A Local Stochastic Algorithm for Separation in Heterogeneous Self-Organizing Particle Systems

Sarah Cannon 💿

- Claremont McKenna College, Claremont, CA, USA
- scannon@cmc.edu
- Joshua J. Daymude D
- Computer Science, CIDSE, Arizona State University, Tempe, AZ, USA
- jdaymude@asu.edu 8

Cem Gökmen 💿

- Georgia Institute of Technology, Atlanta, GA, USA 10
- cgokmen@gatech.edu 11

Dana Randall 12

- Georgia Institute of Technology, Atlanta, GA, USA 13
- randall@cc.gatech.edu14

Andréa W. Richa 15

- Computer Science, CIDSE, Arizona State University, Tempe, AZ, USA 16
- aricha@asu.edu 17

18 – Abstract

We present and rigorously analyze the behavior of a distributed, stochastic algorithm for separation 19 20 and integration in self-organizing particle systems, an abstraction of programmable matter. Such systems are composed of individual computational *particles* with limited memory, strictly local 21 communication abilities, and modest computational power. We consider heterogeneous particle 22 systems of two different colors and prove that these systems can collectively separate into different 23 color classes or *integrate*, indifferent to color. We accomplish both behaviors with the same fully 24 distributed, local, stochastic algorithm. Achieving separation or integration depends only on a single 25 global parameter determining whether particles prefer to be next to other particles of the same color 26 or not; this parameter is meant to represent external, environmental influences on the particle system. 27 The algorithm is a generalization of a previous distributed, stochastic algorithm for compression 28 (PODC '16), that can be viewed as a special case of separation where all particles have the same 29 color. It is significantly more challenging to prove that the desired behavior is achieved in the 30 heterogeneous setting, however, even in the bichromatic case we focus on. This requires combining 31 several new techniques, including the *cluster expansion* from statistical physics, a new variant of the 32 bridging argument of Miracle, Pascoe and Randall (RANDOM '11), the high-temperature expansion 33 of the Ising model, and careful probabilistic arguments. 34

2012 ACM Subject Classification Mathematics of computing \rightarrow Stochastic processes; Theory of 35 computation \rightarrow Self-organization; Theory of computation \rightarrow Random walks and Markov chains 36

- Keywords and phrases Markov chains, Programmable matter, Cluster expansion 37
- Digital Object Identifier 10.4230/LIPIcs.APPROX/RANDOM.2019.54 38
- Category RANDOM 39
- Related Version A full version is available online at https://arxiv.org/abs/1805.04599. 40
- Funding Sarah Cannon: Supported by National Science Foundation (NSF) award DMS-1803325. 41
- Joshua J. Daymude: Supported by NSF awards CCF-1422603, CCF-1637393, and CCF-1733680. 42
- Cem Gökmen: Supported by NSF award CCF-1733812. 43
- Dana Randall: Supported by NSF awards CCF-1526900, CCF-1637031, and CCF-1733812. 44
- Andréa W. Richa: Supported by NSF awards CCF-1422603, CCF-1637393, and CCF-1733680. 45

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Editors: Dimitris Achlioptas and László A. Végh; Article No. 54; pp. 54:1–54:22 Leibniz International Proceedings in Informatics

LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

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46 **1** Introduction

Across many disciplines spanning computational, physical, and social sciences, heterogeneous 47 systems self-organize into both separated (or segregated) and integrated states. Exam-48 ples include molecules exhibiting attractive and repulsive forces, distinct types of bacteria 49 competing for resources while collaborating towards common goals (e.g., [35, 39]), social 50 insects tolerating or aggressing towards those from other colonies (e.g., [30, 20]), and inherent 51 human biases that influence how we form and maintain social groups (e.g., [37, 16]). In 52 each of these, individuals are of different "types": integration occurs when the ensemble 53 gathers together without much preference about the type of their neighbors, while separation 54 occurs when individuals cluster with others of the same type. Here, we investigate these 55 fundamental behaviors of separation or integration as they apply to *programmable matter*, 56 a material that can alter its physical properties based on user input or stimuli from its 57 environment. Instead of studying a particular instantiation of programmable matter, of 58 which there are many [1, 7, 36, 31], we abstractly envision these systems as collections of 59 simple, active computational *particles* that individually execute local distributed algorithms 60 to collectively achieve some emergent behavior. We consider *heterogeneous* particle systems 61 in which particles have immutable *colors*. We seek local, distributed algorithms that, when 62 run by each particle independently and concurrently, result in emergent, self-organizing 63 separation or integration of color classes. 64

This work uses the stochastic approach to self-organizing particle systems first used for 65 *compression*, where (monochromatic) particles self-organize to gather together as tightly as 66 possible [6]. Using this stochastic approach, one first defines an energy function where desired 67 configurations have the lowest energy values. One then designs a Markov chain whose long 68 run behavior favors these low energy configurations. This Markov chain is carefully designed 69 so that all its transition probabilities can be computed locally, allowing it to be translated to a 70 fully local distributed algorithm each particle can run independently. The resulting collective, 71 emergent behavior of this distributed algorithm is thus described by the long run behavior of 72 the Markov chain. Using this stochastic approach, we previously extended our compression 73 algorithm [6] to an algorithm for *shortcut bridging* [2] — or maintaining bridge structures 74 that balance the tradeoff between bridge efficiency and cost — and developed the theoretical 75 basis for an experimental study in swarm robotics [32]. While the process of designing 76 distributed algorithms for self-organizing particle systems via this stochastic approach is 77 fairly well-understood, proving that such algorithms achieve their desired objectives remains 78 quite challenging. In particular, it is not enough to know the desired configurations have the 79 highest long-run probability; there may be so many other, lower probability configurations 80 that they collectively outweigh the desirable ones. This energy/entropy trade-off has been 81 studied in various Markov chains for the purposes of proving slow mixing, but we analyze it 82 directly to show our algorithms achieve the desired objectives with high probability. 83

