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Physically Based, Self-Organizing Cellular Automata

Alan Dorin

School of Computer Science and Software Engineering,
Monash University, Clayton, Australia 3168
ph. +61-3-9905-5524, fx. +61-3-9905-5146
aland@csse.monash.edu.au

Abstract. A physically based system of interacting polyhedral objects is used to model self-assembly and spontaneous organization of complex structures. The surfaces of the polyhedra in the simulation are covered with bonding sites in states akin to those of cellular automata. The bonding sites interact with sites on neighbouring polyhedra to apply forces of attraction and repulsion between bodies and to trigger transitions in their states. Using only these mechanisms, the elements exhibit chaining, membrane and cluster formation, and differentiation / segregation. Examples of each of these phenomena are given along with explanations as to how they are formed. Assembly without the guidance of an external agent or central control is infrequently used in the construction of complex artificial structures, but is the norm for biological construction. This paper presents a model by which the construction of complex structures may be simulated using multiple reactive, artificial agents, acting independently under artificial physical and chemical laws.

Keywords: Artificial Life, Cellular Automata, Physical Modelling, Self - Organization / Assembly, Molecular Dynamics

1 Introduction

Living organisms are problem solvers. Not only at the level at which they seek food, evade predators, construct shelter or play chess, but also at the microscopic level. At this level the components of an organism are continually and co-operatively acting to maintain the organism's physical identity. Organisms are self-assembling, parallel machines whose many and varied components maintain a stable organization under perturbation. This is achieved through the local physical and chemical interactions of the individual elements themselves. There is no external agent or co-ordinating body which acts to place the correct materials, operate the appropriate reactions and so forth within the body of the organism. The parts of the living system independently move into position at the time required for life's processes to proceed.

This paper draws on work in a number of disparate fields to simulate aspects of the defining processes of living things. By simulating the parallel behaviour of usually microscopic components, it is hoped that an understanding of the assembly and maintenance of life may be reached. It is clearly beyond current technology and understanding to fully simulate such processes with anything but extremely remote semblance to the behaviour of actual life. Nevertheless, it *is* becoming feasible to examine at least some of the possibilities, identifying problems of comprehension and computation along the way. With this proviso, the following sections of the introduction outline a few fields which have bearing on the present effort. Section 2 introduces physically-based, Self-Organizing Cellular Automata (SOCA). This is a simulation framework for experiments with collections of rigid, polyhedral elements acting under simulated physical and chemical laws. Section 3 further details the SOCA system and describes a set of experiments with self-assembling structures. In section 4 further research using SOCA is described, then conclusions for this paper are presented. Acknowledgments and a bibliography appear in the final sections.

1.1 Physical Simulation

The non-interpenetration and collision of solids, and their movement under internally and externally generated forces is modelled in the SOCA system. The techniques employed have found wide application in computer graphics and animation, for example [20,27]. Real world, internally generated forces particularly relevant to SOCA include those produced by electro-magnetic attraction and repulsion. Externally generated forces of interest in this study include forces acting between solids, fluids, and the action of gravity or other global forces where applicable.

1.2 Cellular Automata

Cellular Automata (CA) have been widely studied as examples of complex dynamical systems [12,31], under the banner of artificial life [17], and originally as examples of components in a self-reproducing machine [4,11]. The global behaviour usually said to be *emergent* [5] from the local interactions is a source of fascination for researchers struggling to understand complex behaviour in the real world. To some extent, this complexity appears to stem from simple agents or automata operating in complex environments [26].

The cells in a CA grid act in parallel to collectively solve problems. Not necessarily problems in the sense that a chess player or robot controller solves problems, but problems akin to those solved by biological organisms and their components in maintaining their organization [6].

1.3 Philosophy of Biology

Autopoiesis has been coined by Maturana and Varela [19] to describe the organization of living things. The view may be summarized thus: a living thing is the matter contained within a space defined by a set of chemical processes which produce the components of which they themselves are constructed. An organism is a network of self-sustaining, self-bounding chemical processes. Such a view of life places it as a subset of auto-catalytic reactions as described by Kauffman [16] and within the scope described by Prigogine [23]. The extension of this to the virtual space as discussed in [6], includes representational physics and chemistry of relevance to the current study.

