Chapter 1
Systems Design Concepts Mimicking Bio-inspired Self-Assembly

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Abstract Design of complex self-assembly systems requires intelligent solutions that can be manufactured effectively and efficiently. Self-organization is the spontaneous formation of organized structures that can dynamically reconfigure with changing environments. These processes are primarily observed in chemical and biological processes that resemble large-scale ecosystems and in environments as small as biological cells. Inspired by these natural processes, there is also a growing research interest in developing 4D Design and printing technologies in which 3D structures reconfigure with changing stimuli. The 4D design process requires appropriate design, computational and simulation tools aimed at building structures at larger scales that can augment the current engineering design and manufacturing processes. This study presents a new multi-agent framework with two new paradigms called *agents-as-blocks* and *free-agent*. We present further details on these new strategies in the form of preliminary case studies applied to simulating micro-environments of microtubules' self-organization process and through a vibration simulation platform. Our simulation results closely follow the real formation patterns in the microtubules process and show some interesting self-organizing and self-assembling patterns that change with varying geometries, rules, and stimuli in a vibration-platform environment.

Keywords: self-organization, self-assembly, agent-based-models, multi-agent-systems, microtubules, 4D Printing

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1.1 Introduction

Self-organization happens at multiple scales and is studied across various domains, including biology [4, 27], ecology [30], and social systems [31]. For example, in social animals like ants, bees, sheep, fishes, hornbills, etc., simple individual behaviors lead to the strikingly magnified emergent phenomenon that is beyond the scope of the participating individual entities [26]. Collective decision-making, communication, task assignment, and collective exploration are some properties the social animals demonstrate that lead to complex self-organization at swarm and nest levels [15, 28]. Understanding and unleashing nature's potential to develop complex systems can address many of the current design challenges and thus can lead to a new era of engineering design and manufacturing [5, 22].

Self-organization and self-assembly can be defined as the spontaneous organization of entities that leads to emergent patterns, functions, and structures that demonstrate a purpose at a higher level [31]. For example, biological cells further divide and self-organize into tissues and organs, an outcome determined by geometry, physical environment, and chemical signal factors [11]. These processes demonstrate emergent properties that depend on the entities' geometry, interactions, and environment [19]. Studies point to a series of organized transformations leading to a concentration of energy at non-equilibrium states as the reason behind self-organizing patterns [31]. This is subtly different from self-assembly, where the systems tend to form structures at an equilibrium [24, 27], are mainly observed at the micro-scale in biological and chemical processes.

The first macro-level demonstrations of self-assembly were by the mathematician Lionel Penrose using Block Replicators in 1957 [21], which were inspired by the replication of DNA. More recently, the works at the self-assembly lab at MIT by Tibbits' team gained attention for their applications in architectural design and macro-structure formations, including the possibility of industrial-scale assembly applications [19]. Some notable works include studies on *self-replicating spheres*, *aerial assembly*, *fluid assembly chairs*, and *autonomous mass assembly* [17]. Tibbits et al.[18] study various patterns that arise from the suspended magnetized spheres on a vibration platform in a *self-replicating spheres* project. The unique designs of the sphere formed by a combination of smaller magnetic metallic spheres allow them to form new connections, give flexibility and allow divisions. The *aerial assembly project* investigates self-assembly in different environments like water, vacuum, and air.

4D printing is the reconfiguration of 3D printed structures over time in response to an external stimulus [7]. Material selection, also known as shape memory polymers (SMPs), plays a crucial role in allowing the reconfiguration process [20]. The applications of 4D printing range from developing simple visual prototypes to electronic device design, tissue engineering, soft robotics, biomedical devices, and implants [12]. Chu et al. [7] present similar insights and example applications at the macro level and also emphasize the need for addressing challenges related to material selection, computations, and the need for unconventional design strategies for building 4D technologies.

Jari et al. [1] recognize 4D printing as one of the key technologies in the additive manufacturing domain of industry 4.0. Also, Deepak et al., in their review of the 3D and 4D printing technologies in Industry 4.0 [2], present the need for 4D printing in developing smarter biomedical, electronics, aerospace, and automobile designs that also adapt to changing environments and stimuli. Similarly, Demoly et al. [3] highlight the need for 4D printing and self-organizing frameworks for advanced, flexible, and economical manufacturing technologies in the Industry 4.0 initiative.