Here, we focus on separation and integration in heterogeneous systems. Our inspiration 84 comes from the classical Ising model in statistical physics [18, 38], where the vertices of a 85 graph are assigned positive and negative "spins" and there are rules governing the probability 86 that adjacent vertices have the same spin. Connected to the Ising model is classical work 87 from stochastic processes on the Schelling model of segregation [33, 34], which explores 88 how individuals' micro-motives can induce macro-level phenomena like racial segregation 89 in residential neighborhoods. Recent variants of this model from computer science have 90 investigated the degree of individual bias required to induce such segregation [5, 17], and 91 a related distributed algorithm has been developed [29]. Our work differs from those on 92

the Ising and Schelling models because of natural physical constraints on systems of selforganizing, active particles like ours. For example, interpreting particles of one color to be vertices with positive spin and particles of another color to be particles with negative spin, this acts like an Ising model, but on a graph that evolves as particles more. Despite these obstacles, we apply ideas developed for rigorously analyzing the Ising and similar models to prove our distributed algorithm for separation and integration accomplishes the desired goals.

While we are interested in distributed algorithms, it is worth noting that efficient stochastic algorithms for separation can be challenging even with centralized Markov chains. Separation of a region into equitably sized, compact districts has been widely explored recently in the context of gerrymandering, where the aim is to sample colorings of a weighted graph from an appropriately defined stationary distribution [10, 15]. Heuristics for random districting have been discussed in the media, but there are still no known rigorous, efficient algorithms.

106 1.1 Results

We present a distributed algorithm for self-organizing separation and integration that takes 107 as input two bias parameters, λ and γ . Setting $\lambda > 1$ corresponds to particles favoring having 108 more neighbors; this is known to cause compression in homogeneous systems when λ is large 109 enough [6]. For separation in the heterogeneous setting, we introduce a second parameter γ , 110 where $\gamma > 1$ corresponds to particles favoring having more neighbors of their own color. We 111 then investigate for what values of λ and γ our algorithm yields compression and separation. 112 Informally, a particle system is separated if there is a subset of particles such that (i) the 113 boundary between this subset and the rest of the system is small, (ii) a large majority of 114 particles in this subset are of the same color, say c, and (*iii*) very few particles with color 115 c exist outside of this subset. This notion of separation (defined formally in Definition 3) 116 captures what it means for a system to have large monochromatic regions of particles. 117

We prove that for any $\lambda > 1$ and $\gamma > 4^{5/4} \sim 5.66$ such that $\lambda \gamma > 2(2 + \sqrt{2})e^{0.0003} \sim 6.83$, our algorithm accomplishes separation with high probability.¹ However, we prove the opposite for some values of γ close to one; counterintuitively, this even includes some values of $\gamma > 1$, the regime where particles favor having like-colored neighbors. Formally, we prove that for any $\lambda > 1$ and $\gamma \in (79/81, 81/79)$ such that $\lambda(\gamma + 1) > 2(2 + \sqrt{2})e^{0.0003} \sim 6.83$, our algorithm fails to achieve separation (i.e., it achieves integration) with high probability.

1.2 Proof Techniques

Because our distributed algorithm is based on a Markov chain, we can use standard tools such as detailed balance to understand its long-term behavior and prove its convergence to a unique probability distribution π over particle system configurations. This stationary distribution π depends on the input parameters λ and γ . Our main contribution is analyzing π for various ranges of λ and γ , showing that a configuration drawn from distribution π is either very likely (for large γ) or very unlikely (for γ close to one) to be separated.

¹³¹ To show separation occurs when λ and γ are both large, we modify the proof technique of ¹³² *bridging* introduced by Miracle, Pascoe, and Randall [28]. To show separation does not occur ¹³³ when λ is large and γ is small (close to one), we use a probabilistic argument, a Chernoff-type

¹ We say an event A occurs with high probability (w.h.p.) if $\Pr[A] \ge 1 - c^{n^{\delta}}$, where 0 < c < 1 and $\delta > 0$ are constants and n is the number of particles. Our w.h.p. results all have $\delta \in \{1/2, 1/2 - \varepsilon\}$, for arbitrarily small $\varepsilon > 0$.

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¹³⁴ bound, and a decomposition of configurations into different regions. These arguments — ¹³⁵ both for large and small γ — require that the particle system is compressed; i.e., that the ¹³⁶ system has perimeter $\Theta(\sqrt{n})$. However, the arguments from [6] showing compression occurs ¹³⁷ for homogeneous systems when λ is large do not extend to the heterogeneous setting.

