Towards Multi-Level Modeling of Self-Assembling Intelligent Micro-Systems

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ABSTRACT

We investigate and model the dynamics of two-dimensional stochastic self-assembly of intelligent micro-systems with minimal requirements in terms of sensing, actuation, and control. A microscopic agent-based model accounts for spatiality and serves as a baseline for assessing the accuracy of models at higher abstraction level. Spatiality is relaxed in Monte Carlo simulations, which still capture the binding energy of each individual aggregate. Finally, we introduce a macroscopic model that only keeps track of the average number of aggregates in each energy state. This model is able to quantitatively and qualitatively predict the dynamics observed at lower, more detailed modeling levels. Since we investigate an idealized system, thus making very few assumptions about the exact nature of the final target system, our framework is potentially applicable to a large body of self-assembling agents ranging from functional micro-robots endowed with simple sensors and actuators to elementary microfabricated parts. In particular, we show how our suite of models at different abstraction levels can be used for optimizing both the design of the building blocks and the control of the stochastic process.

Categories and Subject Descriptors

I.2 [**Computing Methodologies**]: Artificial Intelligence; I.6.5 [**Simulation and Modeling**]: Model Development—*Modeling methodologies*

General Terms

Theory, Performance, Design

Keywords

aggregation, self-assembly, micro-robotics, Monte Carlo simulations, macroscopic modeling, multi-level modeling

1. INTRODUCTION

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Aggregation is an ubiquitous phenomenon occuring at all scales: atoms and molecules [19], microfabricated parts [3], animals [14], and robotic systems, both with passive objects [1] and robots [9] as building blocks. Also, many functional structures found in nature are generated by a specific type of aggregation, self-assembly, which is essentially *stochastic*, *reversible*, and *directional* [18], i.e. the stability of an aggregate depends on the relative positioning of its building blocks.

This paper investigates and models the self-assembly of distributed intelligent micro-systems (e.g., micro-robots) with minimal requirements in term of sensing, actuation, and control. Among the recent implementations of self-assembling robots at the macroscale, Gross and colleagues demonstrated self-assembly in Swarm-bots, a mobile robot equipped with a gripper [9]. However, since they rely on a full breadth of sensors, including cameras, as well as a neural network as controller, their approach is not really suited to extreme miniaturization (below one millimeter). Klavins and colleagues have demonstrated self-assembly of triangular robotic modules that slide passively on an air table [11]. Here, permanent magnets serve as binding mechanism and the building blocks execute a common graph grammar in order to determine their actions. Once again, we believe that this type of controller is a strongly limiting factor in the context of extreme miniaturization. Garnier et al. [6] achieved a first step towards this direction by successfully implementing bio-inspired probabilistic aggregation in a group of Alice robots, which are only 2 cm in size.

Based on our experience in fluidic self-assembly of microfabricated parts, we believe that future micrometer-sized devices such as micro-robots must rely solely on stochastic self-assembly in order to achieve reliable and controllable collective pattern formation. In this context, we assume that the individual nodes are moving around and colliding in a random fashion; structured aggregates arise owing to the fact that each unit has some preferential binding direction, which makes aggregates with misaligned building blocks less stable. However, the notion of directionality involves an important difficulty: the probability of break-up of an aggregate depends on the relative orientation of its building blocks. Yet, several instances of such building blocks exist in reality, starting with molecules, which are typically assembled by combining two functional groups that we call *sticky ends*, which mediate the aggregation process. Along

the same lines, one can design microfabricated parts that have preferential binding direction according to their surface properties and their shape [13]. Future self-assembling intelligent micro-systems may exploit the same kind of interactions, possibly controlled in real time by changing their geometry, shape, or conformation.

Previous probabilistic models of aggregation [1, 4] and self-assembly [11] did not account for directionality. Zheng and Jacobs [20] proposed a first-order model for the self-assembly of hybrid micro-systems, which does not, however, account for reversibility. In their model, they assume that two assembled building blocks cannot break apart and that they have unique aggregation probability, which must be determined experimentally. Deterministic models of aggregation and flocking (which is conceptually similar to aggregation, but involves a coordinated motion of the aggregate) such as [17, 10] as well as graphical models of multi-robot systems such as [15] are interesting complements, from a system and control perspective, to our probabilistic modeling approach. However, they are not directly applicable to self-assembly processes because they do not account for the intrinsic randomness of these processes.

The present paper presents a suite of models at multiple abstraction levels that are able to cope with the extremely rich combination of features of multi-agent systems; this approach based on multi-level modeling has proven very successful in modeling systems involving robots of a few centimeters [1, 12, 2]. The complexity exhibited by stochastic self-assembly prevents a single model to probe the dynamics of the whole system. This fact motivates a combination of multiple levels of abstractions (e.g., microscopic and macroscopic modeling or multiple levels of microscopic representations) into a consistent multi-level modeling framework. On one hand, one needs microscopic modeling that is able to capture low-level details, namely component direction, shape, material, charge, and so on. On the other hand, one is interested in models that can yield accurate numerical predictions of collective metrics and investigate, possibly formally, macroscopic properties such as the size, the type and the proportion of the resulting aggregates. Multi-level modeling allows fulfillment of both requirements in a very efficient way by building up models at further abstraction levels in order to capture the relevant features of the system. Also, the calibration procedure can leverage the multiple levels, using data collected at a given level for calibrating parameters at one level above. In this paper, we use this methodology to capture directionality at the macroscopic level. Specifically, we start from a spatial microscopic model based on Netlogo [16], a programmable environment for multi-agent simulations (Section 2.1). At this level of abstraction, the position and the velocity of each individual agent is captured, thus making these simulations expensive in terms of both computation and memory requirements. As a result, we relax spatiality in a second type of microscopic model, based on the Monte Carlo method (Section 2.2). In this model, encountering probabilities are calculated using a geometric approximation, and break-up probabilities are shared with other models. Finally, a macroscopic model based on a discretization of the state space is proposed (Section 2.3).