1.4 Self-Organization / Self-Assembly

Self-organization and assembly occur under what may loosely be described as a *physics* without which there are no principles guiding the interaction of components. The SOCA system simulates real world physics and may be used to explore self-assembly and self-organization[1] within the limits imposed by the simulated rules of interaction.

Although they are physical objects, Penrose's wooden machines [22] are similar in spirit to the constructions presented in this paper. The presence of a seed structure in a set of Penrose's machines allows the assembly of more complex machines from the components provided. Once a particular form of machine has been constructed, a mechanical trigger severs it into two or more compound structures with features identical to the seed which began the process.

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[1]The terms self assembly / organization are used so loosely as to have become inter-changeable. A suitable working definition requires only that the terms indicate construction of a unity from components acting under forces / motives internal or local to the components themselves, and arising through their interaction with the environment. That is, assembly or arrangement according to a distributed plan or goal implicit in the structure and behaviour of the parts, not explicitly stated or held by a central controlling entity.

Ingber has built simple machines to model the mechanical properties of cells [15]. His drinking straw and elastic constructions behave in ways not unlike the elements of the SOCA system, although they are unlike the machines of Penrose. Ingber's units form geometric shapes as they find their stable, minimum energy state.

Other authors have explored systems with some similarities to these. A mechanical system of blocks and magnets [14] has been used to study the formation of intermediate products during self-assembly. The simulation of cellular development by Fleischer [10] and the self assembly of the T4 bacteriophage [13] have also been modelled. The physical simulation in the latter model is unsophisticated. Of course there are also many studies of self-organization with no reference to physical simulation in the sense that it is modelled in SOCA, rather a *physics* (although it may not be called such) is modelled according to the researcher's particular needs. Steels [29] investigates the development of language as if it were a self-organizing system. Banzhaf uses binary strings to explore auto-catalysis and metabolic formation [1]. Saitou and Jakiela [24,25] have examined the process of sub-assembly (that is, the ordering of assembly processes within larger scale assembly processes) in detail.

1.5 Reactive, Distributed Artificial Intelligence

Components in many self-assembling systems may be viewed as purely reactive agents. They are unable to plan but respond directly to their surroundings. The stimuli to which a component is capable of responding are dictated by that component's physical composition and properties. This paper shows how simple reactive elements may self-assemble into larger structures without an explicit global plan or complex inter-element communication. The elements rely purely on (simulated) mechanical and chemical properties to realize a plan implicit in their structure and the virtual physics / chemistry of the environment. The resulting structure is not organized by an external agent in the way that, for example, a clock or bridge is built by robots or people. Instead, the structure appears as a result of many local interactions between agents 'responsible' for their *own* behaviour (position / orientation and movement). The systems of interest consist of many reactive artificial agents that interact to spontaneously form at least one complex structure.

Attempts have been made to utilize the emergent properties of interacting reactive agents. Drogoul and Dubreuil [8] demonstrate Eco-Problem-Solving (EPS) after Ferber and Jacopin [9]. The agents in these works aim to satisfy their own goals. The result of their local interactions is a global stable state in which all agents are satisfied and a correct solution to the problem at hand is found. In this respect EPS is similar to the SOCA system presented here. Where EPS differs from SOCA is in the explicit nature of the goals of each agent. The SOCA agents do *not* have explicit goals to satisfy although the system as a whole does have one or many stable states. Perhaps the differences between SOCA and EPS are better understood by making the analogy between SOCA elements and virtual chemicals reacting in various ways to form molecules, an analogy explored in the next subsection.

1.6 Molecular Dynamics & Supramolecular Inorganic Chemistry

Recent papers in supramolecular chemistry grapple with self-assembly [18]. One way of understanding the interactions of groups of molecules is to visualize them according to the shapes they form and the bonding sites the shapes present to their surroundings. Molecules of different types have differently arranged bonding sites which fit together to form large collections of molecules (supramolecules). By some reports [21] it is helpful to visualize molecules as polyhedra whose vertices are bonding sites. The resulting supramolecules are visualized as organized collections of polyhedra[2].