Based on the existing literature and the importance of 4D printing for industry 4.0, we recognize the need to develop appropriate computational tools to support the self-assembly systems design process mimicking 4D printing. Therefore, in this study, we develop a multi-agent framework that proposes the *agents-as-blocks* and *free-agent* design strategies for designing and simulating self-assembling systems structures at multiple levels.

The remainder of this paper is organized as follows. In the next section, we present the multi-agent framework and the generic definitions for artificial self-organizing agents, followed by the introduction to the two novel strategies for demonstrating self-assembly/ self-organization through the behavior-tree framework to define agent rules and behaviors. Finally, we present the results of two case studies obtained by applying the proposed strategies to microtubule self-assembly simulations and demonstrating self-assembly design through vibration platform simulations.

1.2 The Approach

The proposed approach involves developing a multi-agent framework system (MAS) based on agents [15] and their interaction within an environment. These agents can respond to different conditions through various decision-making rules or policies in a decentralized way. More intelligent forms of agents develop consensus towards achieving common or conflicting goals and can learn and adapt to changing environments. Generally, agents can either possess a physical embodiment or be defined logically. For example, in multi-robot systems, each robot has a physical boundary, can interact with other agents through sensors, and interact with the environment through manipulators. On the other hand, as defined by Byrd et al., [6] trading agents are a logical representation or module in software in contrast to the physicality of robot agents. These trading agents can interact and compete with other agents in a trading environment and make decisions like buying, selling, or holding stocks by analyzing the trading information and applying various algorithms. Further, a multi-agent group composition can sometimes be heterogeneous with multiple types of agents that may structurally or functionally be different [8].

A self-organizing behavior can be achieved by carefully controlling the agent properties, group compositions, and environmental parameters. These organizations can either be stable, forming self-assembling patterns at equilibrium or re-configuring depending on the environmental stimuli change. The forming structures and patterns can demonstrate hierarchy, where a larger formation is through smaller intermittent entities. These intermittent structures can also act as agents with emergent characteristics formed from smaller entities. We present a comprehensive diagram in figure 1.1, which details various components in a multi-agent framework for self-organization.

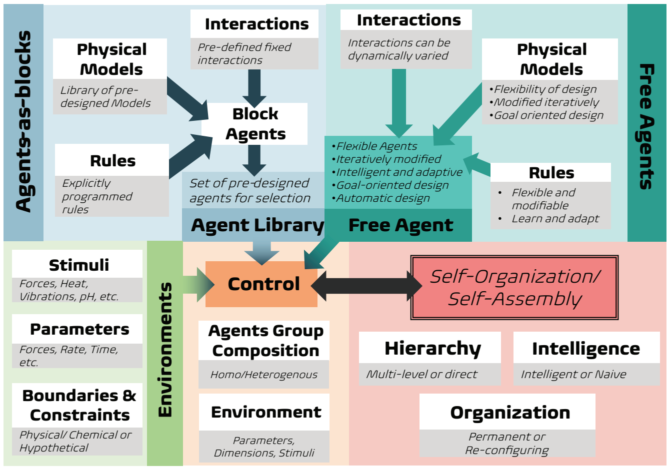

Fig. 1.1 Diagram explaining various components of the MAS framework used in the current study.

1.2.1 Design Strategies

In engineering design, selection and original design processes are prominently followed [16]. Similarly, to form self-organizing structures, a selection design process can be applied by selecting and combining different entities or by building the entities ground up. The design process selection is based on the end goal requirements and constraints. We extend the selection and original design processes to a multi-agent self-organization framework through the design strategies: *agents-as-blocks* and *free-agent* strategies, respectively as shown in figure 1.1.

In the *agents-as-blocks* strategy, an agent library is first developed by adding a wide variety of agents with different model types, rules, and interactions called block agents. From this library, a set of heterogeneous or homogeneous combinations of agents can be selected to demonstrate the desired self-organization patterns. Arriving at the right combinations of agents for a desired self-organizing or self-assembling behavior is challenging and hence would require a few iterations. This iterative selection process can be automated using selection algorithms with a simulator in the loop that runs until an optimal solution is obtained. We term this process the *agents-as-blocks* strategy as this is similar to the selection of the right building blocks of Legos for constructing models. The agents, on the whole, in this strategy are inflexible and inadaptable and go by a fixed set of rules and interactions. Further, this strategy can also lead to the selection of impossible combinations of agents that may fail to demonstrate a self-organizing behavior. And conversely, a desired self-organizing behavior may not have suitable agents available for selection.