2. MATERIALS AND METHODS

The system that we model hereafter is composed of N_0 agents (e.g., mobile robots, microfabricated parts), which we call *building blocks* hereafter. These agents move randomly throughout the environment (e.g., arena, liquid container) and they can, upon collision, bind with each other, thus forming an *aggregate*. The stability of an aggregate depends on the alignment of its building blocks. From the standpoint of an agent, this means that its propensity to leave the aggregate depends on the bearing of its neighbor. For the sake of simplicity, we assume in this paper that building blocks have a single binding site that can handle only one other building block at a time, thus implicitly limiting the system to the formation of dimers. This assumption does not limit the generality of our approach whatsoever as we are specifically interested in capturing the directionality of the aggregation process, and not the size of the aggregates.

Our multi-level modeling framework consists of three models at different abstraction levels: (1) a spatial microscopic model (agent-based), (2) a nonspatial microscopic model (Monte Carlo), and (3) a macroscopic model (mean field approach based on difference equations). The governing principle of our modeling methodology is to build the suite of models from the bottom up while conserving a consistent set of parameters that are shared at all abstraction levels, namely bond energies that determine break-up probabilities. Encountering probabilities are either computed using a geometric approximation (nonspatial microscopic model and macroscopic model) or explicitly simulated using a simple collision routine (spatial microscopic model). Some parameters such as the average velocity of the building blocks are estimated using models at lower abstraction levels.

2.1 Spatial Microscopic Model

Our spatial microscopic model is implemented in Netlogo, a powerful multi-agent simulation environment [16]. In this model, the dynamics of each individual agent is captured. Hereafter, we describe how we model the dynamics of the building blocks and the bonds that mediate the self-assembly.

2.1.1 Building Block Modeling

In our approach, we assume that building blocks are radially symmetric bodies with a mass m, a position $\vec{x} \in \mathbb{R}^2$ of their center of mass, a velocity $\vec{v} \in \mathbb{R}^2$, an orientation θ, and a radius r. The environment has a finite area A_{tot} and has toroidal boundary conditions.

Two building blocks B_1 and B_2 of radius r_1 and r_2, respectively, located at a distance d from each other, collide if and only if $d < r_1 + r_2$. The collision of two building blocks *invariably* leads to the formation of a bond. This assumption will be discussed in further details below.

A building block B_j of mass m undergoes stochastic perturbations of its trajectory, which can be described by a Langevin equation:

$$m\,\dot{\mathbf{v}} = -\gamma\,\mathbf{v} + \mathcal{N}(0, \eta\,\nu_s^2) \qquad (1)$$

where $\mathbf{v}$ is the velocity of the particle, γ is a drag constant for small Reynolds number, and $\mathcal{N}(0, \eta\,\nu_s^2)$ a stochastic force term of variance $\eta\,\nu_s^2$, which is proportional to the agitation of the system represented by the unitless value ν_s^2 (η is a constant term in Newton). For the sake of simplicity, we assume here that an aggregate undergoes, on average, the same stochastic perturbations as its building blocks. This assumption, which is obviously not verified in the case of

large aggregates, shall be relaxed in further work. Equation 1 is obviously relevant to building blocks that undergo Brownian motion, but one could use another equation of motion without restricting the validity of the approach presented in this paper.

The microscopic model captures the conformation of each aggregate, by keeping track of the relative positioning of each building block. Each building block is connected, if part of an aggregate, to other building blocks, called its *neighbors*, through a set of *bonds*. Each bond has a given energy ΔE, which depends on the relative alignment of the building blocks and determines its stability (see Section 2.1.2 for further details).

In this paper, we simplify our model as much as we can: building blocks are represented by circles with a certain orientation and a single preferential binding direction that can handle at most one other building block at a time. The collisions are handled in a purely deterministic fashion based on the relative alignment of the colliding assemblies $\xi = (\theta_1\ \theta_2)^T \in [0, \pi]^2$ (see Figure 1). For the sake of simplicity, we also assume that each individual node can determine the relative orientation of its neighbor with a perfect accuracy.

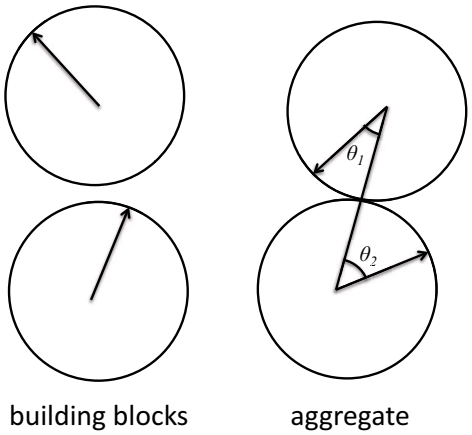


Figure 1: The relative alignment of two aggregated building blocks is given by two angles $\theta_1 \in [0, \pi]$ and $\theta_2 \in [0, \pi]$, i.e. the bearing of each building block with respect to the other. We assume that θ_1 and θ_2 fully determine the energy (and therefore the stability) of the aggregate.

