

Creating a Physically-based, Virtual-Metabolism with Solid Cellular Automata

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Abstract

A physically-based system of interacting polyhedral objects is used to model physical and chemical processes characteristic of living organisms. These processes include auto-catalysis, cross-catalysis and the self-assembly and spontaneous organization of complex, dynamic structures constituting *virtual organisms*. The polyhedra in the simulation are surfaced with bonding sites in states akin to those of cellular automata. These bonding sites interact with sites on neighbouring polyhedra to apply forces of attraction and repulsion between bodies and to trigger transitions in their states. Locally controlled assembly of this kind acts without the guidance of an external agent or central control. Such mechanisms, perhaps a defining property of biological construction, are seldom employed to create complex artificial structures. This paper therefore presents a novel model for the construction of complex virtual structures using multiple reactive, virtual elements, acting independently under virtual physical and chemical laws.

Introduction

At the microscopic 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 components. This paper presents a virtual system which operates on the same principles.

Models of some typical biological structures have been created using a physically-based system of interacting elements called *Self-Organizing (Solid) Cellular Automata* (SOCA) [Dorin 98, 99]. Models of chains and polymers, liposome-like clusters and membranes and a model of cluster reproduction by locally-induced fracture were demonstrated in these earlier publications. Using this simulation framework, new models of catalysis and auto/cross-catalysis are presented here. These models are then combined to create a *virtual organism*, which self-assembles from a set of simulated cross-catalytic reactions. This virtual organism has a simple virtual metabolism and reproduces by fracture in a manner reminiscent of the reproduction of single cells.

Various related fields of study, as well as some proposed areas of application for SOCA are briefly listed below. A

summary of the SOCA system follows. The next section serves as an introduction to chemical reactions and catalysis. A description of SOCA models of irreversible chemical reactions and simulations of catalysis, auto-catalysis and cross-catalysis follow. Finally a virtual organism which self-assembles via the interactions of SOCA elements engaged in virtual cross-catalysis is presented. Proposals for future work and conclusions are then given. Below is a brief summary of material relevant to the present study.

Physical Simulation - Researchers in computer graphics and robotics model solid/fluid interactions for the purpose of visualizing simulated physical processes (e.g. [Sims 94, McKenna & Zeltzer 90]). Similarly, these techniques are applied in the solid cellular automata simulation framework.

Cellular Automata (CA) - CA's have been widely studied as examples of complex dynamical systems [Gardner 71, Wolfram 84], under the banner of artificial life [Langton 86], and as examples of components in a self-reproducing machine [Burks 70, Gardner 70]. The global behaviour, said to be *emergent* [Cariani 91] from local interactions, shares features with that of the processes which maintain an organism [Dorin 96]. This was considered vital in the implementation of a model of life, hence the inclusion of its properties in the SOCA model.

Philosophy of Biology - The work of [Maturana & Varela 80], [Kauffman 93] and [Prigogine 85] to describe the organization of living things 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, auto/cross-catalytic chemical processes. These are taken here to be essential traits of any living thing, and hence necessary features in a model organism with any claim to *virtual* life. The model organism presented below was built with these considerations in mind.

Self-Organization/Assembly - [Penrose 59], [Ingber 98], [Fleischer 95] have presented self-assembling wooden machines, physical models of the mechanical properties of cells and software models of the development of multicelled organisms respectively. These studies are all similar in spirit to that presented here.

Other authors have explored similar systems including a mechanical system of blocks and magnets [Hosokawa et al 95] and a model of the self-assembly of the T4

bacteriophage [Goel & Thompson 98]. [Steels 95] investigates the development of language treating it as a self-organizing system. [Banzhaf 94] uses binary strings to explore auto-catalysis and metabolic formation. [Saitou & Jakiela 95a,95b] have examined the ordering of sub-assembly processes within larger scale construction tasks.

