ABSTRACT
As disciplines converge and new capabilities are developed for programmable materials and self-assembly across length scales and industrial applications, designers will need new models for understanding the fundamental principles within this new paradigm. This paper outlines the key ingredients for self-assembly through a number of recent projects including the BioMolecular Self-Assembly and Chiral Self-Assembly projects. Further possibilities of non-deterministic self-assembly will be highlighted through asymmetrical units, nucleus models and hierarchical assemblies. Finally, opportunities for high-yield self-assembly and future applications for manufacturing and construction scenarios will be outlined. Self-assembly offers a glimpse into a future world of highly programmable, intelligent materials that promise far more adaptive, resilient and efficient built environments.
1 SELF-ASSEMBLY REVOLUTION

We are in a moment of unprecedented capability across length scales and disciplinary boundaries. The line between designer, scientist and engineer is blurring. New materials and capabilities are being developed in both natural and synthetic realms, offering programmability, computation, shape and property change and other life-like qualities. At the nano- and micro-length scales there is a design revolution taking shape through new design tools, like caDNAno and Project Cyborg, which allow scientists to design functional two- and three-dimensional structures for biomedical devices, drug delivery robots or even DNA hard drives (Douglas 2009). The A, C, T and G sequence is then compiled digitally, synthesized and billions of DNA strands self-assemble into functional structures. At a few length scales higher, material scientists are now able to produce self-healing materials, shape-memory materials, granular jammbale systems and micro-fluidic computational devices (Wei 1998). These unbelievable developments fundamentally rely on programmable materials and self-assembly to construct and manufacture functional systems without relying explicitly on human assembly. In the very near future we will likely see these developments influencing the production of architectural materials, infrastructural systems, manufacturing processes and construction techniques. In order to utilize these new techniques and material possibilities to their full potential, we first need to understand the underlying principles of self-assembly, error correction, activation energies and design possibilities for both deterministic and non-deterministic structures. This paper will focus on autonomous self-assembly, rather than self-reconfiguration, and will outline the aforementioned topics in order to highlight the inherent opportunities and constraints of self-assembly systems for future design scenarios.

2 INGREDIENTS FOR SELF-ASSEMBLY

It has been previously demonstrated that there are a number of simple ingredients for self-assembly across length scales and applications: geometry, materials, ambient energy and designed interactions (Figure 1) (Tibbits 2012). These ingredients can be designed around nearly every material, fabrication process and energy source available. For example, if one is working at the human scale, a source of potential energy might be gravity or magnetics. This energy source should then be tuned to the specific geometry and materials that will be acting in accordance to it. Objects might fall, or attract to one another based on their density or geometry. Finally, the objects or components would need to be designed to come together or change state in precise ways due to the influence of the provided energy source. For example, a male/female joint can be designed with a complementary tapering, so that components can come together easily under gravitational or magnetic forces. If the energy source or materials change given a different scale or application, the other ingredients would need to be updated to accommodate those parameters.

3 BIOMOLECULAR SELF-ASSEMBLY PROJECT

The BioMolecular Self-Assembly project, completed for the TED Global Conference in 2012, was a collaboration between molecular biologist Arthur Olson at the Scripps Research Institute, Skylar Tibbits of MIT and Autodesk Inc (Figures 2-5). This project demonstrated molecular self-assembly through tangible physical models (Olson 2007). The project contained three main elements: geometry, component attraction and external energy through random shaking (Figure 1). The geometry and material components were based on various molecular structures including the tobacco plant virus, ferritin protein assembly and catechol dioxygenase enzyme. Each of the molecular structures contained a
patterns of attraction during self-assembly shown through uniquely colored units.