2.1.2 Bond Modeling

A bond is created upon collision of two building blocks, and its energy ΔE is given by a Gaussian-like function of the relative alignment $\xi = (\theta_1\ \theta_2)^T$ of the colliding assemblies:

$$\Delta E(\xi) = -E_{bond} \cdot \exp\left(-\frac{\theta_1^2}{2\,\sigma_{\theta_1}^2} - \frac{\theta_2^2}{2\,\sigma_{\theta_2}^2} \right) \qquad (2)$$

where E_{bond} is the maximal bond energy, σ_{θ_1} and σ_{θ_2} are parameters denoting the misalignment tolerance of each building block, and θ_1 and θ_2 are the angles depicted in Figure 1. This energy function implies that aggregates with properly aligned building blocks have maximal bond energy (in absolute value). We expect this arbitrary energy function to be flexible and meaningful enough to be applied to a large body of target systems.

In our case, we assume that all building blocks have the same tolerance of misalignment, and the bond energy can therefore be written

$$\Delta E(\xi) = -E_{bond} \cdot \exp\left(-\frac{\theta_1^2 + \theta_2^2}{2\,\sigma_\theta^2} \right). \qquad (3)$$

where the parameter σ_θ can be tuned as a function of the building block properties (shape, surface properties, etc.)

To determine the policy of bond destruction, we use a model similar to the well-known *law of mass action* in chemistry. We know that the equilibrium constant K of a reaction

$$A + B \underset{k_-}{\overset{k_+}{\rightleftharpoons}} AB \qquad \text{with } K = \frac{k_+}{k_-} \qquad (4)$$

can be written as a function of the energy ΔE of the formed bond:

$$K = \frac{k_+}{k_-} = \exp\left(\frac{-\Delta E}{E_B} \right) \qquad (5)$$

where k_+ and k_- are the forward and backward rate constants, respectively, and E_B is the mean energy of the particles in the system, if they are thermally randomized to the Maxwell-Boltzmann distribution.

One can interpret the rate constants k_+ and k_- as probabilities of bond formation and destruction. Now, recall that we assumed above that all collisions lead to an aggregation regardless of the energy of the formed, which is similar to setting $k_+ = 1$. Therefore, the probability that one bond of energy ΔE will break up in the next time interval $[t, t + T]$ can be written:

$$p_b \equiv k_- \cdot T = \exp\left(\frac{\Delta E}{E_B} \right) \cdot T \qquad (6)$$

In the systems we are investigating, one cannot assume that the kinetic energies of the building blocks are randomized to any specific distribution. Furthermore, the system agitation is not limited to thermal agitation. Hence, the term E_B has to be replaced by a parameter $\alpha\,\nu_s^2$, that is, an energy term (α is a constant term in Joule) proportional to the agitation of the system, in its most general sense (see also Equation 1). Therefore, the breakup probability p_b of a bond of energy $\Delta E(\xi)$ can be written:

$$p_b(\xi) = \exp\left(\frac{\Delta E(\xi)}{\alpha\,\nu_s^2} \right) \cdot T \qquad (7)$$

2.2 Nonspatial Microscopic Model

NetLogo offers an interesting framework for spatial modeling, but it is expensive both in term of memory and computation. Indeed, the simulation stores the position, the orientation, and the neighbors of each agent. Also, it must determine at each iteration and for each pair of agents whether a collision occured or not. Hereafter, we describe a Monte Carlo approach, which does not capture spatiality, i.e. it does not keep track of the position and orientation of each individual. It is a stochastic microscopic model that, in contrast to macroscopic models (see Section 2.3), does not rely on a mean field assumption and a single representation for the whole multi-unit system. Indeed, each collision event is sampled individually and bonds are represented individually, even though it keeps track only of the total, absolute,

and discrete number of single building blocks. Furthermore, the algorithm stores only one piece of information about bonds: the relative positioning ξ of the building blocks they are connecting. Figure 2 outlines the pseudocode of the algorithm.

Since our model is nonspatial, collisions must be handled in a probabilistic fashion. Using a geometric approximation, the probability of encountering between two building blocks of radius r is written

$$p_c \sim \frac{\widehat{v}\, T\, w_d}{A_{tot}} \tag{8}$$

where $\widehat{v}$ is the average velocity of the building blocks (Equation 1), T the sampling time, $w_d = 2\,r$ is the diameter of the building blocks, and A_{tot} is the total area of the arena [12].