Reactive, Distributed Artificial Intelligence - Attempts have been made to utilize the emergent properties of interacting reactive agents [Drogoul & Dubreuil 92, Ferber & Jacopin 91]. 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 solution to the problem at hand is found.

Molecular Dynamics and Supra-molecular Inorganic Chemistry - Papers in supra-molecular chemistry grapple with self-assembly [Lawrence et al 95]. The interactions of groups of molecules may be visualized according to the shapes they form and the bonding sites these present to their surroundings. Molecules have characteristically arranged bonding sites which link to other molecules to form large *supra-molecules*. It is helpful to visualize molecules as polyhedra whose vertices are bonding sites [Muller et al 95], the resulting supra-molecules are visualized as organized collections of polyhedra¹. SOCA are an ideal choice for models of these phenomena.

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 and analytically-derived impulses prevent bodies from interpenetrating in a manner similar to that of [Baraff 89].

The fluid model incorporates viscosity acting on the bodies as fluid drag. 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. In keeping with the fluid models found in [Dorin 94, Wejchert & Haumann 91], effects of solids on the fluid medium are ignored, only effects of the fluid on solids within it are considered.

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

¹The models described in the supra-molecular chemistry literature visualize bonding sites at the vertices 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.

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.

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.

Here is a sample force table from [Dorin 98] intended to model the interactions of ferrous bar-magnets.

| | inert | blue | green |
|-------|-------|------|-------|
| inert | 0.0 | 0.0 | 0.0 |
| blue | 0.0 | -1.0 | +1.0 |
| green | 0.0 | 1.0 | -1.0 |

Tab1 Sample force table

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. (Therefore inert faces are usually omitted from force tables altogether.)

When a blue face on a solid element (read down the left column of the table) encounters a green face on a neighbouring element (read across the top row of the table), a force acting at the centre of the blue face is generated (read from the cell where the relevant row and column intersect) in a direction towards the centre of the green face [Fig1] (and vice versa since elements in this example have identical symmetrical transition tables). The strength of the force is attenuated across space according to an inverse-square law.

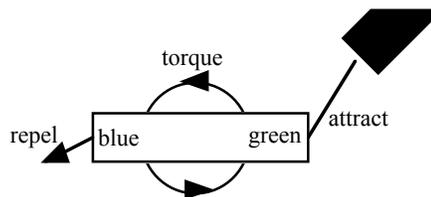


Fig1 Torque on simulated bar magnet

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, it may only *trigger* a response dictated by the *transition* table of the neighbouring body.

A sample transition table [Tab2] from [Dorin 98] appears below. It was used to construct organized collections of elements which reproduced by fracture. (I.e. when they reach a threshold size they split to form two collections, each of which then continues to grow until

reaching the threshold and once again splitting. Details are provided in the earlier paper.)

| | | | |
|-------|---------|------|------------|
| | green | blue | red |
| green | 8,red,0 | - | 1,red,0 |
| blue | - | - | - |
| red | - | - | 10,green,0 |

Tab2 Transition table for fracturing cluster formation
(tuple: threshold, transition, priority)

The table states that if a green face (read down left column) encounters green faces on other elements (read across top row) the interaction specified in the table (in the cell where the relevant row and column intersect) will become active.

This green/green interaction states that if the current green face simultaneously encounters eight green neighbours, it will change state to red. The third value in the cell is a priority for the interaction used to select from a set of interactions whose requirements are met simultaneously. This feature is not used in the experiments here and is omitted from the tables below.

The table above also specifies interactions for changing a green face in the presence of one red neighbour to a red face, and a red face in the presence of ten red faces to a green face.

A force table and transition table is specified for each element in the SOCA system. To date, all experiments have been performed using elements with identical force and transition tables. This simplifies the specification of the transitions required to obtain a desired outcome.

For the following experiments, the face of an element may be in one of the states *yellow*, *magenta*, *cyan*, *blue*, *green*, *red* or *grey* (after the colours in which they are drawn) or in the *inert* state. The strength of each applied force is here independent of the surface area of the face on which it acts. The density of all elements is identical unless otherwise stated.