Different number of elements: twelve in the tobacco plant virus, eight in the ferritin assembly and four in the catechol enzyme (Figure 3). We produced five hundred glass beakers containing the different molecular structures. Each beaker contained a single molecular structure colored either white, red or black, which could be shaken hard enough to break the structure apart, or consistently yet randomly to allow for the self-assembly of the complete geometry. The colored components could be mixed and matched with each other to demonstrate the variety of patterns or probabilities of self-assembly (Figure 4). For example, the tobacco plant virus contained twelve pentamer units, each with five sides, which could be connected to any one of the five sides of the neighboring part and so on. This produces an enormous array of different patterns (roughly $11! \times 5^{12}$ ) that can form the same molecular structure (Olson 2007). For example, if a beaker is filled with an equal number of black and white components, there is a great potential for different patterns to arise; sometimes an alternating pattern would emerge versus a different pattern where half of the dodecahedron was black and the other half was white. This variability nearly guarantees, due to the probability of the attraction orientations, that none of the molecular structures would be assembled in exactly the same way during subsequent trials, yet the overall global structure would always remain the same. This ability to generate the same global structure, despite allowing variability of the individual components, demonstrates one of the reasons that molecular structures are so robust and successful at self-assembling.

Within each beaker, there was a highly precise pattern of attraction designed into each of the components. This pattern of attraction allowed the components to come together, error-correct and collectively self-assemble the molecular structure (Figure 5). Each component has a number of faces and each face contains at least two magnets in order to correctly align a neighboring unit. The pattern of those magnets (positive or negative) can be manipulated in order to produce auto-aligned units and right/ left-handedness. The pattern of magnetic attraction acts as a programmed code in the physical materials, instructing the units on their placement and correct formation for state change. Error correction was demonstrated by having weak local bonds. For example, two single units come together in a fairly weak manner, given that only one of their faces is participating in a magnetic connection. However, as more units are added, the structure becomes increasingly stronger because each unit is held in place through a greater number of connections. If at any point a unit connects in the wrong orientation, the connection produced will be a weak one (only one of the two face-magnets will be participating in a connection), and therefore the dangling unit will eventually fall off. This process of weak local bonding that collectively adds up to stronger structures can be also seen in biological error correction in DNA and other systems (von Neuman 1965).
4 CHIRAL SELF-ASSEMBLY PROJECT

A second exhibit, the Chiral Self-Assembly project, was produced for Autodesk University in Las Vegas as a collaboration between molecular biologist Arthur Olson at the Scripps Research Institute, Skylar Tibbits of MIT and Autodesk Inc (Figures 6–7). This project was an opportunity to explore biomolecular chirality, or the ability for a structure to have a right-handed and left-handed pattern (Olson 2007). As demonstrated in the precise magnetic patterns of the BioMolecular Self-Assembly project, we were previously able to produce error-correcting structures and an encoded mechanism to dictate the successful formation of closed structures.

In the Chiral Self-Assembly project we aimed to further exploit this technique by demonstrating self-sorting structures. Given a large container with a completely mixed number of right-handed (yellow) and left-handed (black) pieces that were shaken randomly, we were able to demonstrate that two distinct and sorted structures (completely black and completely yellow) emerged where the right-handed units found one another and the left-handed units found one another without errors (Figure 6). The right-handed and left-handed units had opposite patterns of attraction which allowed them to repel the incorrect units while only attracting their mating pairs (Figure 5). This meant that for any particular unit, if you looked at one of the individual faces there would be a pattern where the left magnet was positive and the right magnet was negative. For the oppositely colored unit, the opposite would have been true: the left magnet would have been negative and the right magnet positive.

An interesting observation developed based on the speed of assembly. The Chiral Self-Assembly project showed that randomly mixed components can be self-sorted through random agitation given that they have smartly encoded attraction patterns and geometry. However, the speed for successful assembly was far slower than that of only a single unit. At first this might be obvious, since it was assembling two distinct structures. However, we observed that the speed was, on average, much more than twice as slow for successful self-sorting. We are hypothesizing that this is because of the process of error correction and competition at any stage. A single unit may bump into many other units at any one moment and in this case there was roughly a 50 per cent chance that they would be bumping into an opposite-colored unit, which reduces the probability of quickly assembling. This means that the units are actually competing against one another and error correction takes much longer. However, if we were to include far more of the right-handed units than what is needed to make a complete structure, we probably could have ensured that successful assembly of both the right-handed and left-handed structure would have been faster. The right-handed structure would have been “programmed” to assemble first, leaving only left-handed units to be quickly assembled afterwards. There are many interesting studies yet to be conducted in this area of research in the hope that they lead to possible scalability for potential manufacturing applications, larger-scale error-correcting structures or even safety applications where materials only come together under very specific pre-programmed conditions.

