopted the *interactive evolutionary method* [17, 13, 5] to make possible interactive design of interesting structures and collective behaviors in swarm chemistry. Using this simulator, a human experimenter,

1 http://bingweb.binghamton.edu/~sayama/SwarmChemistry/

Table 2. Kinetic parameters involved in the simulation of agent behavior. Unique values are assigned to these parameters for each agent i as its own kinetic properties.

Name	Min	Max	Meaning	Unit
R^i	0	300	Radius of local perception range	pixel
V_n^i	0	20	Normal speed	pixel step^{-1}
V_m^i	0	40	Maximum speed	pixel step^{-1}
c_1^i	0	1	Strength of cohesive force	step^{-2}
c_2^i	0	1	Strength of aligning force	step^{-1}
c_3^i	0	100	Strength of separating force	pixel^2 step^{-2}
c_4^i	0	0.5	Probability of random steering	—
c_5^i	0	1	Tendency of pacekeeping	—

or *alchemist*, can actively participate in the selection, perturbation, and blending of swarm populations by subjectively selecting preferred swarm behaviors. Interactive evolution has already been applied to the designs of swarm behavior for scientific and educational purposes [11, 14]. Our work presented here is distinct from the earlier studies in that it evolves self-organizing patterns in heterogeneous swarm populations.

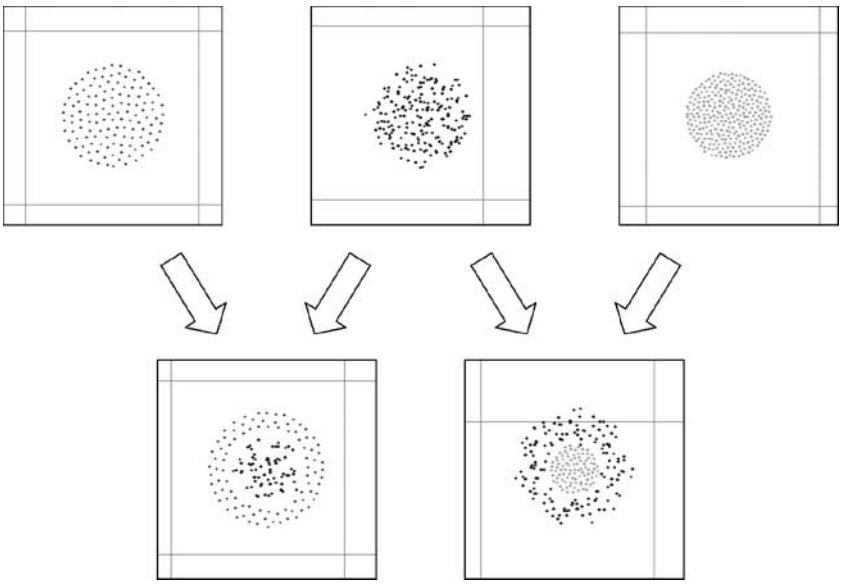

Figure 1. Chemical reactions in swarm chemistry. Each dot represents one agent. Agents are colored by taking their (c_1^i, c_2^i, c_3^i/100) values as their (R, G, B) values, respectively. Colors are converted to grayscale in this article. Top: Swarms of three different chemical species (homogeneous populations made of identical agents). Kinetic parameters (from left to right, in (R, V_n, V_m, c_1, c_2, c_3, c_4, c_5) format): (260.37, 0.84, 12.55, 0.69, 0.59, 47.16, 0.49, 0.9), (185.11, 10.86, 19.97, 0.53, 0.05, 19.12, 0.05, 0.44), (211.12, 16.22, 1.13, 0.73, 0.89, 15.82, 0.39, 0.54). Bottom: Results of reactions (spatial patterns formed after blending two swarms of different species). Blending different chemical species produces different patterns. Gray lines are references drawn at an interval of 300 pixels to show the scale of the image.

We also note that evolutionary computation techniques, such as genetic algorithms, could be implemented to acquire some types of swarm behaviors automatically. However, we did not choose to do so, because setting an easily measurable metric for automated fitness evaluation would necessarily limit the diversity and novelty of potential outcomes.

Figure 2 shows a screenshot of our swarm chemistry simulator. Several different swarms are simultaneously simulated and demonstrated in their respective frames. A user can select up to two preferred swarms by clicking on the frames in which those swarms are simulated.

To produce a next generation of swarms, we used a unique set of evolutionary operators that are different from other typical genetic operators such as point mutation or crossover operators. Specifically, we used the following two operators:

- *Perturbation:* If just one swarm is selected by the user, perturbed swarms will be generated by repetitive random resampling of agents from the selected swarm up to a modified total population size (with $\pm 80\%$ possible variations; the population in a swarm can be up to 300). They will form the next set of swarms, together with the original swarm preserved as is and a new swarm of randomly generated species, which is introduced to diversify the available options.