We instead turn to the *cluster expansion* from statistical physics to show our separation 138 algorithm achieves compression for large enough γ . The cluster expansion was first introduced 139 in 1937 by Mayer [27], though a more modern treatment can be found in the textbook [12] 140 where it is used to derive several properties of statistical physics models including the Ising 141 and hard-core models. In the past year, the cluster expansion has received renewed attention 142 in the computer science community due to the recent work of Helmuth, Perkins, and Regts 143 that uses the cluster expansion to develop approximate counting and sampling algorithms 144 for low-temperature statistical physics models on lattices including the Potts and hard-core 145 models [14]. Subsequent work has considered similar techniques on expander graphs [19] and 146 random regular bipartite graphs [23]. Inspired by the interpolation method of Barvinok [4, 3], 147 these works give algorithms for estimating partition functions that explicitly calculate the 148 first $\log n$ coefficients of the cluster expansion. We use the cluster expansion differently, to 149 separate the volume and surface contributions to a partition function. 150

The cluster expansion is a power series representation of $\ln Z$ where Z is a polymer 151 *partition function.* We relate each of our quantities of interest to a particular polymer 152 partition function, and then use a version of the Kotecký-Preiss condition [21] to show that 153 the power series in the cluster expansion is convergent for the ranges of parameters we are 154 interested in. We then use this convergent cluster expansion to split our polymer partition 155 functions into a volume term, depending only on the size of the region of interest, and a 156 surface term, depending only on its perimeter. This separation into volume and surface terms 157 turns out to be the key to our compression argument, both for large γ and for γ close to one. 158 While splitting partition functions into volume and surface terms is not a new idea in the 159 statistical physics literature (for example, Section 5.7.1 of [12] uses it to derive an explicit 160 expression for the infinite volume pressure of the Ising model on \mathbb{Z}^d with large magnetic 161 field), we are the first to bring this approach into the computer science literature. We are 162 hopeful it will be useful beyond its specific applications in this paper. 163

164 **2** Background

We begin by defining our amoebot model for programmable matter and stating a few key results. We then extend the amoebot model to heterogeneous particle systems and formally define what it means for a system to be separated or integrated. We conclude with the necessary terminology and results on Markov chains.

169 2.1 The Amoebot Model

In the *amoebot model*, introduced in [9] and fully described in [8], programmable matter 170 consists of individual, homogeneous computational elements called *particles*. In its geometric 171 variant, particles are assumed to occupy nodes of the triangular lattice $G_{\Delta} = (V, E)$ and 172 can move along its edges (see Figure 1a). Each node in V can be occupied by at most one 173 particle at a time. Each particle occupies either a single node in V (i.e., it is *contracted*) or 174 a pair of adjacent nodes in V (i.e., it is *expanded*), as in Figure 1b. Particles move via a 175 series of *expansions* and *contractions*: a contracted particle can expand into an unoccupied 176 adjacent node to become expanded, and completes its movement by contracting to once 177 again occupy a single node. 178



Figure 1 (a) A section of the triangular lattice G_{Δ} . (b) Expanded and contracted particles (black dots) on G_{Δ} (gray lattice). Particles with a black line between their nodes are expanded.

Two particles occupying adjacent nodes are said to be *neighbors*. Each particle is *anonymous*, lacking a unique identifier, but can locally identify each of its neighboring locations and can determine which of these are occupied by particles. Each particle has a constant-size local memory that it can write to and its neighbors can read from for communication. In particular, a particle stores whether it is contracted or expanded in its memory. Particles do not have any access to global information such as a shared compass, coordinate system, or estimate of the size of the system.

The system progresses through *atomic actions* according to the standard asynchronous 186 model of computation from distributed computing (see, e.g., [25]). A classical result under 187 this model states that for any concurrent asynchronous execution of atomic actions, there 188 exists a sequential ordering of actions producing the same end result, provided conflicts that 189 arise in the concurrent execution are resolved. In the amoebot model, an atomic action 190 corresponds to the activation of a single particle. Once activated, a particle can (i) perform 191 an arbitrary, bounded amount of computation involving information it reads from its local 192 memory and its neighbors' memories, (ii) write to its local memory, and (iii) perform at 193 most one expansion or contraction. Conflicts involving simultaneous particle expansions 194 into the same unoccupied node are assumed to be resolved arbitrarily such that at most 195 one particle moves to some unoccupied node at any given time. Thus, while in reality many 196 particles may be active concurrently, it suffices when analyzing algorithms under the amoebot 197 model to consider a sequence of activations where only one particle is active at a time. 198

¹⁹⁹ 2.2 Terminology and Results for Homogeneous Particle Systems

We now recall the relevant terminology and notation from our previous work on compression [6]. 200 A particle system arrangement is the set of vertices of the triangular lattice G_{Δ} occupied 201 by particles. Two arrangements are equivalent if they are translations of each other; we 202 define a particle system *configuration* to be an equivalence class of arrangements. An *edge* 203 of a configuration is an edge of G_{Δ} where both endpoints are occupied by particles. A 204 configuration is *connected* if for any two particles in the system, there is a path of such edges 205 between them. A configuration has a *hole* if there is a maximal, finite, connected component 206 of unoccupied vertices in G_{Δ} . 207

As we justify with Lemma 6, our analysis will focus on connected, hole-free configurations. The *boundary* of such a configuration σ is the closed walk \mathcal{P} on edges of σ that encloses all particles of σ and no unoccupied vertices of G_{Δ} . The *perimeter* $p(\sigma)$ of configuration σ is the length of this walk, also denoted $|\mathcal{P}|$. The following bounds the number of configurations with a given perimeter.