Algorithm 1: Pseudocode of the Monte Carlo simulation

input : a time span **tspan** and a total number of building blocks N_0
output: one realization of the time evolution of the system

data structures:
– $\mathcal{B}_i$ denotes the i-th buidling block, with $i = 1, \ldots, N_0$
– N is the number of single building blocks, initially N_0
– N_c is the number of single building blocks that collided ($N_c \leq N$)
– $\mathbf{\Xi_c} = (\xi_1, \ldots, \xi_{N_c})$ is the vector of aggregates that have just been formed, with $\xi_i = (\theta_{1,i}, \theta_{2,i})$ the relative alignment of the aggregate i
– $\mathbf{\Xi_a} = (\xi_1, \ldots, \xi_{N_a})$ is the vector of all aggregates, initially empty
– N_a denotes the total number of aggregates, i.e. the size of $\mathbf{\Xi_a}$

foreach t **in** tspan **do**
– Generate a random vector $\mathbf{X}^c = (x_1^c, \ldots, x_N^c)$ with $x_i^c \sim U(0,1)$
– Compute n_c the number of building blocks $\mathcal{B}_i$ that collided, i.e. that satisfy the condition $x_i^c < p_c \cdot N$ (Equation 8)
– Generate a random vector of relative alignments $\mathbf{\Xi_c} = (\xi_1, \ldots, \xi_{n_c})$ with $\xi_i = (\theta_{1,i}, \theta_{2,i})$ and $\theta_{d,i} \sim U(0, \pi)$
– Append $\mathbf{\Xi_c}$ to $\mathbf{\Xi_a}$ and let $N_a \leftarrow \texttt{size}(\mathbf{\Xi_a})$
– Generate a random vector $\mathbf{X}^s = (x_1^s, \ldots, x_{N_a}^s)$ with $x_i^s \sim U(0,1)$
– Remove from $\mathbf{\Xi_a}$ all aggregates ξ_i that broke up, i.e. that satisfy the condition $x_i^s < P_b(\xi_i)$ (Equation 7)
– Let n_b be the number of ξ_i removed from $\mathbf{\Xi_a}$
– Let $N \leftarrow N + 2\,n_b - 2\,n_c$
end

Figure 2: Pseudocode of the non-spatial Monte Carlo simulation.

2.3 Macroscopic Model

Both agent-based and Monte Carlo simulations are computationally expensive stochastic models, which only provide a single realization of the time evolution of the system. As a result, one must *always* perform several runs in order to obtain statistically meaningful results. Hereafter, we describe a macroscopic model of directional aggregation, which allows one to overcome these limitations. Our model is a time-discrete difference equation system, where k denotes the current iteration (time step) and kT the actual time, with T the sampling time, which is left out in the equations for the sake of simplicity, and should be chosen small enough in comparison to the system time constants/dynamics.

Capturing Directionality at the Macroscopic Level

First, we shall notice that one can describe the dynamics of each building block B by a Markov chain with a set of states $\mathcal{X}$. The state space $\mathcal{X}^{(\mathrm{B})}$ shall be discrete, finite, and it must reflect the type of the aggregate s that the robot is a part of. Unfortunately, the space $\mathcal{S}$ of aggregate's types is not discrete. Indeed, even though we can distinguish between single building blocks and pairs in a discrete manner, pairs take continuous energy values. As a consequence, we need to discretize $\mathcal{S}$ in order to obtain a discrete and finite state space $\mathcal{X}^{(\mathrm{B})}$. Now, a pair is fully defined by the relative positioning of its building blocks ξ, which is a two-dimensional vector. Fortunately, the symmetry of Equation 3 allows one to simplify this definition to a scalar, that is, the norm of the relative positioning, denoted

$$\theta^2 = ||\xi||^2 = \theta_1^2 + \theta_2^2 \in [0, 2\pi^2], \tag{9}$$

which can be easily discretized into a set of K averaged values $\widehat{\theta}_i^2$ given by

$$\widehat{\theta}_i^2 = \left(i - \frac{1}{2}\right) \cdot \frac{2\pi^2}{K} \quad \text{with } i = 1, 2, \ldots, K. \tag{10}$$

Therefore, the state space of the Markov chain is given by

$$\mathcal{X}^{(\mathrm{B})} = s_i \in \mathcal{S}_d \tag{11}$$

with $\mathcal{S}_d$ the discretized space of aggregate's types, with s_0 representing single building blocks, s_i pairs with an averaged relative positioning norm $\widehat{\theta}_i^2$ with $i = 1, 2, \ldots, K$ and a binding energy

$$\Delta E(s_i) = E_{bond} \cdot \exp\left(\frac{\widehat{\theta}_i^2}{2\,\sigma_\theta^2}\right). \tag{12}$$

Therefore, the probability for a building block B to aggregate with another building block into a pair of averaged relative positioning norm $\widehat{\theta}_i^2$ is

$$P\big(\mathcal{X}^{(\mathrm{B})}(k+1) = s_i \,|\, \mathcal{X}^{(\mathrm{B})}(k) = s_0\big) = 1. \tag{13}$$

Similarly, the probability for a building block B to leave a pair with an averaged relative positioning norm $\widehat{\theta}_i^2$ is given by

$$P\big(\mathcal{X}^{(\mathrm{B})}(k+1) = s_0 \,|\, \mathcal{X}^{(\mathrm{B})}(k) = s_i\big) : \mathcal{S}_d \to [0,1] \tag{14}$$

and will be denoted $p_l(s_i)$. A pair will break up if one or both of its building blocks leaves. Therefore, the probability $p_b(s_i)$ for a pair of type s_i to break up (Equation 7) can be written

$$\begin{aligned} p_b(s_i) &= 1 - (1 - p_l(s_i))^2 \\ &= p_l(s_i) \cdot \big(2 - p_l(s_i)\big) \\ &= \exp\left(\frac{\Delta E(s_i)}{\alpha\, \nu_s^2}\right). \end{aligned} \tag{15}$$

Using a set of difference equations, one can summarize the average state transitions of each individual Markov dynamical system, and thus keep track of the number of aggregates of type $s \in \mathcal{S}_d$. We write N_i the average number of aggregate of type s_i.