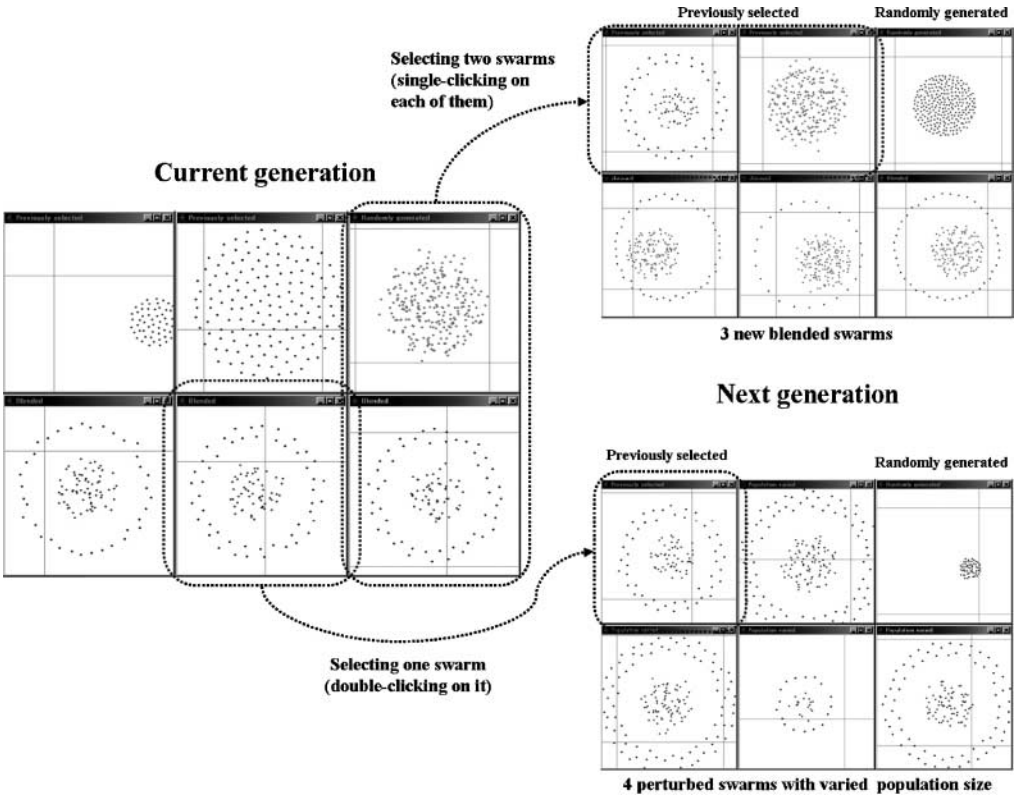

Figure 2. Left: Screenshot of the swarm chemistry simulator. Several swarms are simultaneously simulated on a screen (number of frames can be changed). The simulated space has no boundaries, so that the distribution of agents could be infinitely large due to diffusion. The simulator dynamically rescales the viewing size so that the most significant cluster should always be tracked within the frame. Right: Results of selection operations in the swarm chemistry simulator. A user can select up to two swarms by clicking on the respective frames. If two swarms are selected, three new blended swarms will be generated at different ratios between the two (top). If just one swarm is selected, it will be replicated four times through random resampling with varied population sizes (bottom).

- *Blending:* If two swarms are selected by the user, blended swarms will be generated at randomly determined ratios between the two selected swarms (ranging from 20:80 to 80:20). The number of agents in each of the new swarms is set to the average of those in the two selected swarms. The new blended swarms will be part of the next set of swarms, together with the original two as well as a new swarm of randomly generated species.

We also implemented a simple point mutation operator that introduces random variations of each of the kinetic parameters; insertion, duplication, and deletion operators that add or delete chemical species; and an interactive interface by which the user can manually edit the kinetic parameter settings. These features were not used when producing the results presented in this article.

By repeating this interactive selection process, the experimenter can explore a variety of dynamics and potentially create a novel, complex dynamic structure. This design cycle continues indefinitely until the application is manually quitted.

4 Results

We have conducted preliminary exploration of possible dynamics in swarm chemistry and have found several characteristic outcomes of chemical reactions in this model world, which are summarized in what follows.