▶ Lemma 1 ([6], Lemma 4.3). For any $\nu > 2 + \sqrt{2}$, there is an integer $n_1(\nu)$ such that for all $n \ge n_1(\nu)$, the number of connected, hole-free particle system configurations with n particles

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²¹⁵ and perimeter k is at most ν^k .

Let $p_{min}(n)$ be the minimum possible perimeter for a configuration of n particles; it is easy to see that $p_{min}(n) = \Theta(\sqrt{n})$. Given any $\alpha > 1$, a configuration of n particles is said to be α -compressed if $p(\sigma) \le \alpha \cdot p_{min}(n)$. The following lemma establishes a concrete upper bound on $p_{min}(n)$.

▶ Lemma 2. For any $n \ge 1$, there is a connected, hole-free particle system configuration of n particles with perimeter at most $2\sqrt{3}\sqrt{n}$. That is, $p_{min}(n) \le 2\sqrt{3}\sqrt{n}$.

Proof. This lemma follows easily from noting that hexagonal configurations of n particles have perimeter on the order of $2\sqrt{3}\sqrt{n}$; a proof can be found in Appendix A.1.

224 2.3 Heterogeneous Particle Systems

Generalizing previous work on the amoebot model in which all particles are homogeneous and indistinguishable, we assume that each particle P has a fixed color $c(P) \in \{c_1, \ldots, c_k\}$ that is visible to itself and its neighbors, where $k \ll n$ is a constant. We extend the definition of configuration given in Section 2.2 to include both the vertices of G_{Δ} occupied by particles as well as the colors of those particles. An edge of configuration σ with endpoints occupied by particles P and Q is homogeneous if c(P) = c(Q) and heterogeneous otherwise.

We further extend the original model by allowing neighboring particles to exchange their positions in a *swap move*. Swap moves have no meaning in homogeneous systems as all particles are indistinguishable, but they grant heterogeneous systems flexibility in allowing particles trapped in the interior of the system to move freely.² These swap moves are not necessary for the correctness of our algorithm or our rigorous analysis, but enable faster convergence in practice.

In this paper, we study heterogeneous systems with k = 2 color classes. As discussed in Section 5, our algorithm performs well in practice for larger values of k and we expect our proof techniques would generalize without needing significant new ideas. However, this generalization would be cumbersome; thus, for simplicity, we restrict our attention to systems with colors $\{c_1, c_2\}$. For 2-heterogeneous systems, we can formally define separation with respect to having large monochromatic regions.

▶ Definition 3. For $\beta > 0$ and $\delta \in (0, 1/2)$, a 2-heterogeneous particle system configuration σ is said to be (β, δ) -separated if there is a subset of particles R such that:

- ²⁴⁵ **1.** There are at most $\beta \sqrt{n}$ edges of σ with exactly one endpoint in R;
- **246 2.** The density of particles of color c_1 in R is at least 1δ ; and
- **3.** The density of particles of color c_1 not in R is at most δ .

²⁴⁸ Unpacking this definition, β controls how small a boundary there is between the monochro-²⁴⁹ matic region R and the rest of the system, with smaller β requiring smaller boundaries. ²⁵⁰ The δ parameter expresses the tolerance for having particles of the wrong color within the ²⁵¹ monochromatic region R: small values of δ require stricter separation of the color classes, ²⁵² while larger values of δ allow for more integrated configurations. Notably, R does not need ²⁵³ to be connected.

² In domains where physical swap moves are unrealistic, colors could be treated as in-memory attributes that could be exchanged by neighboring particles to simulate a swap move.

254 2.4 Markov Chains

A thorough treatment of Markov chains can be found in the standard textbook [22]. A Markov chain is a memoryless random process on a state space Ω ; for our purposes, Ω is finite and discrete. We focus on discrete time Markov chains, where one transition occurs per *iteration* (or *step*). Because of its stochasticity, we can completely describe a Markov chain by its transition matrix M, which is an $|\Omega| \times |\Omega|$ matrix where for $x, y \in \Omega$, M(x, y) is the probability, if in state x, of transitioning to state y in one step. The *t*-step transition probability $M^t(x, y)$ is the probability of transitioning from x to y in exactly t steps.

A Markov chain is *erqodic* if it is both *irreducible* (i.e., for all $x, y \in \Omega$ there is a t such that 262 $M^t(x,y) > 0$ and aperiodic (i.e., for all $x \in \Omega$, $gcd\{t: M^t(x,x) > 0\} = 1$). A stationary 263 distribution of a Markov chain is a probability distribution π over Ω such that $\pi M = \pi$. 264 Any finite, ergodic Markov chain converges to a unique stationary distribution given by 265 $\pi(y) = \lim_{t\to\infty} M^t(x,y)$ for any $x, y \in \Omega$; importantly, for such chains this distribution is 266 independent of starting state x. To verify π' is the unique stationary distribution of a finite 267 ergodic Markov chain, it suffices to check that $\pi'(x)M(x,y) = \pi'(y)M(y,x)$ for all $x, y \in \Omega$ 268 (the detailed balance condition; see, e.g., [11]). 269

Given a state space Ω , a set of allowable transitions between states, and a desired 270 stationary distribution π on Ω , the Metropolis-Hastings algorithm [13] gives a Markov chain 271 on Ω with those transitions that converges to π . For separation, the state space contains 272 particle configurations and transitions correspond to configurations that differ by one particle 273 move; the stationary distribution π favors well-separated configurations; and we calculate 274 transition probabilities according to the Metropolis-Hasting algorithm (using a Metropolis 275 *filter*). Importantly, we choose π so that these transition probabilities can be calculated by 276 an individual particle using only information in its local neighborhood. 277

²⁷⁸ **3** The Separation Algorithm

We now present our stochastic, local, distributed algorithm for separation. Our algorithm achieves separation by biasing particles towards moves that both gain them more neighbors overall and more like-colored neighbors. We use two bias parameters to control this preference: $\lambda > 1$ corresponds to particles favoring having more neighbors, and $\gamma > 1$ corresponds to particles favoring having more neighbors of their own color.