We address the shortcomings of the *agents-as-blocks* strategy by introducing the *free-agent* strategy based on the original design process. Compared to a selection design process, an original design provides the advantage of flexibility and accuracy and overcomes availability and selection limitations. Thus, in a *free-agent* strategy, similar to the original design process, agents can be designed freely without any restrictions on models, rules, and interactions. The design complexity of the agent can be varied and depends on the desired outcome, and thus an agent can either be explicitly designed for the desired behavior or can be built by combining properties from a set of models, rules, and interactions.

The iterative modifications in a *free-agent* strategy are at the property level in contrast to the iterative selection in the *agents-as-blocks* strategy. Further, *free-agents* can also be designed to be intelligent and adaptive through policies that represent their behavior rules. The *free-agent* design process can also be automated at the property level through property selection algorithms. Additionally, a stable *free-agent* can also be added to the agent library for future use as part of the *agents-as-blocks* strategy, as the agent selection process in *agents-as-blocks* is faster and less complex than the *free-agent* design process.

1.3 Case Studies

We present two case studies for each of the proposed *agents-as-blocks* and free agent strategies. The first case study focuses on the self-assembly simulation of dynamic instability in microtubules. Our second case study is on the self-organization of macro-sized agents on a vibration platform, similar to the self-replicating spheres, and autonomous mass assembly studies by Tibbits et al. [17] Finally, we present some simulation results on self-organization for both the case studies.

1.3.1 Case Study #1: Microtubule Self-Assembly Simulations

Microtubules are complex networked protein structures responsible for many crucial intra-cellular processes in eukaryotic cells [23]. These are highly dynamic polymers undergoing continuous assembly and disassembly [25]. The building blocks in these structures are globular proteins of types α and β that combine to form *Heterodimers* (dimers). Structurally these are hollow cylinders with *heterodimers* arranged on their walls, forming a helical structure. Each level has 13 members in a eukaryotic cell with an approximate diameter of 25 nm. Microtubules undergo a continuous growth and shrinkage process through the assembly and disassembly of their structures controlled by MAPs (Microtubule Association Proteins) [29], generally starting from centrosomes or sometimes in the cytoplasm. The dimers in a microtubule are activated by bonding with GTPs, and these activated dimers can bond with other active dimers to form a microtubule. In this process, a biological cell consumes energy to maintain the concentrations of GTP that favor polymerization [9]. The activated dimers in the main microtubule structure de-hydrolyze turning GTP to GDP over time, deforming the bonds in the tubulins, thus inducing strains and making the structure unstable. An unstable dimer detaches itself, leading to depolymerization of the microtubule.

In our previous work [10], we presented the formation of protofilaments and ring substructures using agent-based models. We also analyzed the effect of factors like GTP concentration, GTP to GDP transition delays [9], and bonding probabilities on

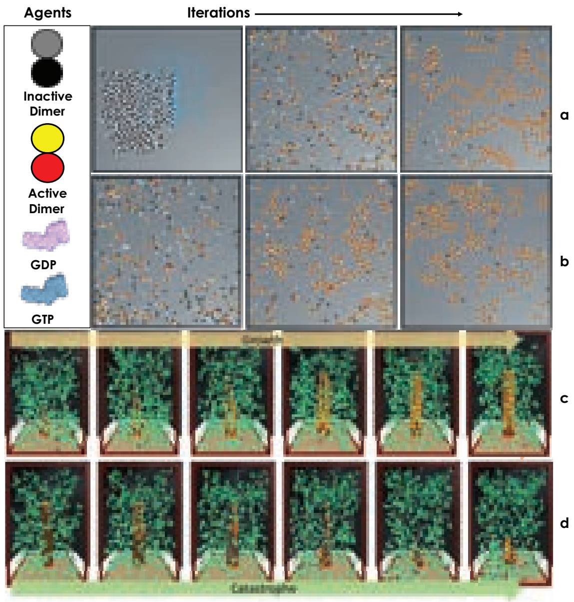

Fig. 1.2 Snapshots of simulations obtained during the a) Self-organization of protofilament sub-structures over time b) Self-organization of ring sub-structures. c & d) Growth and shrinkage of microtubules demonstrating dynamic instability.