4.1 Spontaneous Segregation

In most cases, agents spontaneously form clusters of the same species and segregate themselves from other chemical species when blended, even though they have no capability to distinguish themselves from other species. This is because of the difference in their kinetic parameter settings, which causes the difference in the local environments they "prefer." It is generally very rare for a swarm made of two different species to remain mixed, with some exceptions where one or both of the species are insensitive to local environmental conditions (this may happen if, e.g., the perception range or the maximum speed of agents is very small).

4.2 Production of Movements

Reaction in swarm chemistry may produce a new macro-scale dynamic movement of the swarm, which may be considered an example of the emergence of autonomous motion in pre-biotic systems [9]. Movements typically arise when an asymmetric relationship is established between the two chemical species, one as a chaser and the other as an escaper. Such movements based on chasing may take a couple of different forms, as shown in Figure 3.

4.3 Encapsulation and Restriction of Movements

Chemical reaction in swarm chemistry can also form multiple closed layers in a population, where a subpopulation of one species is encapsulated in a dynamically formed membrane made of agents of the other species (Figures 1, 4). This sometimes restricts the movement of swarms of originally mobile species (Figure 5), creating an internal rotation or oscillation inside the structure.

4.4 Interactive Design of Complex Structures

Swarm chemistry may be applied to the heuristic design of robust distributed systems. Our simulator enables one to interactively and incrementally build artificial chemical systems toward desirable structures and/or behaviors (Figure 6). Because the previously selected swarms (i.e., the best designs obtained so far) are always preserved and simulated on screen (Figure 2), the designer can compare the new results of blending or variation with the previous achievement and decide whether or not the most recent changes should be incorporated into the design.

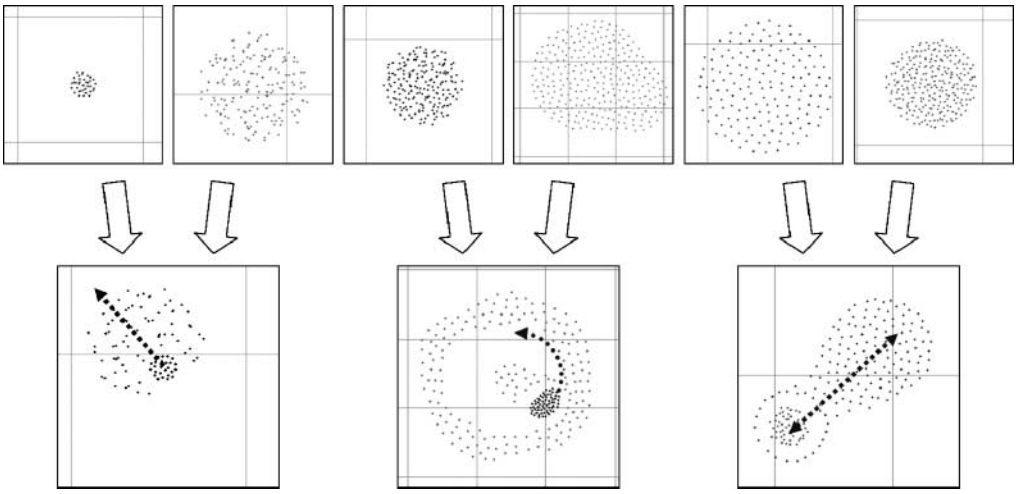

Figure 3. Production of movements as a result of reaction in swarm chemistry. Left: Linear motion. Blending two swarms of originally immobile species results in a polarized cluster, and their chasing and escaping behaviors create a linear motion of the entire population. Middle: Rotation. The small cluster rotates counterclockwise inside the other cluster. Right: Linear oscillation. The small cluster is continuously attracted by the main body of the population made of the other species and keeps moving back and forth through it. Kinetic parameters of the six species in the top row (from left to right, in (R, V_n, V_m, c_1, c_2, c_3, c_4, c_5) format): (231.53, 2.72, 26.49, 0.89, 0.0, 23.23, 0.47, 0.78), (292.29, 15.44, 25.33, 0.98, 0.46, 94.01, 0.29, 0.16), (241.98, 6.93, 5.43, 0.59, 0.02, 26.39, 0.17, 0.77), (74.54, 1.24, 36.59, 0.11, 0.84, 51.18, 0.3, 0.41), (86.89, 1.8, 22.26, 0.57, 0.35, 80.8, 0.35, 0.64), (70.55, 5.52, 7.39, 0.97, 0.45, 35.51, 0.45, 0.06).

Sample products of such iterative design are shown in Figure 7, where the designers tried to create some biological-looking structures. The first example self-organizes into a shape that resembles a horseshoe crab, and it actually moves in the direction it heads in. The second example forms a biological cell-like structure, including nucleus and membrane, and shows very chaotic, aggressive movement after its self-organization. The designs of these final products are specified in the form of a *recipe*, a list of the kind and the number of agents that describes the composition of the swarm population. What the designer is doing is to design and control the structure and behavior of the product indirectly by modifying the contents of the recipe.