In order to leverage powerful techniques from Markov chain analysis and statistical physics 284 to prove the correctness of our algorithm, we design our algorithm to follow certain invariants. 285 First, assuming the initial particle system configuration is connected, our algorithm ensures 286 it remains connected; this is necessary because particles have strictly local communication 287 abilities so a disconnected particle is unable to communicate with or even find the rest of 288 the particles. Second, our algorithm eventually eliminates all holes in the configuration, and 289 no new holes are ever formed. This is necessary because our proof techniques only apply to 290 hole-free configurations. Third, once all holes have been eliminated, all moves allowed by our 291 algorithm are *reversible*: if a particle moves from node u to an adjacent node v in one step, 292 there is a nonzero probability that it moves back to u in the next step. Finally, the moves 293 allowed by our algorithm suffice to transform any connected, hole-free configuration into any 294 other connected, hole-free configuration. 295

Our algorithm uses two locally-checkable properties that ensure particles do not disconnect the system or form a hole when moving (our first two invariants). We use the following notation. For a location ℓ — i.e., a node of the triangular lattice G_{Δ} — let $N_i(\ell)$ denote the particles of color c_i occupying locations adjacent to ℓ . For neighboring locations ℓ and ℓ' , let

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 $N_i(\ell \cup \ell')$ denote the set $N_i(\ell) \cup N_i(\ell')$, excluding particles occupying ℓ and ℓ' . When ignoring

color, let $N(\ell) = \bigcup_i N_i(\ell)$; define $N(\ell \cup \ell')$ analogously. Let $\mathbb{S} = N(\ell) \cap N(\ell')$ denote the set

of particles adjacent to both locations. A particle can move from location ℓ to ℓ' if one of the following are satisfied:

³⁰⁴ \triangleright Property 4. $|\mathbb{S}| \in \{1, 2\}$ and every particle in $N(\ell \cup \ell')$ is connected to exactly one particle ³⁰⁵ in \mathbb{S} by a path through $N(\ell \cup \ell')$.

 $_{306}$ \triangleright Property 5. $|\mathbb{S}| = 0$, and both $N(\ell) \setminus \{\ell'\}$ and $N(\ell') \setminus \{\ell\}$ are nonempty and connected.

Note these properties do not need to be verified for swap moves, since swap moves do not 307 change the set of occupied locations and thus cannot disconnect the system or create a hole. 308 We now define the Markov chain \mathcal{M} for separation. The state space Ω of \mathcal{M} is the set 309 of all connected heterogeneous particle system configurations of n contracted particles, and 310 Algorithm 1 defines its transition probabilities. We note that \mathcal{M} , a centralized Markov 311 chain, can be directly translated to a fully distributed, local, asynchronous algorithm \mathcal{A} that 312 can be run by each particle independently and concurrently to achieve the same system 313 behavior. This translation is much the same as for previous algorithms developed using the 314 stochastic approach to self-organizing particle systems [6, 2]; we refer the interested reader to 315 those papers for details. Importantly, this translation is only possible because all probability 316 calculations and property checks in \mathcal{M} use strictly local information available to the particles 317 involved. Simulations of \mathcal{M} can be found in Section 3.2. 318

Algorithm 1 Markov Chain \mathcal{M} for Separation and Integration

Beginning at any connected configuration σ_0 of *n* particles, repeat:

- 1: Choose a particle P uniformly at random; let c_i be its color and ℓ its location.
- 2: Choose a neighboring location ℓ' and $q \in (0, 1)$ each uniformly at random.
- 3: if ℓ' is unoccupied then
- 4: P expands to occupy both ℓ and ℓ' .
- 5: Let $e = |N(\ell)|$ (resp., $e_i = |N_i(\ell)|$) be the number of neighbors (resp., of color c_i) P had when contracted at location ℓ , and define $e' = |N(\ell')|$ and $e'_i = |N_i(\ell')|$ analogously.
- 6: **if** (i) $e \neq 5$, (ii) ℓ and ℓ' satisfy Property 4 or 5, and (iii) $q < \lambda^{e'-e} \cdot \gamma^{e'_i-e_i}$ then
- 7: $P \text{ contracts to } \ell'.$
- 8: else P contracts back to ℓ .
- 9: else if ℓ' is occupied by particle Q of color c_j then

10: **if** $q < \gamma^{|N_i(\ell') \setminus \{P\}| - |N_i(\ell)| + |N_j(\ell) \setminus \{Q\}| - |N_j(\ell')|}$ **then** *P* and *Q* perform a swap move.

319 3.1 The Stationary Distribution of Markov Chain \mathcal{M}

In this section, we prove that Markov chain \mathcal{M} maintains the four invariants described previously and then characterize its stationary distribution.