The geometry of the elements used in the following examples was arrived at after some experimentation but is not mandatory. The system is sensitive to changes in dimensions of its elements. Largely this is because 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. Inter-element collisions in these simulations are elastic (the coefficient of restitution, epsilon, equals one).

Modelling Chemical Systems

A simple model reaction may be simulated between 100 randomly placed cubic SOCA elements. Each of these may be given five grey sides and one coloured side which, to begin with, is either red or blue (50% each of red/blue). These elements shall be referred to as blue-faced and red-faced respectively, similarly for other elements with single coloured faces.

The reaction $\text{red} + \text{blue} \Rightarrow \text{cyan} + \text{magenta}$ may be simulated using the transition table [Tab3] and an empty force table. The transition table contains entries which convert a blue-faced element to a cyan one in the presence of red, and a red-faced element to a magenta one in the presence of blue.

| | | | | | |
|---------|------|--------|--------|------|---------|
| | grey | red | blue | cyan | magenta |
| grey | - | - | - | - | - |
| red | - | - | 1,mag. | - | - |
| blue | - | 1,cyan | - | - | - |
| cyan | - | - | - | - | - |
| magenta | - | - | - | - | - |

Tab3 Transition table: $\text{red} + \text{blue} \Rightarrow \text{cyan} + \text{magenta}$

A graph showing the concentrations of red and cyan-faced elements for this irreversible process is given [Fig2]. Concentrations of red and cyan elements are drawn. Magenta and blue concentrations are symmetrical to these. In this simulation, elements are initiated with random velocities. Their reaction only occurs when the blocks are within each other's predetermined *neighbourhood region*. This depends on chance movements since no inter-element forces act in this run.

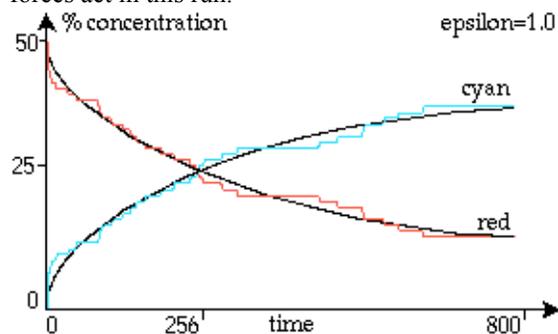


Fig2 Element concentration vs. time for reaction:
 $\text{red} + \text{blue} \Rightarrow \text{magenta} + \text{cyan}$

This graph is the expected outcome for a simple irreversible chemical reaction in which the reactants are being gradually consumed [Dorin 99]. The most notable feature is the intersection of the curves after 256 time steps. This point of equal concentration of cyan and red will be compared with the results in the following section.

Catalysis

A catalyst is a substance which binds substrate molecules (reactants) to its surface. The substrate molecules are held proximate to one another and in the correct orientation for them to interact to form the reaction's products [Beck et al. 91, p178]. Once the bound molecules have reacted, the catalyst is freed in an unaltered state allowing it to bind more substrate.

A virtual catalyst to drive the $\text{red} + \text{blue} \Rightarrow \text{magenta} + \text{cyan}$ reaction must bind to red and blue faces, bringing them together so that they can react. This may be achieved using

a cubic element with two adjacent (not opposite) binding sites, green and yellow, which attract red and blue faces respectively, but repel cyan and magenta faces so as to free itself once the reaction has occurred. Here are the force and transition tables for the system [Tab4].

| | grey | green | blue | red | cyan | mag. | yellow |
|--------|------|-------|------|------|------|------|--------|
| grey | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| green | 0 | 0 | 0 | +500 | 0 | -500 | 0 |
| blue | 0 | 0 | 0 | 0 | 0 | 0 | +500 |
| red | 0 | +500 | 0 | 0 | 0 | 0 | 0 |
| cyan | 0 | 0 | 0 | 0 | 0 | 0 | -500 |
| mag. | 0 | -500 | 0 | 0 | 0 | 0 | 0 |
| yellow | 0 | 0 | +500 | 0 | -500 | 0 | 0 |