The system described in this paper is ideal for the simulation of such behaviour. To date, self-assembly in chemistry has been examined by mixing real chemicals. Efforts have been made to utilize simulated Newtonian physics to allow models of molecules constructed from empirical data to fall into natural minimum energy states, a practice called *molecular dynamics*. The system presented in this paper allows for the full simulation of the movement of rigid polyhedra acting under the influence of forces centered on bonding sites across their geometry. It should be of interest to those exploring the chemistry of self-assembly.

2 The SOCA System

The elements in the SOCA system are simulated, rigid, convex polyhedra suspended in a fluid. The densities and geometric properties of the elements may be specified. Collisions are detected, analytically derived impulses prevent bodies from interpenetrating. The implementation details of this are in many respects similar to those of Baraff [2].

The fluid model incorporates viscosity acting on the bodies as fluid drag. A vector field specifying the direction of fluid flow at any location in space is also modelled. For the purposes of this paper the fluid is stationary at large scales. Small scale Brownian motion helps 'jiggle' the elements in the fluid into stable states. Effects of solids on the fluid medium are ignored, only effects of the fluid on solids within it are considered. This is in keeping with the fluid models found in [7, 30].

In addition to the above properties, the faces of each element have a state visualized as their colour. This is analogous to the state of a CA cell. Lookup tables stored with each element dictate the behaviour of a face depending on its current state and the state of the faces on *other* elements within its vicinity.

Faces may apply forces to the bodies on which they lie in response to the presence or absence of faces on other elements in particular states. The forces act at the center of the face in question and therefore provide linear and angular acceleration to the element on which they lie. The scale of the force generated is determined using a lookup table particular to the element on which the face resides. This value may be scaled according to the surface area of the face and the range over which the neighbouring face is detected.

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[2]The models described in the supramolecular chemistry lierature visualize bonding sites at the verteces of the polyhedra. This scheme was not adopted for the experiments described here although modification of the SOCA software to emulate the chemist's approach is trivial.

There exists a special 'inert' state similar to the quiescent or background state of CA's. An inert face does not interact with any faces around it.

Besides generating a force, a face may undergo a change of state. This is triggered, like the application of forces, by the presence or absence of faces on other elements in particular states and at particular distances. It is not possible for a face on one polyhedron to control the behaviour of a face on another. The face may however *trigger* a response dictated by the transition table of the neighbouring body.

In sections 3.1 and 3.2, the properties of SOCA elements utilizing empty transition tables are explored. Section 3.3 on the formation of clusters of SOCA elements, utilizes the transition table to alter the state of the elements according to their environment. The properties of dynamic SOCA elements, elements with faces which change in such a way as to produce mobile or active structures, are not discussed in this paper.

3 Self-Assembling Structures

For the following experiments, the face of an element may be in one of the states 'blue', 'green', 'grey' or 'red' (after the colours in which they are drawn) or in the 'inert' state[3].

The dimensions of the elements used in the following examples were arrived at after some experimentation but are not mandatory. The system is sensitive to changes in dimensions of its elements for various reasons. Most notably, short or small elements are less stable than long elements under forces tending to align them in specific directions. This is due to the reduced lever arm available on a short element for the application of torque. [Fig 1]

Additionally, the difference between forces experienced by a pair of opposite faces, say on a cube is less than the difference between opposite end caps on a long rectangular prism because in the SOCA system, as in real life, forces attenuate across space. In these experiments all forces between element faces obey the standard inverse square law of force propagation. The strength of each force is independent of the surface area of the face on which it acts. The density of all elements is identical unless otherwise stated.

3.1 Chaining

A tube or cord is a geometric structure along which energy or matter may pass. It is a continuous structure able to span distances with a minimum expenditure of energy and material. Long, narrow, flexible, structures play vital roles throughout the natural and artificial worlds. Elephants marching around a ring, ropes, chains, wires, threads, tendons, muscle fibres, arteries, veins, capillaries, nerve cords, sinuses, hairs, all these things loosely fit into this category.