5 NEW MODELS FOR NON-DETERMINISTIC SELF-ASSEMBLY

The Chiral Self-Assembly project highlighted a plethora of new possibilities for programming self-constructing and error-correcting assemblies, leading us to develop a number of new models for non-deterministic self-assembly. Non-deterministic assemblies are an interesting field of research given that the final outcome is not always known or desired to be a predetermined entity (Figure 8). As a design tool, non-deterministic structures offer the potential to utilize material mediums embedded with specific logics and possibly decision-making, to collaborate with humans in developing possible new design outcomes or global structures that were not previously known. This is distinctly different than generating random structures where a number of parts are put together in
arbitrary ways. This is also very different from deterministic structures that come together to produce structures that were previously known. Deterministic structures are often useful, especially in the case of manufacturing or other industrial applications where one might want complete control over the outcome. However, it is often the middle zone with oscillations between determinism and non-determinism that is the most difficult and potentially the most interesting (Wolfram 2002). We will outline three categories of prototypes for non-deterministic structures including asymmetrical units, nucleus models and hierarchical non-determinism.

Our first prototypes were focused on developing identical units that would allow for a certain degree of structural variability when self-assembled. In other words, we searched for determinate single-unit geometries that would lead to indeterminacy when observed at the level of multiple-unit interactions. In order to address the question of indeterminacy versus arbitrariness, we set the additional constraint of designing single-unit geometries whose assembly would lead to closed structures, thereby preventing indefinite growth. We developed units that can assemble either into a torus or a sphere (Figure 9), and units that assemble into spherical shapes with unique surface patterns (Figure 10).

The non-radially symmetrical unit still relies on the dodecahedron backbone and thus takes advantage of the high degree of probability leading to self-assembly, yet certain edges are missing and thus produce irregular patterns. These patterns help to demonstrate the number of possible orientations for each unit in combination with the large number of possible locations for each unit around the sphere.

A second set of prototypes were developed to investigate nucleus models as a method for creating irregular assemblies. These systems consist of a series of identical pieces that, along with an interchangeable nucleus, give rise to different recognizable geometries (Figure 10). The potential of such systems lies in the ability to create highly specialized assemblies by simply designing a unique center piece, and combining it with mass-produced, standard parts. The idea of introducing a specialized element into a pool of standardized parts in order to generate a specific product or assembly has been used successfully in bioengineering (Huang 2007). This precedent suggests that the reuse and reprogramming of standardized parts is in fact an efficient technique when aiming for high system specificity, while also minimizing the number of uniquely designed components.

A final type of self-assembly structure utilizes hierarchical assembly as a method for creating irregular structures. If we look at the BioMolecular and Chiral Self-Assembly projects, we can see local non-deterministic structures where units move around stochastically and connect to arbitrary neighbors. However, when the parts come together, they form deterministic structures. Similarly, if we want to develop further non-deterministic structures we
can imagine producing another level of assembly. This type of third-order would allow the deterministic closed structures (for example, the dodecahedrons) to connect to one another in non-deterministic ways so as to produce irregular assemblies at this higher-order level (Figure 12). In this example, there were a fixed number of “Siamese” units that were produced with two faces, back-to-back, so that when a closed structure is created, there are certain units that have open faces on the outside to connect to neighboring units. The non-deterministic order of the first level and the number of “Siamese” units in the mix would help to shape the potential global irregular structures that could emerge; however, they could not be predicated without being tested or simulated. These irregular hierarchies could potentially be infinitely built on top of one another to produce deterministic and non-deterministic structures cyclically.

Hierarchical non-deterministic self-assembly may theoretically relate to biological orders of complexity (primary, secondary, tertiary, and quaternary structures). It may also be analogous to the lower levels of cellular division and specialization that can lead to somewhat determined human form while allowing a vast diversity of traits, features and specialized cell-types to be expressed. This type of local non-determinism, middle-determinism, and global non-determinism can be seen as a design tool that, when seeded with embedded logics and given enough room to differentiate and explore the search space, could produce highly “evolved” solutions for specific environments or contexts that may be difficult to predict beforehand. Further, this type of hierarchical material can be viewed as a fully recyclable “programmable matter,” as suggested by Neil Gershenfeld and George Popescu in their work on digital materials (Popescu 2007). These materials could start out as deterministic units at the smallest scale, then be assembled stochastically to form again deterministic macro-units, then build contextually guided connections, ultimately producing highly differentiated systems at various length scales. For example, the same programmable micro-material may self-produce a brick that is then self-assembled hierarchically to build a house. When the materials are not needed or fail, they could be broken down to determined levels and recycled for other functions.