The average number of single building blocks N_s is given by the following difference equation

$$N_s(k+1) = 2\,\langle \mathbf{p_b}\ \mathbf{N_p}(k)\rangle - p_c \cdot N_s(k)^2 \tag{16}$$

with

$$\mathbf{p_b} = \big(p_b(s_1), \ldots, p_b(s_K)\big)^T$$
$$\mathbf{N_p}(k) = \big(N_1(k), \ldots, N_K(k)\big)^T$$

and p_c is the collision probability (Equation 8) and $\langle \cdot\ \cdot \rangle$ is the scalar product. The scalar term $\langle \mathbf{p_b}\ \mathbf{N_p}(k)\rangle$ is the average number of pairs that broke up at iteration k. The term $p_c \cdot N_s(k)^2$ is the average number of building blocks

that collided and formed a pair at iteration k. Similarly, the number of pairs of type s_i with $i = 1, \ldots, K$ is given by the following difference equation

$$N_i(k+1) = f(i) \cdot \frac{p_c \cdot N_s(k)^2}{2} - p_b(s_i) \cdot N_i(k) \qquad (17)$$

where $f(i) : \mathbb{Z}_+ \to [0, 1]$. The term $p_b(s_i) \cdot N_i(k)$ is the average number of pairs of type s_i that broke up at iteration k. The term $p_c \cdot N_s(k)^2$ is the average number of building blocks that collided and formed a pair at iteration k, regardless its type. Since two building blocks are needed to form a pair, this term is divided by two. Furthermore, since all formed pairs are not of type s_i, the function $f(i)$ determines the fraction of formed aggregates that are actually of type s_i.

Hence, the function $f(i)$ shall be a discretized version of the probability density of the random variable Z, which denotes the probability that a formed aggregate has a relative positioning norm $\theta^2 \in [0, 2\pi^2]$. Now, since $\theta^2 = \theta_1^2 + \theta_2^2$, one can write $Z = X^2 + X^2$, where X is a random variable that denotes the probability that θ_1 or θ_2 take a specific value in $[0, \pi]$. We assume that X is uniformly distributed, i.e. $X \sim U(0, \pi)$. Therefore, we have that $X^2 \sim Beta(0, \pi, \frac{1}{2}, 1)$ [8] and its probability density is given by

$$f_{X^2}(x) = \frac{(x/\pi)^{-1/2}}{\int_0^\pi (u/\pi)^{-1/2}\, du} = \frac{1}{2}\left(\frac{x}{\pi}\right)^{-1/2} \quad \text{with } x \in [0, \pi^2]$$

Now, the probability density of $Z = X^2 + X^2$ is given by the convolution of the probability density of X^2 with itself [8]:

$$\begin{aligned} f_Z(z) &= f_{X^2}(z) \star f_{X^2}(z) \\ &= \frac{1}{4}\int_{-\infty}^{\infty} \left(\frac{z-\tau}{\pi}\right)^{-1/2} \left(\frac{\tau}{\pi}\right)^{-1/2} d\tau \end{aligned} \qquad (18)$$

Since $z \in [0, 2\pi^2]$, we need to normalize $f_Z(z)$ such that

$$f_Z(2\pi^2) = 0 \quad \text{and} \quad \int_{-\infty}^{\infty} f_Z(z)\, dz = 1,$$

which leads to

$$f_Z(z) = \begin{cases} \frac{1}{4\pi} & \text{if } z \in [0, \pi^2] \\ \frac{1}{\pi^2} \arctan\left(\frac{\pi}{\sqrt{z-\pi^2}}\right) - \frac{1}{4\pi} & \text{if } z \in [\pi^2, 2\pi^2] \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, the function $f(i)$ is given by

$$f(i) = \int_{l(i)}^{u(i)} f_Z(z)\, dz \quad \text{with} \begin{cases} l(i) &= \frac{2\pi^2}{K}(i-1) \\ u(i) &= \frac{2\pi^2}{K} i \end{cases} \qquad (19)$$

with $l(i)$ and $u(i)$ the lower and upper bound, respectively, of the i-th subinterval of $[0, 2\pi^2]$.

Capturing Self-Alignment at the Macroscopic Level

All the aforementioned models assume that mitigated bonds either break up or remain unchanged. However, in reality, two aggregated building blocks may change their relative alignment because of random mitigation of their common bond. Indeed, the agitation of the system and collisions with other aggregates may cause the bond to change its energy state without breaking up, thus resulting in a change in the alignment of the aggregate. Our macroscopic model can be easily extended in order to take this phenomenon, which we call *self-alignment*, into account. To achieve that, we just need to modify slightly the difference equations governing the dynamics of pairs (Equation 17) such that pairs of type s_i can turn into pairs of type s_{i-1} and s_{i+1} at certain rate $a_-(i)$ and $a_+(i)$, respectively. As a result, the number of pairs of each type is given by the following system of difference equations:

$$\begin{aligned} N_1(k+1) &= f(1) \cdot \frac{p_c \cdot N_s(k)^2}{2} - p_b(s_1) \cdot N_1(k) \\ &\quad + a_-(2) \cdot N_2(k) - a_+(1) \cdot N_1(k) \\ N_i(k+1) &= f(i) \cdot \frac{p_c \cdot N_s(k)^2}{2} - p_b(s_i) \cdot N_i(k) \\ &\quad + a_-(i+1) \cdot N_{i+1}(k) - a_-(i) \cdot N_i(k) \\ &\quad + a_+(i-1) \cdot N_{i-1}(k) - a_+(i) \cdot N_i(k) \\ N_K(k+1) &= f(K) \cdot \frac{p_c \cdot N_s(k)^2}{2} - p_b(s_K) \cdot N_K(k) \\ &\quad - a_-(K) \cdot N_K(k) + a_+(K-1) \cdot N_{K-1}(k) \end{aligned}$$

where $i = 2, \ldots, K-1$. Unfortunately, determining the form of $a_+(i)$ and $a_-(i)$ is not straightforward and these rates may depend strongly on the nature of the interactions among the building blocks. In this paper, we assume that these rates are proportional to the break-up probability of the aggregate, i.e. $a_+(i) = a_-(i) = a \cdot p_b(s_i)$, where a is a constant parameter, which defines the ratio between self-alignment and break-up rates. This form accounts for the fact that self-alignment and break-up are both due to the role of agitation in mitigating the bonds, and that stable bonds are less likely to change their energy state as well. Whether this form is realistic enough to probe self-alignment phenomena of real systems remains an open question, which is beyond the scope of this paper and will be therefore adressed in future work.

3. RESULTS AND DISCUSSION

If not stated otherwise, the parameters are set as follows in all experiments: $E_{bond} = 5.0$ J, $m = 1.0$ kg, $r = 0.3$ m, $\gamma = 1.0$ kg $\cdot$ s^{-1}, $\alpha = 1$ J, $\eta = 1$ N, $\sigma_\theta = \frac{\pi}{180}$ rad, and $\nu_s^2 = 0.4$. All models share the exact same set of parameters, except for the average velocity $\widehat{v}$ of the building blocks, which is sampled from the spatial microscopic simulation (one could also solve Equation 1).

Difference equations are solved by numerical integration for 25000 time steps (time discretization of the system $T = 1$ s) with $N_s(0) = N_0 = 1000$ and a discretization $K = 3000$. In all experiments, we performed 10 runs of the Monte Carlo simulation and 10 runs of the agent-based simulation, both for 25000 s.

Available performance metrics of the system include the yield $Y(k)$ (i.e., the proportion of pairs with respect to the total number of aggregates[1] at iteration k), of course, but also a measure of the average misalignment of the aggregates at iteration k, denoted $M(k)$. These two metrics can be described by the following formulae:

$$Y(k) = \frac{\sum_{i=1}^K N_i(k)}{N_s(k) + \sum_{i=1}^K N_i(k)} \qquad (20)$$

$$M(k) = \frac{\sum_{i=1}^K N_i(k) \cdot \hat{\theta}_i^2(k)}{\sum_{i=1}^K N_i(k)} \qquad (21)$$

[1]Here, single building blocks are counted as an aggregate.

For $N_0 = 1000$, all models show a good agreement (Figure 3), even though the Monte Carlo simulation and the macroscopic model exhibits a slightly faster convergence, which is probably due to their non-spatiality. Indeed, a building block that is surrounded by stable aggregates may take quite some time before encountering another free building block. This suboptimal mixing tends to slow the process down; this phenomenon is not captured by non-spatial models.

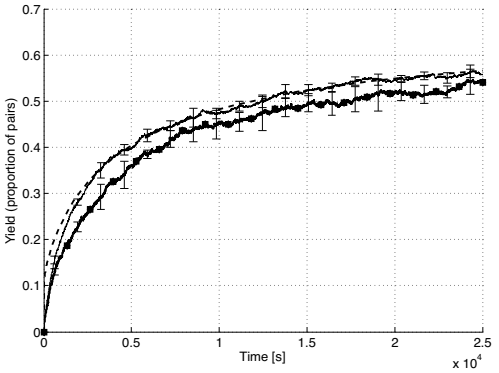


Figure 3: Comparison of the dynamics of the system (proportion of pairs) predicted by the macroscopic model with $K = 3000$ (dashed), the Monte Carlo simulation (continuous), and the agent-based simulation (bold).

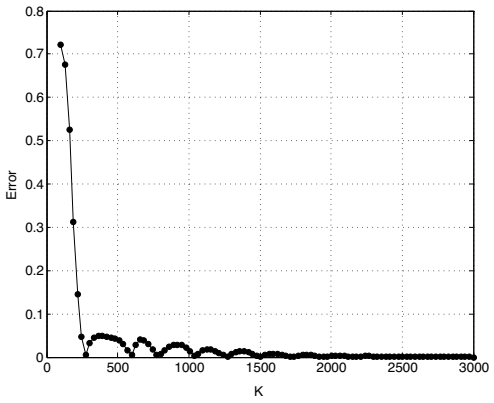


Figure 4: Error in the prediction of the macroscopic model with different values of $K \in [100, 3000]$ with respect to a baseline prediction with $K = 3000$. Interestingly, in the close neighborhood of $K = 276$, the error is small (approximately 0.6%) whereas it attains 4% for $K = 657$.