A common behaviour in chemistry and a useful property of many artefacts is referred to here as 'chaining'. For example, polymerization is chemical chaining in which many identical molecules or repeated sets of molecules link up end to end to

[3]Figures are rendered as clearly as possible within the limits imposed by black and white reproduction. The figure captions are written to clarify the orientation of the bodies. Colour figures are available from the author should they be required.

form a molecular tube, cord or similar. A chain of metal rings is an artificial example of this structure, rope a variation on the theme. Chaining is a simple way to create tubes and cords from many identical elements.

To model chaining in the SOCA system, elements of length eight times the width of their square cross section were set up to act like ferrous magnets, one end cap in the green state, the other blue. The mid-sections of the elements were inert for this experiment. As with magnets it was arranged that opposite poles attract and like poles repel. Under these conditions all elements have the same transition table (since all magnets behave alike). Table 1 shows the forces between faces for this experiment.

	Inert	Blue	Green
Inert	0.0	0.0	0.0
Blue	0.0	-1.0	+1.0
Green	0.0	+1.0	-1.0

Table 1. Force table for ferrous magnet simulation

A positive force indicates a direction *towards* the neighbouring face (attraction), a negative force a direction *away* from the neighbouring face (repulsion). Interactions between inert faces and any other face always result in a force of 0.

When a blue face on a SOCA element encounters a green face on a neighbouring element, a force acting at the center of the blue face is generated in a direction towards the center of the green face (and vice versa because each element has the same transition table) [Fig 1]. As indicated above, the strength of the force is scaled to decay according to an inverse square law.

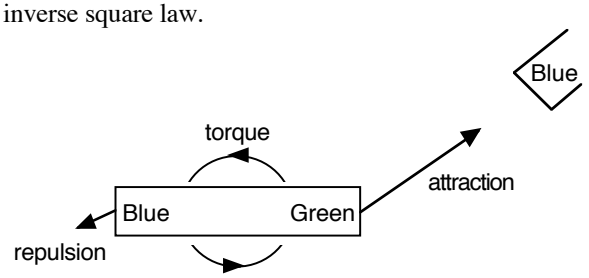

Fig. 1. Diagram illustrating resultant torque on a body undergoing attraction at one end, repulsion at the other

An environment homogeneously populated with elements of this type organizes itself into element pairs. Sometimes a short chain of three elements arises, but this is unstable and is hardly the desired behaviour [Fig 2a]. The stable state for the elements is a pair aligned head to tail (ie. blue to green and green to blue). From a distance, the net attraction or repulsion to the end point of one of these pairs is zero since the forces generated by blue and green ends cancel out.

To encourage chaining, the inert sides of the elements were replaced with grey sides. Table 2 shows the forces acting between elements in the new system.

	Inert	Grey	Blue	Green

Inert	0.0	0.0	0.0	0.0
Grey	0.0	-0.25	0.0	0.0
Blue	0.0	0.0	-1.0	+1.0
Green	0.0	0.0	+1.0	-1.0

Table 2. Force table for ferrous magnet simulation with repulsion along the length of the bodies

Table 2 is the same as table 1 but for the addition of a small repulsive force between the grey lengths of the SOCA elements. The small repulsion prevents pairs of elements from mating at both ends and encourages chaining [Fig 2a,b&c]. The stable form for a system of these elements, like those above, is a circle. In this case it is a circle of circumference greater than the degenerate two-link 'circle' (pair) in the earlier experiment and requires the chaining of more than two elements to be complete. The circumference of the minimum stable circle is proportional to the force applied between pairs of grey faces.