Tab4a Force table for catalyzed reaction
red + blue => cyan + magenta

| | grey | green | blue | red | cyan | mag. | yellow |
|--------|------|-------|--------|--------|------|------|--------|
| grey | - | - | - | - | - | - | - |
| green | - | - | - | - | - | - | - |
| blue | - | - | - | 1,cyan | - | - | - |
| red | - | - | 1,mag. | - | - | - | - |
| cyan | - | - | - | - | - | - | - |
| mag. | - | - | - | - | - | - | - |
| yellow | - | - | - | - | - | - | - |

Tab4b Transition table for catalyzed reaction
red + blue => cyan + magenta

The figure [Fig3] shows the randomly placed elements of one virtual catalyst (green/yellow) and reactants (red and blue-faced elements). Frame two shows the red face having been pulled towards the green face of the now re-oriented catalyst. Likewise the blue face is approaching the catalyst's yellow face. Frame three depicts the newly created cyan and magenta products, brought about by the combination of the red and blue model substrate bound to the catalyst. In this frame, the yellow face of the catalyst has rotated out of view due to the repulsion between it and the cyan face. As can be seen also, the green face has rotated away from the magenta face due to the repulsive force between them.

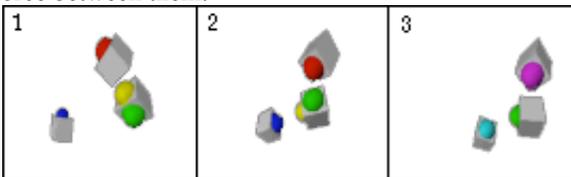


Fig3 Images from a catalyzed irreversible reaction

A run of the reaction commencing with 50 red-faced, 50 blue-faced and 10 yellow/green catalyst elements produced concentration plot [Fig4]. The virtual catalyst clearly speeds up the production of magenta and cyan from red and blue. The point at which equal concentrations of all elements was reached with the catalyst present appears at 150 simulation time units. The un-catalyzed reaction required 256 time units [Fig2] before reaching this point.

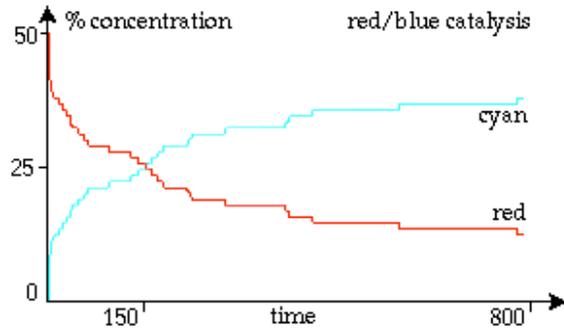


Fig4 Element concentration vs. time for catalyzed reaction red + blue => magenta + cyan

Auto-catalysis

A process of *auto-catalysis* may be illustrated as shown [Fig5] after [Prigogine & Stengers 85, p134]. This represents the production of (more) B from A, in the presence of B. The process is an example of a *positive feedback loop*, in conventional notation: $A+B \Rightarrow B+B$.



Fig5 Auto-catalytic loop

Auto-catalysis may be modelled using solid cellular automata elements which commence with two green end caps and four grey sides each. Here are the force and transition tables for the model involving the conversion of such elements into polyhedra with blue end caps replacing the original green ones [Tab5].

| | grey | green | blue |
|-------|------|-------|------|
| grey | -1 | -1 | -1 |
| green | -1 | 0 | +100 |
| blue | -1 | +100 | -100 |

Tab5a Force table for auto-catalysis

| | grey | green | blue |
|-------|------|-------|---------|
| grey | - | - | - |
| green | - | - | 1, blue |
| blue | - | - | - |

Tab5b Transition table for auto-catalysis

These tables state that a green face in the presence of a blue face will undergo a transition to create another blue face. The blue catalyst has an affinity for green faces and vice versa. Green faces are not attracted to, nor repelled from each other. But blue catalyst *is* repelled from others of its kind.