6 HIGH-YIELD SELF-ASSEMBLY

The levels of hierarchical determinism versus non-determinism require one key ingredient: many parts. This requirement has led to a branch of research investigating high-yield self-assemblies. The idea behind high-yield assemblies is to study systems with many parts, the amount of energy required to produce a high-yield of assembly and the success rate of the structures built. We were...
able to test the self-assembly of eighteen macro-structures, each made with twelve parts, totaling 212 identical parts in the system (Figure 12). We poured the separate pieces into a container and agitated them continuously for several minutes, which led to a series of observations.

The first observation was that it takes nearly the same amount of stochastic agitation to self-assemble only one dodecahedron as it does to self-assemble many of them. This is an exciting finding, in that it suggests that the amount of energy required to manufacture a single part is not directly proportional to that required to manufacture many parts. The second observation is that we were left with fourteen successful assemblies and more than four partial assemblies. This means that the incomplete assemblies were in configurations that could not be further connected. However, there were more partially complete assemblies than would have completed the eighteen initial structures. Further, the yield could be counted as fourteen complete over eighteen total or 78 per cent with nearly the same energy as just one assembly. This output could be increased in one of two ways. One solution is to add more units to the system with a type of “smart pouring” where a sensor could detect the number of required units to complete the assemblies and give more time. The second solution is that the system could increase the amount of agitation so as to break apart the remaining elements, then cycle-down the agitation to self-assemble them again. Either way, a system of high-yield self-assembly is an exciting potential for manufacturing processes in the future where precision placement and determined time to produce a component is replaced with stochastic smart interactions and high-yield to low-energy input. Similarly, we would need to switch our evaluation metrics to probabilistic time frames rather than precise part-production times with the understanding that overall times would decrease, and local part-times are indeterminate. A future area of study includes guided mutations in high-yield systems by utilizing irregular assembly components in large numbers that interact and propagate non-deterministic patterns across the field.

7 FUTURE APPLICATIONS

The prospect of self-assembly stretches from the unprecedented design revolutions happening at the nano- and micro-length scales all the way through large-scale industrial applications. We have outlined a number of projects that explore the concepts of self-assembly, chirality, hierarchical orders and non-deterministic, irregular structures. These principles can be seen as the
fundamental design opportunities and constraints given within this world of programmable materials and physical self-organization. In order to utilize self-assembly as an industrial technique we need to first understand the governing orders of complexity, hierarchies and possible solution space that can emerge from bottom-up construction. The opportunities that have been highlighted within the fields of irregular assemblies, whether through nucleus models, asymmetrical units or hierarchical assembly, may ultimately be utilized as design tools for physical “computation” or generative solutions. These tangible models of irregular self-assembly may also lead to future insights into the origins of life problem or new understandings in biological assembly, order and specialization (Gillet 2005).

Deterministic models of self-assembly and high-yield systems can potentially have far-reaching applications in manufacturing or construction where ambient energies can be supplied to self-construct determined and precise structures. In manufacturing, the processes of sorting or sifting can be seen as a type of self-organization of non-homogenous particles through random agitation. In the future, we imagine that these processes will go further and be utilized for constructing new types of products that cannot be made with current assembly techniques. For example, complex structures with internal and external intricacies that cannot be produced with traditional processes like injection molding may be possible. Similarly, self-assembly could be utilized as a process for reducing energy input while maintaining high output with error-correcting material systems. In a broad sense, we see a future of highly adaptive products, resilient infrastructural systems and self-constructing/repairing techniques that utilize smarter materials to respond to internal logics and external stimuli. New models of construction will be needed in scenarios where current techniques no longer work; where old models are too dangerous, expensive or energy-intensive. Thus, smarter materials and self-constructing systems may be the key to developing a future of highly responsive and efficient built environments.

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WORKS CITED


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