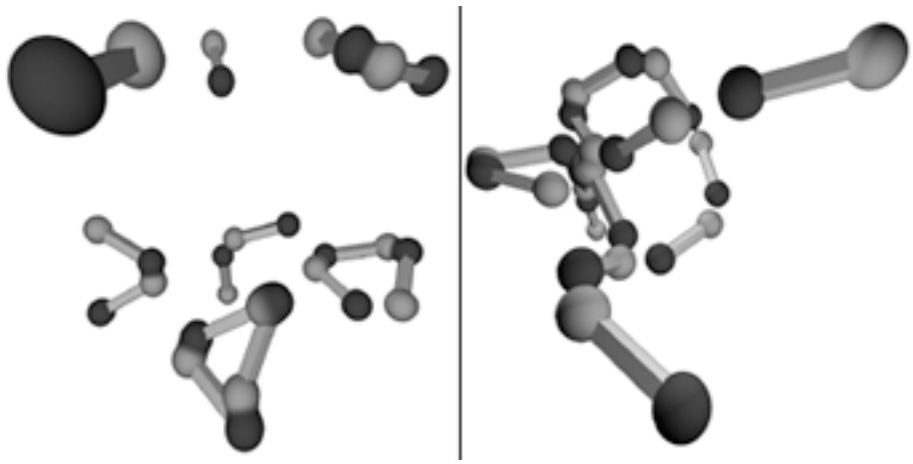

Fig. 2a & b. Chaining blue ends to green ends, elements form:
(a) small clumps (No repulsion along element lengths as in Table 1.),
(b) compact chains (Slight repulsion along element lengths).

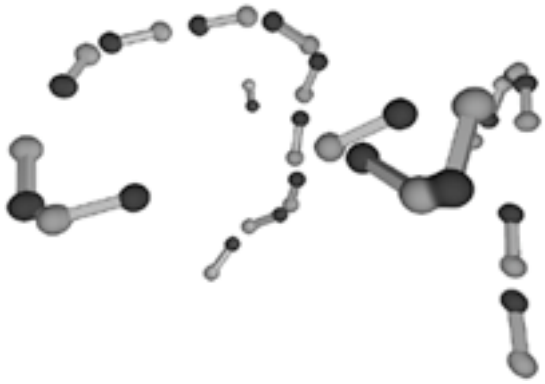

Fig. 2c. Chaining blue ends to green ends - long extended chains of elements (Repulsion along element lengths as in Table 2)

As has been shown, without any repulsion between grey faces the minimum stable 'circle' has a 'circumference' of two elements. Circles containing nine elements have been observed. In theory larger structures could be formed but in practice these are not easily assembled. This seems to be due to the inevitable presence of twists and turns in the chain which keep the two free ends from meeting. The grey faces of all elements in the chain repel one another and keep the structure from attempting to self-intersect. They resist the pull of the free ends to form a clean circle and tend to meander. The resulting structure has more in common with a helix than a circle.

Under conditions where the minimum circle size has been established, circles larger than the minimum stable circle have nevertheless been seen to form. Should an element of one of these large circles be dislodged by a collision with an element from outside, the circle may close out the dislodged element and form a structure closer in circumference to the minimum stable circle.

3.2 Boundary Formation

In many circumstances in the natural and artificial worlds, it is useful to separate something from its surroundings by means of a material barrier. The cell membrane is such a barrier, as are the skin and the walls of the stomach. A bottle and a balloon are artificial barriers.

Table 3 illustrates one way in which SOCA elements can be made to self-assemble into a boundary. All green faces attract one another, all blue faces repel one another. The effect is to have the elements' green faces forming the inside surface of a spherical boundary. The blue faces settle into a minimum energy outer surface. [Fig 3]

	Inert	Blue	Green
Inert	0.0	0.0	0.0
Blue	0.0	-1.0	0.0
Green	0.0	0.0	+1.0

Table 3. Force table for boundary formation

The boundaries formed using table 3 are unstable and slow to form. The instability manifests itself as oscillations in the arrangements of the elements and an insecure hold on components within the structure. A more stable configuration can be achieved using the behaviour specified by table 4.

	Inert	Grey	Blue	Green
Inert	0.0	0.0	0.0	0.0
Grey	0.0	-1.0	0.0	0.0
Blue	0.0	0.0	-4.0	-1.0
Green	0.0	0.0	-1.0	+4.0

Table 4. Force table for boundary formation with repulsion along the length of the bodies

Repulsion between faces along the length of the elements in the grey state (as opposed to the inert state) proves to be a useful stabilizer. Additionally, a small amount of repulsion between blue and green faces accelerates assembly by forcing 'un-linkable' ends apart. By altering the ratio of repulsion between the grey / grey and green / green faces to the attraction between blue / blue faces, boundaries of different diameter may be assembled. The repulsive forces must not be so great as to force the elements too far apart or the attractive forces will be insufficient to orient the elements over the greater diameter of the structure.