Lemma 6. If the particle system is initially connected, it remains connected throughout the execution of \mathcal{M} . Moreover, \mathcal{M} eventually eliminates any holes in the initial configuration, after which no holes are ever introduced again.

Proof. This follows directly from analogous results for compression [6]. Although the separation and compression algorithms assign different probabilities to particle moves, the set of allowed movements is exactly the same, excluding swap moves that do not change the set of occupied nodes of G_{Δ} , so they cannot disconnect the system or introduce a hole.

Lemma 7. Once all holes have been eliminated, every possible particle move is reversible; that is, if there is a positive probability of moving from configuration σ to configuration τ , then there is a positive probability of moving from τ to σ .

Proof. Suppose, for example, that a particle P moves from location ℓ to ℓ' . In the next time step, it is possible for P to be chosen again (Step 1) and for ℓ to be chosen as the position to explore (Step 2). Because Properties 4 and 5 are symmetric with respect to ℓ and ℓ' , whichever was satisfied in the forward move will also be satisfied in this reverse move. Finally, the probability checked in Condition (*iii*) of Step 7 is always nonzero, so all together there is a nonzero probability that P moves back to ℓ in this reverse move. Swap moves can be shown to be reversible in a similar way.

 $_{339}$ **Lemma 8.** Markov chain \mathcal{M} is ergodic on the space of connected, hole-free configurations.

Proof Sketch. One can show that \mathcal{M} is irreducible (i.e., the moves of \mathcal{M} suffice to transform any configuration to any other configuration) similarly to the proof of the same fact for compression [6]: it is first shown that any configuration can be reconfigured into a straight line; then, the line can be sorted by the color of the particles; finally, by reversibility (Lemma 7), the line can be reconfigured into any configuration. Additionally, it is easy to see that \mathcal{M} is aperiodic: at each iteration of \mathcal{M} , there is a nonzero probability that the configuration does not change. Thus, because \mathcal{M} is irreducible and aperiodic, we conclude it is ergodic.

Because \mathcal{M} is finite and ergodic, it converges to a unique stationary distribution π that we now characterize. For a configuration σ , let $h(\sigma)$ be the number of heterogeneous edges in σ .

→ Lemma 9. For $Z = \sum_{\sigma} (\lambda \gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}$, the stationary distribution of \mathcal{M} is:

$$\pi(\sigma) = \begin{cases} (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}/Z & \text{if } \sigma \text{ is connected and hole-free;} \\ 0 & \text{otherwise.} \end{cases}$$

Proof Sketch. By Lemma 6, when \mathcal{M} starts at a connected configuration it eventually 351 reaches and remains in the set of configurations that are connected and hole-free. Thus, 352 disconnected configurations and configurations with holes have zero weight at stationarity. 353 In Appendix A.2, we show using detailed balance that the unique stationary distribution of 354 \mathcal{M} can be written, for σ connected and hole-free, as $\pi(\sigma) = \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}/Z_e$ where $e(\sigma)$ is the 355 number of edges and $a(\sigma)$ is the number of homogeneous edges of σ and $Z_e = \sum_{\sigma} \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}$. 356 This can be rewritten as in the lemma using two facts: (i) since every edge is either 357 homogeneous or heterogeneous, $e(\sigma) = a(\sigma) + h(\sigma)$; and (ii) for any connected, hole-free 358 configuration σ , $e(\sigma) = 3n - p(\sigma) - 3$, a result shown in [6]. 359

³⁶⁰ The remainder of this paper will be spent analyzing this stationary distribution.

361 3.2 Simulations

We supplement our rigorous results with simulations that show separation occurs for even 362 better values of λ and γ than our proofs guarantee, indicating that our proven bounds are 363 likely not tight. We simulated \mathcal{M} on heterogeneous particle systems with two colors, using 50 364 particles of each color. Figure 2 shows the progression of \mathcal{M} over time with bias parameters 365 $\lambda = 4$ and $\gamma = 4$, the regime in which particles prefer to have more neighbors, especially 366 those of their own color. The simulation ran for nearly 70 million iterations, but much of the 367 system's compression and separation occurs in the first million iterations. Separation still 368 occurs even when swap moves are disallowed, but takes much longer to achieve. 369

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Figure 2 A 2-heterogeneous particle system of 100 particles starting from an arbitrary initial configuration after (from left to right) 0; 50,000; 1,050,000; 17,050,000; and 68,250,000; iterations of \mathcal{M} with $\lambda = 4$ and $\gamma = 4$.

Figure 3 compares the resulting system configurations after running \mathcal{M} from the same 370 initial configuration for the same number of iterations, varying only the values of λ and γ . 371 We observe four distinct phases: compressed-separated, compressed-integrated, expanded-372 separated, and expanded-integrated. We rigorously verify the compressed-separated behavior 373 (i.e., when λ and γ are large), and do the same for the compressed-integrated behavior (i.e., 374 when λ is large and γ is small). We do not give proofs for expanded configurations; in fact, 375 our current definition of separation may not accurately capture what occurs in expanded 376 configurations. 377