A remarkable feature of these products, and all other products that can be obtained in swarm chemistry, is that they are inherently *self-organizing.* Agents are initially mixed randomly, but they quickly find their own places to sit in and collectively form the shape of the final product (Figure 7). This self-organization process is found to be highly reproducible and robust to perturbations such as minor variations in system sizes and addition or removal of a small number of agents.

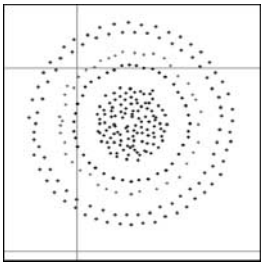

Figure 4. Typical multilayer structure made of agents of several different chemical species. Distribution of kinetic parameters (in (number of agents) × (R, V_n, V_m, c_1, c_2, c_3, c_4, c_5) format): 94 × (288.73, 2.09, 10.98, 0.87, 0.21, 86.72, 0.01, 0.98), 42 × (171.96, 8.47, 28.86, 0.85, 0.71, 55.9, 0.2, 0.74), 41 × (174.34, 5.66, 8.8, 0.59, 0.35, 33.43, 0.02, 0.08), 113 × (226.1, 3.83, 29.64, 0.4, 0.6, 13.48, 0.37, 0.17).

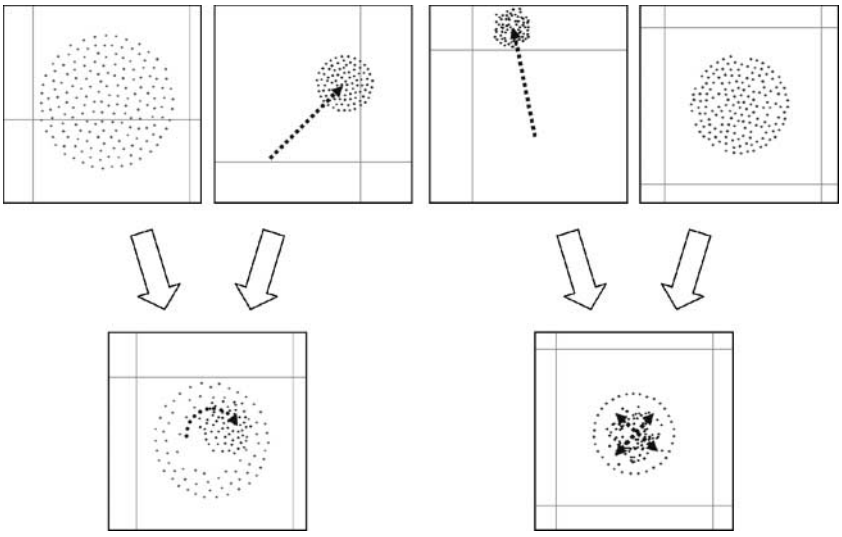

Figure 5. Encapsulation of subpopulations of originally mobile species into an immobile membrane structure made of agents of other species. The movements of the mobile agents are restricted and transformed into internal rotation (left) or oscillation (right). Kinetic parameters of the four species in the top row (from left to right, in (R, V_n, V_m, c_1, c_2, c_3, c_4, c_5) format): (278.56, 10.88, 1.23, 0.26, 0.78, 27.69, 0.07, 0.77), (89.41, 8.12, 18.29, 0.4, 0.51, 13.3, 0.03, 0.58), (116.78, 16.82, 30.15, 0.46, 0.22, 8.47, 0.2, 0.87), (246.36, 0.02, 20.62, 0.91, 0.12, 47.96, 0.41, 0.77).

The shape of the final product must be indirectly woven into the recipe; however, there is neither an articulated blueprint nor a central controller that coordinates the arrangement of the agents. The entire process is driven solely by local kinetic interaction between agents. It would be difficult to predict the final outcome without carrying out explicit numerical simulation. While it is generally hard to manually design such a distributed self-organizing system, our approach with interactive, iterative heuristic design appears to be effective in reconciling the inconsistency between self-organization and manual design.