In this example, the number of elements in the boundary also effects its diameter. In each case the system settles into its state of minimum energy. The more elements there are, the more tightly packed they must be to form a sphere of some diameter, the higher the attraction on the inner surface needed to counter the repulsion between grey faces tending to expand the structure.

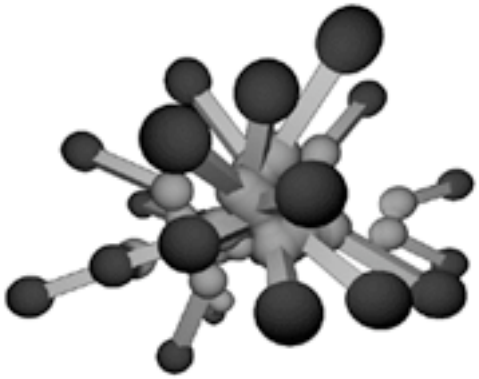

Fig. 3. Boundary formation, green end caps inward, blue outward

The boundary presented mimics to some degree the formation of liposomes [3]. Fatty acids in water orient their hydrophilic heads outward to form a hollow sphere which isolates the acid's hydrophobic tails from the water [Fig 4]. Single surface spheres like those created by the SOCA elements are formed by fatty acids surrounding droplets of oil placed in water.

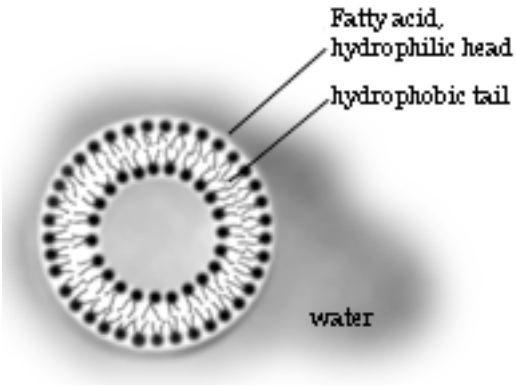

Fig. 4. Liposome formation

3.3 Cluster Formation

It is not always desirable to have all SOCA elements participating in the formation of one structure like the membrane above. It may be necessary to assemble a complex structure hierarchically. To illustrate, a simple bridge constructed of steel girders is not assembled one girder at a time. A few girders are first bolted to one another and to a floor to form a sub-unit of the bridge. Several of these sub-units are then joined to form the complete bridge. How may hierarchical subassembly be achieved in SOCA?

A means of ensuring that SOCA elements self-assemble in stages triggered by their environmental conditions is required. This mechanism is implemented in the manner of Cellular Automata. The SOCA elements have, in addition to the table of forces generated between faces, a lookup table storing the transitions a face of a particular state may undergo when it encounters faces on neighbouring elements. This table contains, for each face state and each state it may encounter on a neighbouring face, a threshold which triggers the application of the transition. The transition itself, and its priority are also stored. The neighbourhood region falls within a constant range of a face's center.

A transition table may, for example, tell a green face that if it detects within its neighbourhood three red faces on other elements it should change to the red state with a priority of 2. The priority value is used to choose between rules triggered simultaneously. Low values indicate high priorities. Thus the transition table provides a means of testing environmental conditions and behaving accordingly. This enables elements to 'differentiate' in a manner analogous to biological cells. When a given set of environmental conditions are met, some change in the structure of an element may be triggered to alter the way it interacts with its environment. This may be understood as a *virtual chemical reaction*.

To create many dispersed clusters of elements arranged like those discussed in section 3.2, the following transition and force tables were utilized. These tables were arrived at through experimentation, since no automated means of reverse-engineering them from the specification of a desired emergent behaviour is (yet) available.