4 Summary of Results and Proofs

Here we summarize our results and proofs; details have been omitted due to length constraints. 379 We want to know for which values of λ and γ separation does or does not occur. Our 380 proof techniques only apply to compressed configurations, so we must first show that Markov 381 chain \mathcal{M} achieves compression for the values of λ and γ we are interested in. Previous proofs 382 of compression in homogeneous particle systems break down for heterogeneous systems, so 383 we utilize the *cluster expansion* to overcome this obstacle. The cluster expansion comes from 384 statistical physics and allows us to rewrite a sum over collections of disjoint objects in terms 385 of a sum over collections of overlapping objects. This latter sum is often much easier to 386 work with. For the cluster expansion to be useful, the formal power series it involves must 387 be convergent. We highly recommend Chapter 5 of [12] to learn more about the cluster 388 expansion. Here we present only the relevant definitions and results from this chapter. 389

In a *polymer model*, we consider a finite set Γ , the elements of which are called *polymers*. We will consider polymers that are collections of edges of G_{Δ} having certain properties; for large γ , our polymers are minimal cut sets that we call *loops*, and when γ is close to one, our polymers are connected edge sets with an even number of edges incident on each vertex. Formally, polymers only need to satisfy:

- Each polymer $\xi \in \Gamma$ has a real weight $w(\xi)$.³
- ³⁹⁶ There is a notion of pairwise *compatibility* for polymers.

³⁹⁷ Polymers are typically compatible when they are well-separated in some sense. Our loop ³⁹⁸ polymers will be compatible when they share no edges, and our even polymers will be ³⁹⁹ compatible when they are not incident on any of the same vertices. We say a collection of ⁴⁰⁰ polymers $\Gamma' \subseteq \Gamma$ is *compatible* if all polymers in Γ' are pairwise compatible.

³ In general $w(\xi)$ can be complex, but for our purposes it will always be a (positive or negative) real number.



Figure 3 A 2-heterogeneous particle system of 100 particles starting in the leftmost configuration of Figure 2 after 50,000,000 iterations of \mathcal{M} for various values of the parameters λ and γ .

⁴⁰¹ The *polymer partition function* is defined as:

402
$$\Xi = \sum_{\substack{\Gamma' \subseteq \Gamma \\ compatible}} \prod_{\xi \in \Gamma'} w(\xi).$$

⁴⁰³ Many partition functions of spin systems, such as the Ising model or the hard-core lattice ⁴⁰⁴ gas model, can be written in this form as polymer partition functions. Such an abstract sum ⁴⁰⁵ can sometimes be hard to analyze, but the *cluster expansion* gives a way of rewriting this ⁴⁰⁶ expression in terms of a sum over subsets $\Gamma' \subseteq \Gamma$ where many polymers are incompatible; ⁴⁰⁷ because incompatible polymers 'touch,' we can enumerate such collections more easily and ⁴⁰⁸ thus such sums are often easier to work with

Formally, consider an ordered multiset $X = \{\xi_1, \xi_2, \dots, \xi_m\} \subseteq \Gamma$. Let H_X be the *incompatibility graph* on vertex set $\{1, 2, \dots, m\}$ where $i \sim j$ whenever ξ_i and ξ_j are incompatible. We say that the X is a *cluster* if H_X is connected.⁴ Let |X| = m denote the number of polymers in cluster X (with polymers counted with the appropriate multiplicities).

⁴¹³ The *cluster expansion* is the formal power series for $\ln \Xi$ given in Equation 2. Often this ⁴¹⁴ power series does not converge, but the *Kotecky-Preiss condition* guarantees convergence ⁴¹⁵ and is often easy to verify [21]. The following theorem states the Kotecky-Preiss condition ⁴¹⁶ (Equation 1) and the cluster expansion of Ξ .

⁴¹⁷ ► **Theorem 10** ([12], Chapter 5). Let Γ be a finite set of polymers ξ with real weights $w(\xi)$ ⁴¹⁸ and a notion of pairwise compatibility. If there exists a function $a : \Gamma \to \mathbb{R}_{>0}$ such that for ⁴¹⁹ all $\xi^* \in \Gamma$,

$$\sum_{\substack{\xi \in \Gamma:\\ incompatible}} |w(\xi)| e^{a(\xi)} \le a(\xi^*), \tag{1}$$

421 ξ, ξ^{*} incompatible

420

⁴ Many sources define clusters to be unordered multisets, necessitating additional combinatorial terms in the cluster expansion; for simplicity, we assume clusters are ordered.

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then the polymer partition function Ξ satisfies

$$_{423} \qquad \ln \Xi = \sum_{X: \ cluster} \frac{1}{|X|!} \left(\sum_{\substack{G \subseteq H_X: \\ connected, \\ spanning}} (-1)^{|E(G)|} \right) \left(\prod_{\xi \in X} w(\xi) \right), \tag{2}$$

where $G \subseteq H_X$ means G is a subgraph of H_X . 425

The cluster expansion is derived and this theorem is proved in Chapter 5 of [12], for a slightly 426 different (but equivalent) definition of a cluster. 427

We apply the cluster expansion twice, with two different notions of polymers and com-428 patibility. In both cases, our polymers will be connected edge sets $\xi \subseteq E(G_{\Delta})$, and we use 429 that to state a general result here. Let Γ be an infinite set of such polymers that is invariant 430 under translation and rotation of polymers. Two polymers in Γ will be compatible if they 431 are well-separated in the model-dependent sense described above. Polymers are incompatible 432 when they are 'too close;' for a polymer $\xi \in \Gamma$, let $[\xi] \subseteq E(G_{\Delta})$ be the minimal edge set 433 such that if ξ' is not compatible with ξ , then ξ' must contain an edge of $[\xi]$. We use brackets, 434 consistent with the notation of [12], because this is a type of *closure* of a polymer. For our 435 loop polymers, which are compatible if they share no edges, $[\xi] = \xi$. For our even polymers, 436 which are compatible if they are not incident on any of the same vertices, $[\xi]$ is all edges that 437 share an endpoint with an edges of ξ . We denote the size of this edge set as $|[\xi]|$. 438