Also, the accuracy of the macroscopic model degrades as K decreases, especially at the steady state, where the system is governed by the smallest break-up probabilities. However, as depicted by Figure 4, the error depends on K in a strongly non-linear fashion, and there are multiple local minima where the macroscopic model performs well in spite of a small value of K. These non-linearities arise from the interplay between the discretization of the space of aggregate's types $\mathcal{S}$ and the actual form of the function $f(i)$. The computational cost of the model being proportional to K, an interesting solution would consist in using a non-uniform discretization of the space $\mathcal{S}$ so that the error is minimized. Nevertheless, as shown by Figure 4, even small K (e.g., around 600) are appropriate for qualitatively probing the dynamics of the system. Note however that these "good" values of K vary as a function of the control and design parameters of the system. However, for $K \geq 2000$, we consistently observed excellent quantitative agreement with other models, with very few variations of the error.

Another potential source of inaccuracy of our macroscopic model is related to the small numbers of individual building blocks N_0. In Figure 5, one can clearly see that the accuracy of the macroscopic model with respect to the Monte Carlo simulation degrades gracefully as N_0 decreases; for $N_0 = 50$, the macroscopic model actually predicts a much faster growth of the pair ratio than that observed in Monte Carlo simulations, whereas an almost perfect match is observed for $N_0 = 500$. Indeed, the predictions of deterministic difference equations are valid only for large populations of individuals. Stochastic modeling represents a potential solution to this problem [7], which may become crucial in the case of centimeter-scale robotic systems that usually involve only a few tens of units.

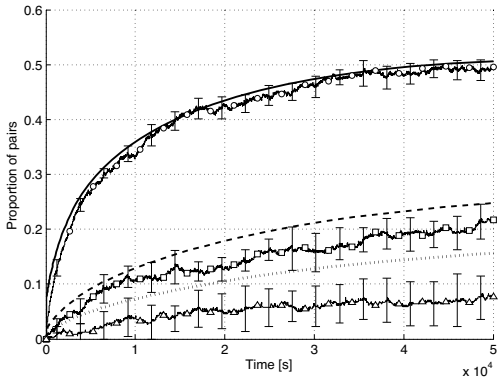


Figure 5: Comparison of the long run prediction (50000 s) of the agent-based simulation ($N_0 = 50$, triangles; $N_0 = 100$, squares; $N_0 = 500$, circles) and the macroscopic model ($N_0 = 50$, dotted line; $N_0 = 100$, dashed line; $N_0 = 500$, continuous line) for different total number of individual building blocks N_0.

3.1 Model-based Design and Control of Self-Assembling Systems

Models become really useful when one is interested in optimizing a given process, in particular when the behavior of the system is strongly non-linear and counter-intuitive. In this paper, we investigate an idealized system with two design parameters, i.e. the maximal bond energy E_{bond} and the misalignment tolerance σ_θ, as well as one control parameter, i.e. the agitation of the system ν_s. In reality, the design parameters would translate into properties of the self-assembling agents such as their shape, their surface chemistry, or the type of interaction force mediating the self-assembly process. For instance, capillary forces tend to be longer range and much stronger than purely hydrophobic interaction. As a result, the former would have a higher misalignment tolerance than the latter, as well as a larger maximal bond energy.

As stated before, the yield is not the unique performance metrics of the system, and one may want to optimize also

the average misalignment M. In this regard, the misalignment tolerance σ_θ of the building blocks plays a key role. Indeed, as depicted by Figure 6, while a large misalignment tolerance increases the yield, it also worsen the alignment of the aggregates. Note that the relationship between σ_θ and M is linear whereas the one between σ_θ and Y is not. Therefore, one can find an interesting tradeoff between a high yield (around 96%) and a quite good alignment (around 0.62) for a misalignement tolerance of 0.5 radians (35.5 degrees). This type of information is crucial when designing and optimizing a new system, and it would be prohibitively expensive to achieve such systematic exploration of the parameter space using realistic simulations and even a priori impossible using real hardware.

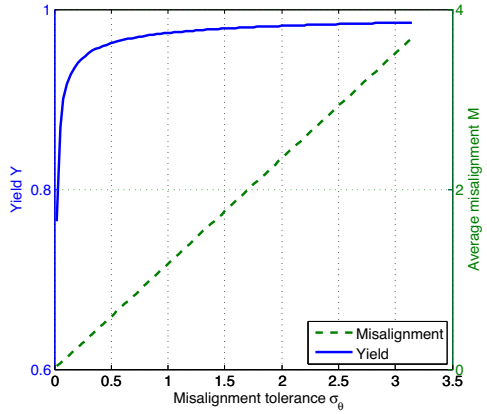


Figure 6: Influence of the misalignment tolerance σ_θ (in radians) on both the yield $Y(k)$ and the average misalignment of the aggregates $M(k)$ at $k = 25000$. Note the nearly perfect linear relationship between the average misalignment and the misalignment tolerance.

Our macroscopic models can also be used for optimizing the control of the system. For instance, we investigate how the yield of the system varies as a function of the agitation ν_s. To this end, we systematically vary the parameter ν_s in the interval $[0, 1]$ with a granularity of 0.01 (Figure 7). Interestingly, the relation between the yield and the agitation is strongly non-linear and exhibits an optimum around $\nu_s^\star = 0.15$.