the sub-structure formation. To simulate the microtubule self-assembly, we developed a multi-agent simulator following the *agent-as-blocks* strategy that simulates the formation of microtubules and their intermittent structures. In this case, the agents were designed following the *free-agent* strategy and were added to an agent library. From this library, various combinations were tested for different behaviors that closely resemble the microtubule formation in-vivo. The agent design was based on a literature review, where approximate geometries resembling the real structure were developed. The control rules were based on the protein characteristics that were embedded in the form of behavior trees [14, 13].

1.3.2 Case Study #2: Self-organizing Systems Design and Organization

The second case study deals with self-organizing systems design with varying building blocks and the resulting final structures through the development of a vibration simulation platform. The simulator and agents were developed in Unity 3D combined with CAD models. The agent design process follows the *free-agent* strategy, where the user can select a physical structure or design one as per the requirement. The rules are picked from a pre-made set or can be exclusively designed using behavior trees. The user can finally assemble the right combinations as required for testing the self-organization process.

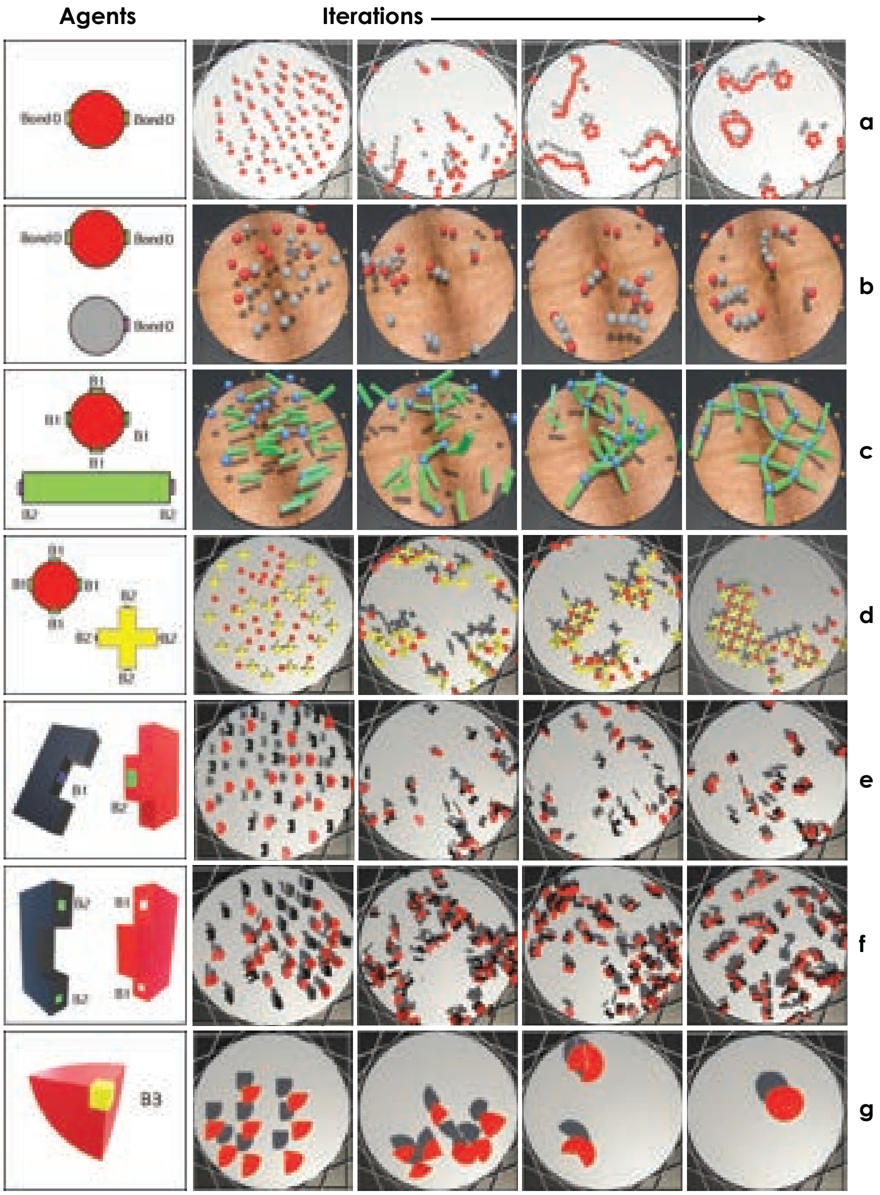

Fig. 1.3 a) A spherical agent with two bond 0 sites forming chains and rings b) Two different spherical agents forming linear chains. c) Spherical and Cuboid-shaped agents forming grid structures. d) Sphere and cross-shaped agents form uniform mesh lattice structures. e) Puzzle pieces as agents with a single bond location forming small plates f) Puzzle pieces as agents with changed bonding location forming a chain, arch, and plate patterns g) A quarter sphere self-assembling into a sphere.

The vibration platform has a circular disc surface suspended over a rigid base platform. An invisible enclosure is designed around the vibration plate to ensure the agents remain within a boundary while the simulations are in progress. The vibration plate has 3-Degrees of Freedom, and the frequency and amplitude of vibration along the three-axis can be varied during run time. The vibrations along all the axes follow a sinusoidal pattern. At the same time, the vibrations along the x and y axes can be switched between elliptical (for both clock and counterclockwise directions) and linear patterns. In an elliptical pattern, the amplitude along the x and y axes translates to the major and minor axes' lengths in an ellipse, respectively.

For our current study, we utilized stock models like sphere and cuboid and customized physical models for an agent. To simplify the rule selection process, we designed bond entities that are massless, cubical structures designed to interact with other agents within a specific range. The interaction rules for the bonds are designed in a behavior-tree structure and are programmed to react selectively. For example, in the current case study, we used Bond 0, 1, 2, and 3. A Bond 0 can bond with one other Bond 0, a Bond 1 can bond with a Bond 2 only, and a Bond3 can bond with any number of Bond 3s. We combined the physical structures and bonds during the agent design process, mimicking chemical bonds and magnets. Some of the results obtained forming different structures are presented in figure 1.3.