The conversion of green faces to blue at first proceeds slowly, but as more catalyst is produced and dispersed by

repulsion through the collection of raw green material, the reaction rate increases until the SOCA space contains nothing but dispersed blue-faced elements [Fig5]. (Some of the blue elements have been dispersed beyond the camera's view in frame four).

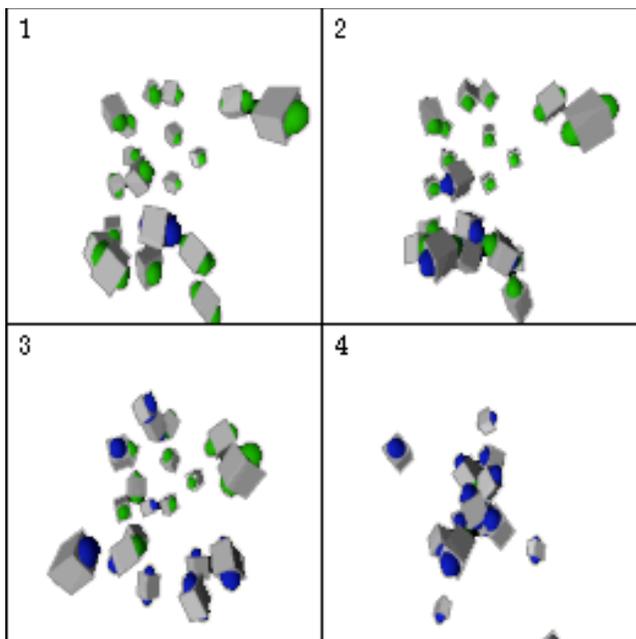


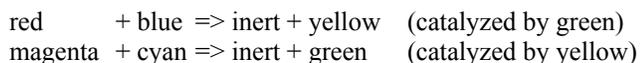
Fig5 Images from an auto-catalytic reaction

Cross-catalysis

The process of cross-catalysis is modelled in this section. Also, what is sought in this section is a virtual chemical process which is not only self-sustaining, but forms and maintains a dynamic, recognizable virtual structure. As indicated in the introduction, this would constitute an example of virtual life.

The SOCA elements of this experiment are cubes with faces in any of the states: inert, grey, green, yellow, blue, red, magenta, cyan or black. The simulation commences with elements randomly oriented and positioned.

Cross-catalysis involves two reactions which occur simultaneously, each producing as a product a catalyst for the other. This may be written in terms of SOCA face-states:



Hence a red face is converted to an inert face in the presence of a blue face. The blue face is simultaneously converted to a yellow face. Similarly, the magenta face is converted to inert and the cyan face which causes this is converted to green. A green face catalyzes the red/blue interaction, and a yellow face catalyzes the magenta/cyan interaction. The catalysis operates as described earlier.

A system commencing with a 25% mixture of elements,

each with one face coloured red, blue, cyan or magenta, will approach a concentration of 50% inert elements, and 25% each of yellow and green-faced elements. The further each reaction goes, the more catalyst it produces for the other reaction in the pair, which in turn produces more catalyst for the first, until the supply of reactants is exhausted. Hence this simulation combines auto-catalysis and catalysis of an irreversible reaction. Each reaction produces catalyst for its own acceleration indirectly by accelerating the other process in the pair.