We expect the same type of complex behavior to appear in real systems since the role of agitation is always two-fold: it tends to favor aggregation by increasing the average velocity of the particles (and therefore the number of collisions) *while* favoring disaggregation by making aggregates less stable. Therefore, one key design question arises: in terms of yield and misalignment, is a system with strong agitation and stable bonds preferable to a system with low agitation and unstable bonds? Figure 8 shows how each performance metric is influenced by these parameters. As expected, highest yields are achieved within the zone of moderate agitation and high bond energies; this zone also corresponds to the lowest average misalignments. These results emphasize the crucial role of agitation for optimizing, and more generally, controlling self-assembly processes.

However, as stated before, mitigated bonds do not necessarily break up; they may only change their energy state, thus resulting either in a better or worse relative alignment

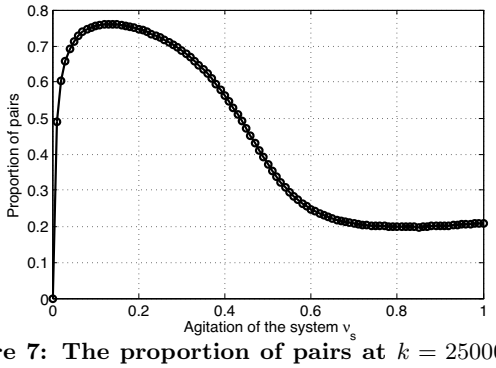
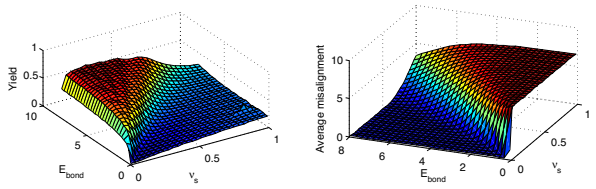


Figure 7: The proportion of pairs at $k = 25000$ as a function of the agitation of the system ν_s. An optimum can be observed around $\nu_s^\star = 0.15$. Generally speaking, high yields (higher than 70%) are achieved by a moderate agitation (between 0.05 and 0.3).



(a) (b)

Figure 8: Yield $Y(k)$ (a) and average misalignment $M(k)$ (b) at $k = 25000$ for two systematically varying parameters: the agitation of the system $\nu_s \in [0, 1]$, and the maximal bond energy $E_{bond} \in [0, 8]$ (900 runs of the macroscopic model with $N_0 = 1000$, $K = 1500$). Both high yields and small misalignments are achieved with moderate agitation and high bond energies.

of the building blocks. Interestingly, this phenomenon of bond mitigation, which we call *self-alignment*, does not impede the self-assembly process. On the contrary, because stabler bonds tend to be less likely to change their energy state, self-alignment allows the system to converge more quickly towards its equilibrium, as depicted by Figure 9. This observation, however, is obtained using a model that still needs to be validated at lower abstraction levels. This task is challenging because the exact impact of agitation and collisions with other building blocks on the energy state variations of the bonds is difficult to capture at the microscopic level and/or in realistic simulations, and goes beyond the scope of this paper.

More generally, one limitation of the models presented above is that they do not account for the detailed embodiment of the building blocks, which can usually be captured only using realistic physical simulations. Furthermore, we observed in recent studies using a real swarm of miniaturized robots [5] that the embodiment of the building blocks can play a critical role in the self-assembly process. For instance, the embodiment generates geometric obstructions that make bonds less likely to form; often this is due to large chains obstructing the paths of other robots, or aggregates forming near walls where further aggregation is not possible.

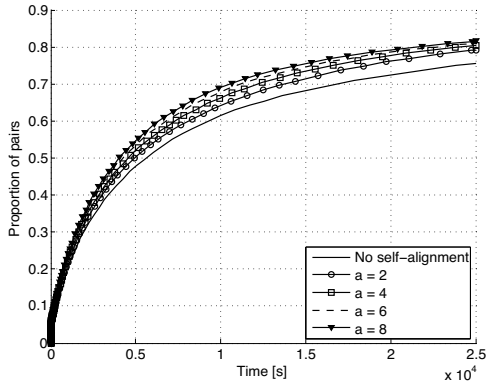


Figure 9: Comparison of the system dynamics predicted by the macroscopic model with and without self-alignment, and for different values of the rate parameter a. As expected, self-alignment speeds up the convergence of the system to the steady state.

4. CONCLUSION

The suite of models at multiple levels presented in this paper is not only capable of capturing directionality in aggregation processes, but it also provides an insight into what design and control parameters are optimal in term of yield and alignment quality of the aggregates. While this paper emphasizes an "horizontal", methodological, platform-independent approach, it must be noted that our modeling framework is applicable to a wide range of self-assembling systems since very few fundamental assumptions are made about the nature of the system, thus making our approach suitable for a full breadth of target platforms ranging from centimeter-scale mobile robots down to micro-robots or, more generally, micro-electro-mechanical systems.

In the future, we envision to extend our formalism to both of these platforms, in particular regarding the development of stochastic models for coping with small populations of building blocks and robots. More importantly, we aim at validating and calibrating our models with real robotic experiments at different length scales.

Last, this paper emphasizes the utmost importance of agitation for controlling self-assembly. However, one important limitation of our approach is precisely that it relies on a first order approximation for modeling agitation of the system, and more particularly its influence on the stability of the bonds. Developing faithful models of agitation and understanding the complex interplay between agitation and bond stability in various real systems is one of our objective for future research.

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