In figure 1.3, the spherical agents in *a* are designed similar to Tibbits' reconfiguring spheres [17], with bond type 0 on two opposite ends, and these agents formed chain and ring patterns. In *b*, the agents from *a* were combined with spherical agents with only one bond. These new agents ended in the terminal positions, thus leading to chain structures predominantly. We designed a spherical structure with four B1 bonds and combined it with a cuboid structure with two terminal B2 bonds in *c*, which formed grid structures. The quad bond spheres in *c* were combined with a cross-shaped agent that formed mesh lattice structures in *d*. In *g* a 3D sphere is formed from its symmetric wedges. In this case, a single bond B3 can stick with any number of B3 bonds that are fixed at a corner of the wedge.

The structures in *e* and *f* are formed from the same agent physical structures. However, they differ in the location of the bonds. While the agents in *e* self-organized into plate structures, the agents in *f* formed plates, chains, and arch patterns, whose composition also varied with the frequency and amplitude of the vibration platform. These are some examples to show the effect of interaction rules and geometry on the self-organization process.

1.4 Summary and Conclusions

In this study, a multi-agent approach with *agents-as-blocks* and *free-agent* design strategies framework for designing 4D self-organizing and self-assembling systems is developed. In both design strategies, we treated self-organizing entities as agents with a physical structure, interactions, and rules. *agents-as-blocks* is a designed selection-based strategy where pre-designed agents are introduced into an environment and tested for self-organization. On the other hand, *free-agent* strategy allows users to design or choose a combination of structures, interactions, and rules for designing agents. The two case studies presented demonstrate a successful self-organization process and possible designs. In the microtubule self-assembly simulations, we showed the formation of sub-structures like protofilaments and rings followed by the formation of a complete microtubule that undergoes both growth and shrinkage processes. In the second case study, we showed examples of designing free agents based on simple principles, and many interesting structures were observed, along with some significant variations that were affected by simple changes in agent properties. In the future, we plan to categorically investigate the effect of parameters on each simulation platform for designing and synthesizing self-assembled structures for multiple applications.

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