Cross-catalysis may be established using the SOCA transition and force tables [Tab6]. Unlike the catalyst used with the irreversible reaction, (which had yellow and green faces to bring blue and red faces into proximity), the catalyst in the current reaction has a single face which attracts both reactants. I.e. the green-faced catalyst attracts *both* blue and red, and the yellow-faced catalyst attracts *both* cyan and magenta. This is not a necessary feature of the catalyst, as has been shown, but it does reduce the complexity of the force and transition tables.

| | grey | green | blue | red | cyan | mag. | yellow |
|--------|------|-------|------|------|------|------|--------|
| grey | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| green | 0 | 0 | +500 | +500 | 0 | 0 | 0 |
| blue | 0 | +500 | 0 | 0 | 0 | 0 | 0 |
| red | 0 | +500 | 0 | 0 | 0 | 0 | 0 |
| cyan | 0 | 0 | 0 | 0 | 0 | 0 | +500 |
| mag. | 0 | 0 | 0 | 0 | 0 | 0 | +500 |
| yellow | 0 | 0 | 0 | 0 | +500 | +500 | 0 |

Tab6a Force table for cross-catalysis

| | grey | green | blue | red | cyan | mag. | yellow |
|--------|------|-------|---------|---------|---------|---------|--------|
| grey | - | - | - | - | - | - | - |
| green | - | - | - | - | - | - | - |
| blue | - | - | - | 1,yell. | - | - | - |
| red | - | - | 1,inert | - | - | - | - |
| cyan | - | - | - | - | - | 1,green | - |
| mag. | - | - | - | - | 1,inert | - | - |
| yellow | - | - | - | - | - | - | - |

Tab6b Transition table for cross-catalysis

The virtual cross-catalytic reactions proceed more and more rapidly once the first random collision between reactants creates a catalyst. An amount of catalyst can even be included at the start of the simulation to kick-start the reactions. In either case, the conversion of reactant into product occurs in a manner like that described for auto-catalysis. The process is not quite as rapid as in the earlier case, due to the need for separate elements to be pulled towards the catalyst.

It was also found that the inert by-product of the reactions initially remains near the catalyst where it interferes with the catalysis by colliding with approaching raw material. This may be responsible for slowing down the conversion of raw material to some extent, but the degree to which this is true has not been tested. If interference from inert bodies is seen as a problem, they

can be removed from the system by any of the means discussed in [Dorin 99].

This simple cross-catalysis offers little for discussion beyond what has already been presented on catalysis and auto-catalysis. However at a simple level, the cross-catalytic reactions operate in the manner of a virtual organism. They require raw material to be fed into the system (red, blue, cyan, magenta), which is acted upon to produce (inert) waste material and material for the maintenance of the same set of processes, the catalyst (yellow and green). What is lacking is the assembly and maintenance of a recognizable topology for the virtual organism. This is now addressed.

Topology and Cross-catalysis

A suitable topology for the solid cellular automata is a cluster created in [Dorin 98]. This is a robustly assembled and easily maintained formation in which a collection of elements have one of their faces pulled towards the group's center by mutual attraction. The opposite faces are forced by mutual repulsion to fan out radially, away from the group's center. Using the transition table [Tab2], such clusters may be made to fracture like dividing cells. This property will be useful for creating and maintaining a dynamic topology in a virtual organism.

The assembly of a cluster from cross-catalysis by-products like those of the previous section is achieved by introducing coloured faces opposing the blue and cyan faces on the elements which have them. Each blue or cyan-faced element is given a grey face on the side opposite the pre-existing coloured face. The force table given shortly [Tab7] is set up for mutual attraction between grey faces. This attraction does not accelerate the red/blue interaction because the red elements do not have grey back-faces. Similarly, the magenta/cyan interaction is not accelerated by the grey/grey attraction.

The grey/grey attraction does however pull blue and cyan-faced elements together. They usually meet with their grey faces pointing towards one another. When each of these elements meets the other reactant in its pair, as specified by the cross-catalytic reactions, its blue or cyan face is converted to yellow or green accordingly. The grey back-faces are unmodified by this interaction so what remains is a pair of catalysts (one green and one yellow), bound at their back by mutual attraction between grey faces.