5 Conclusion

We have proposed swarm chemistry as a new artificial chemistry framework, which uses populations of semi-autonomous agents as chemical reactants and considers the emergence of new spatiotemporal

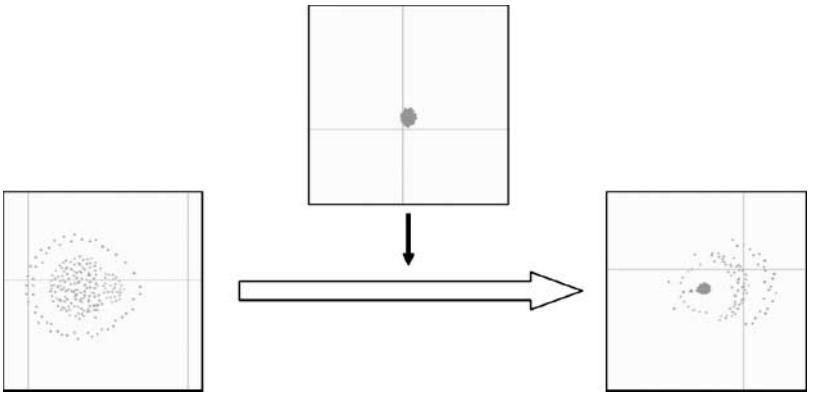

Figure 6. Addition of agents of a new chemical species to the existing swarm as a method to incrementally build artificial structure in swarm chemistry.

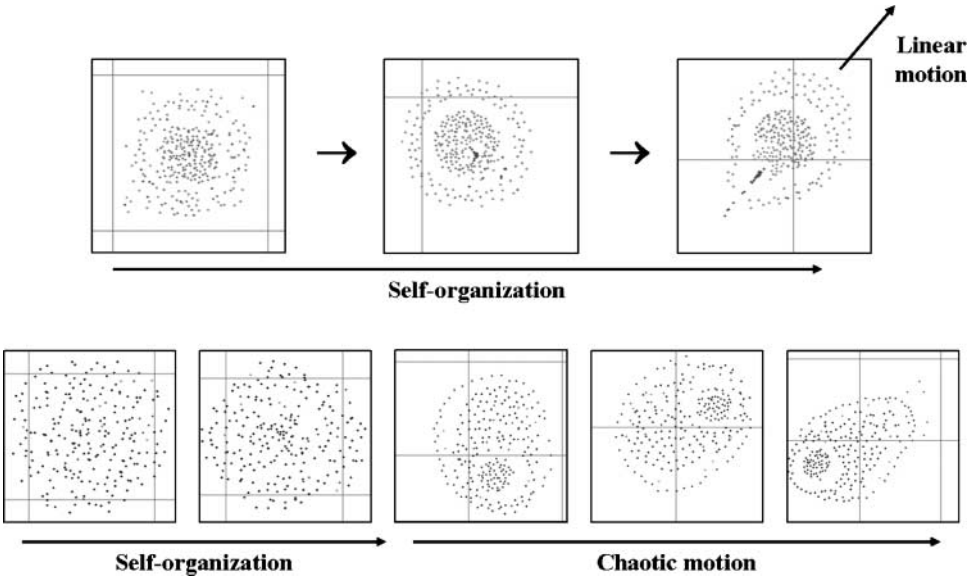

Figure 7. Examples of complex structures made of several different chemical species, designed using our interactive simulator. The swarms self-organize from initially random states to a shape that looks like a horseshoe crab (top), or a biological cell-like structure that shows active chaotic movement after self-organization (bottom).

patterns as the outcomes of chemical reaction. We also developed a prototype of the interactive simulator and illustrated several characteristic phenomena frequently observed in the reaction processes in swarm chemistry, as well as its potential for heuristic design of robust, self-organizing distributed systems. We anticipate several practical applications of this work, including (a) introduction and dynamic control of self-organized heterogeneous swarms for particle swarm optimization [10, 3], (b) distributed formation control of unmanned aerial vehicles (UAVs) in aerospace and/or military applications [15], and (c) interactive generation of aesthetically appealing dynamic patterns for artistic purposes [17].

Our model is unique in that the agents we use are fairly simple. They have no lengthy self-regulating instructions like a genome in a biological cell; they always remain the same, with no potential to differentiate. Also, the agents have no capability to identify or distinguish themselves from other species. They look identical to each other, and therefore no sophisticated communication exists between them. This component simplicity would strengthen swarm chemistry as a model of distributed artificial systems, especially in view of real-world implementations where the simplicity of modules is of particular concern.

The swarm chemistry project is still at its launching stage, and there are a number of things yet to be done. Future tasks include (a) analytical and numerical investigations of the properties of each chemical species and the effects of kinetic parameters on pattern formation, (b) exhaustive computational investigation of possible outcomes of the interactions of multiple species, (c) implementation and evaluation of dynamic self-replication and self-maintenance of complex patterns, and (d) hardware implementation and demonstration using mobile robotic modules.

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