	Inert	Grey	Green	Blue	Red
Inert	0	0	0	0	0
Grey	0	-1	-1	-1	0
Green	0	-1	+70	-30	-2
Blue	0	-1	-30	-60	-20
Red	0	0	-2	-20	+70

Table 5a. Force table for cluster formation

	Inert	Grey	Green	Blue	Red
Inert	-	-	-	-	-
Grey	-	-	-	-	-
Green	-	-	8,Red,0	-	1,Red,0
Blue	-	-	-	-	-
Red	-	-	-	-	10,Green,0

Table 5b. Transition table for cluster formation
(cell data triple: threshold, transition, priority)

The SOCA system commences with a random arrangement of polyhedra like those of the previous section. They have grey lengths and opposite end caps of green and blue. As can be seen in table 5a, green faces attract one another quite strongly, blue faces repel one another slightly less strongly. Blue and green faces repel one another around half as strongly as the blue faces repel one another. Green, blue and grey faces are all repelled weakly by nearby grey faces. So far this is similar to the membrane forming system discussed in section 3.2. In fact, to begin with this is exactly the kind of behaviour which occurs.

Unlike in section 3.2, the transition table in this case acts to trigger changes in clusters of elements. Where a green face exceeds the threshold of 8 green neighbours, it is instructed by the transition table to change state to red with the highest priority (0). The same table also says that any green face which exceeds the threshold of 1 red neighbour should become a red face itself, also with priority 0.

The effect of this state changing is that 8 green faces in close proximity all become red. The force table 5a shows that red faces are strongly attracted to one another (as were the green faces) but that red and green faces weakly repel one another. Hence, the effect is to discourage further addition of green elements to the cluster which behaves like a small membrane of section 3.2, red faces inward, blue faces outward. The rule in the bottom right most corner of the transition table ensures that a red face encountering more than 10 red neighbours, will change into a green face with priority 0. This prevents large clusters of red / blue elements forming by expelling excess bodies and changing them back into the raw blue / green state.

The result of operating this SOCA system is illustrated [Fig 5]. The clusters sit apart due to the repulsion between their blue outer surfaces. Some clusters do not reach their quota of 8 elements and so remain green on the inside. Other clusters which have undergone the green / red transition fracture to form smaller units. Still other structures form with more than 10 elements, some hovering around the green / red transition. This complexity is the nature of a fully physically based model.

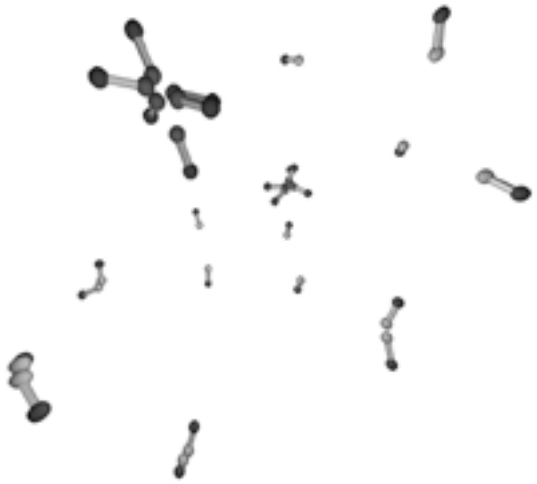

Fig. 5. Clusters of elements with red or green end caps inwards, blue end caps outwards

4 Future Work

The SOCA system is capable of simulating a vast range of emergent behaviours, far more than can be covered by this introductory paper. Work is under way to sub-assemble small groups of elements like the clusters in section 3.3, into larger groups which self-assemble into still larger configurations. Early experiments show that the SOCA elements are also capable of self-assembly into simple machines through the use of their transition tables. Elementary oscillators and rotary motors have been constructed and provide promise of further interesting results. Autocatalysis is also being investigated within the SOCA system.

5 Conclusions

A system of interacting rigid polyhedral units acting under simulated chemistry and physics has been shown to be useful for the study of self-organization and assembly. It has been demonstrated that physically based Self-Organizing Cellular Automata (SOCA) may feasibly simulate some of the basic interactions of the sub-units of living systems. Chaining, the linking of identical elements to form long, slender structures has been modelled. The formation of clusters and membrane like structures similar to liposomes has also been reproduced. The differentiation and segregation of groups of SOCA elements has been modelled by changing the state of SOCA elements according to their environmental conditions.

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