If individual blue or cyan-faced elements meet others which have already been converted to catalysts, their grey faces are still attracted to the catalyst's grey back-face. The elements sit beside one another until the blue or cyan face interacts with a red or magenta face to become a catalyst itself. Once again, two catalysts (one yellow, one green), are left back to back in a cluster.

Sometimes several green, yellow, blue or cyan elements form a cluster. Nevertheless, the same process unfolds during which these are converted into a cluster of yellow and green catalysts. The more green catalysts there are in a

cluster, the more this cluster will accelerate the local production of yellow catalyst, and vice versa. Hence clusters form with approximately equal numbers of green and yellow-faced catalyst elements.

This then is the formation of a recognizable topology, but it is not yet a dynamic topology. Organisms continually consume material from the environment, convert it to the material they need to build themselves and discard any waste material. The virtual structure as described simply 'grows'. It consumes red, blue, cyan and magenta from the environment, and produces inert waste. But the virtual body of this organism continually accrues yellow and green catalyst. Once material has formed a part of the virtual body it is not removed or exchanged for fresh material.

The final addition to the model is the specification of an additional transition. When a grey face has three grey neighbours, it is converted to an inert face. This breaks the bond of a catalyst to its cluster and it is pulled from the group by any neighbouring reactant, or is left to drift freely about the space. Alternatively, by introducing weak repulsive forces between yellow and green faces (these must not be strong enough to break the bond formed by their opposing grey faces), the yellow or green catalyst with an inert back-face will be forced out of the cluster to be replaced by a fresh yellow or green element with a grey back-face, as it is produced.

Although this scheme does indeed give the desired dynamic topology, it also has an unwanted side-effect. If three blue or cyan elements come into proximity due to attraction between their grey back-faces, these grey faces may be converted into inert faces and the blue or cyan elements can never form a part of a catalyst cluster. Thus additional waste is produced along with the catalyst which participates in the virtual organism.

To counter this, and to answer a question frequently posed by those who believe that reproduction is a necessary feature of life, an additional transition has been added to the model. The transition and force tables for the model incorporating all of the above interactions as well as the new transition are given [Tab7].

The extra transition requires that when a grey element has four grey neighbours, instead of being transformed to an inert face, it is converted to a black face. This black face is repelled from all grey faces, but attracted to other black faces. In addition, the black face will undergo a transition back to grey if it comes within range of five black neighbours.

| | grey | green | blue | red | cyan | mag. | yellow | black |
|--------|------|-------|------|------|------|------|--------|-------|
| grey | +500 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| green | 0 | -100 | +500 | +500 | 0 | 0 | -100 | -100 |
| blue | 0 | +500 | 0 | 0 | 0 | 0 | 0 | 0 |
| red | 0 | +500 | 0 | 0 | 0 | 0 | 0 | 0 |
| cyan | 0 | 0 | 0 | 0 | 0 | 0 | +500 | 0 |
| mag. | 0 | 0 | 0 | 0 | 0 | 0 | +500 | 0 |
| yellow | 0 | -100 | 0 | 0 | +500 | +500 | -100 | -100 |
| black | -100 | -100 | 0 | 0 | 0 | 0 | -100 | +500 |

Tab7a Force table for cross-catalysis/dynamic topology

| | grey | green | blue | red | cyan | mag. | yellow | black |
|--------|---------|-------|---------|---------|---------|---------|--------|--------|
| grey | 4,black | - | - | - | - | - | - | - |
| green | - | - | - | - | - | - | - | - |
| blue | - | - | - | 1,yell. | - | - | - | - |
| red | - | - | 1,inert | - | - | - | - | - |
| cyan | - | - | - | - | - | 1,green | - | - |
| mag. | - | - | - | - | 1,inert | - | - | - |
| yellow | - | - | - | - | - | - | - | - |
| black | - | - | - | - | - | - | - | 5,grey |

Tab7b Force table for cross-catalysis/dynamic topology

When four grey (or five black) faces meet up, an element is expelled from the group to start its own cluster. The asymmetry between the numbers of neighbours required to convert between grey and black (i.e. four grey and five black faces, instead of four of each) prevents repeated oscillations between the black and grey states by a group of elements, each with the requisite number of neighbours.

A rendering of the present experiment is reproduced [Fig6]. Two collections of catalyst are numbered. These clusters of grey and black-backed yellow and green elements are easily spotted amongst the other inert, blue, red, cyan and magenta material.

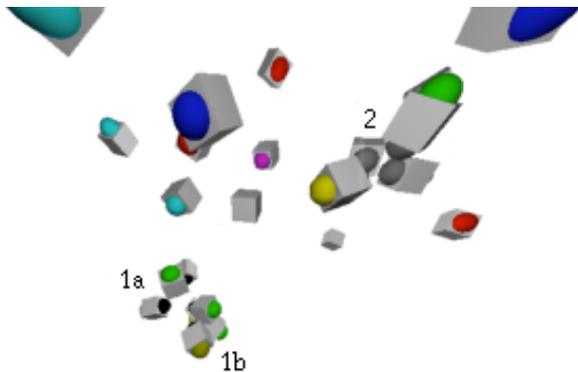


Fig6 Dynamic, fracturing clusters, formed by cross-catalysis

Clusters one and two arose from the same roots. Initially a single large cluster grew as all elements with grey faces were attracted towards a central location. This group exceeded its quota of grey elements and fractured. The figure clearly shows cluster one undergoing this process again as the number of elements in its body exceeds the quota permitted by the transition table.

Using the transition and force tables as they stand, there is no waste catalyst, it may all participate in the construction of virtual life. The catalyst is regularly expelled from a given structure and replaced by new material. Hence the clusters' topologies are dynamic.

Material is consumed in the production of the yellow and green building blocks. These blocks operate for awhile within a structure before removal and replacement. Waste produced by the bodies is left to float about the space. The structures *metabolize* in a simple (virtual) sense.

Additionally, although it is *not* required for a model of life, the structures are able to reproduce. They do this by fracture during which their virtual metabolism is not interrupted, as is true of real biological reproduction and metabolism. This example of virtual life, a representation of certain aspects of real life, is complete.

Conclusion and Future Work

A physical model of interacting molecules has been presented. The model contains virtual polyhedra with faces in states akin to those of cellular automata. These states may be used to govern the interactions between elements and so simulate various chemical reactions.

Presented in this paper were simulations of irreversible reactions, catalyzed irreversible reactions as well as auto and cross-catalysis. These simulations were amalgamated to produce a model of a simple virtual organism capable of self-assembly and maintenance. The model was also capable of reproduction by fracture whilst maintaining its virtual metabolism.

The construction of more complex static structures using SOCA has been described in [Dorin 98]. Dynamic structures which behave in ways similar to *gliders* and *spinners* from Conway's *Game of Life* have also been produced [Dorin 99]. In the future it is hoped to combine all of these models to construct virtual organisms with more complex physical forms capable of simple locomotion in a manner similar to that of a glider.

Acknowledgments

The author would like to thank Damian Conway for his supervision during the completion of the PhD from which this work arose. Also due thanks are those who provided practical and philosophical suggestions and additional information during the candidature including: David Baraff, Kurt Fleischer, Kevin Korb, Humberto Maturana, Jon McCormack, Craig Reynolds, Karl Sims.

"The chief difficulty Alice found at first was in managing her flamingo: she succeeded in getting its body tucked away, comfortably enough, under her arm, with its legs hanging down, but generally, just as she had got its neck nicely straightened out, and was going to give the hedgehog a blow with its head, it *would* twist itself round and look up in her face, with such a puzzled expression that she could not help bursting out laughing", Carroll, L. *Alice's Adventures In Wonderland* parallel Alan's Adventures with SOCA.

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