We will be interested in some finite region $\Lambda \subseteq E(G_{\Delta})$, and we say $\Gamma_{\Lambda} \subseteq \Gamma$ is all polymers 439 of Γ whose edges are contained in Λ . Let $\partial \Lambda$ be an edge set such that a cluster containing an 440 edge in Λ and an edge not in Λ must contain an edge of $\partial \Lambda$. We will consider loop polymers 441 with edges from $E_{\mathcal{P}}^{int}$, the set of edges with at least one endpoint strictly inside boundary \mathcal{P} , 442 so in this case we use $\Lambda = E_{\mathcal{P}}^{int}$ and $\partial \Lambda$ the edges in \mathcal{P} . For even polymers, we use $\Lambda = E_{\mathcal{P}}$, 443 all edges on or inside \mathcal{P} , and $\partial \Lambda$ is all edges with one endpoint on \mathcal{P} and the other outside. 444

The following states the key fact about the cluster expansion that we will need. Namely, 445 when a certain mild condition is satisfied, we can use the cluster expansion to give upper and 446 lower bounds on the polymer partition function for Λ in terms of a volume term, depending 447 only on $|\Lambda|$, and a surface term, depending only on $|\partial\Lambda|$. 448

► Theorem 11. Let Γ be an infinite set of polymers $\xi \subseteq E(G_{\Delta})$ that is closed under 449 translation and rotation, and let $\Lambda \subseteq E(G_{\Delta})$ be finite. If there is a constant c such that for 450 any edge $e \in E(G_{\Delta})$, 451

$$\sum_{\substack{\xi \in \Gamma: \\ e \in \xi}} |w(\xi)| e^{c|[\xi]|} \le c,$$

then for any Λ the partition function 454

455
$$\Xi_{\Lambda} := \sum_{\substack{\Gamma' \subseteq \Gamma_{\Lambda} \\ compatible}} \prod_{\xi \in \Gamma'} w(\xi)$$

satisfies 456

457
$$e^{\psi|\Lambda|-c|\partial\Lambda|} \le \Xi_{\Lambda} \le e^{\psi|\Lambda|+c|\partial\Lambda|}$$

for some constant $\psi \in [-c, c]$ that is independent of Λ . 458

⁴⁵⁹ We prove this theorem in Appendix A.3.

This result is the key step needed to show that when λ and γ are both large, compression 460 occurs; as our techniques for establishing separation first require configurations to be com-461 pressed, this is a necessary first step. For compression, we look at the partition function $Z_{\mathcal{P}}$ 462 for different fixed boundaries \mathcal{P} , where $Z_{\mathcal{P}}$ is the sum over all configurations σ with boundary 463 \mathcal{P} of their weights $(\lambda \gamma)^{-|\mathcal{P}|} \cdot \gamma^{-h(\sigma)}$. We cannot analyze $Z_{\mathcal{P}}$ directly, so we instead relate $Z_{\mathcal{P}}$ 464 to a specific polymer partition function $\Xi_{\mathcal{P}}^{\mathcal{L}}$ which does have a cluster expansion. Using the 465 sufficient condition of Theorem 10, we show the cluster expansion for $\Xi_{\mathcal{P}}^{\mathcal{L}}$ is convergent when 466 $\gamma > 4^{5/4}$. We then use this expression of $\ln \Xi_{\mathcal{P}}^{\mathcal{L}}$ as a convergent power series and Theorem 11 467 to bound $\Xi_{\mathcal{P}}^{\mathcal{L}}$ in terms of a *volume term*, depending only on the number of particles n, and a 468 surface term, depending only on $|\mathcal{P}|$, the length of boundary \mathcal{P} . 469

Lemma 12. When $\gamma > 4^{5/4}$, for c = 0.0001, there exists a constant $\psi \in [-c, c]$ that depends on γ but is independent of \mathcal{P} such that

$$_{472} \qquad e^{(3n-3)\psi - 3c|\mathcal{P}|} \le \Xi_{\mathcal{P}}^{\mathcal{L}} \le e^{(3n-3)\psi + 3c|\mathcal{P}|}$$

This means, in particular, that the ratios of $\Xi_{\mathcal{P}}^{\mathcal{L}}$ and $\Xi_{\mathcal{P}'}^{\mathcal{L}}$ for different boundaries \mathcal{P} and 473 \mathcal{P}' that enclose the same number n of particles can be bounded by an expression that is 474 exponential in the lengths of these boundaries but independent of n. This is essential to our 475 compression argument, which will focus on boundaries of various lengths. We note that it is 476 straightforward, using the previous lemma, to get similar bounds on $Z_{\mathcal{P}}$, the quantity we are 477 actually interested in. We use this to apply a Peierls argument similar to the one used to 478 show compression in [6]. This argument relates the total weight of undesirable configurations 479 - those with boundaries longer than $\alpha \cdot p_{min}$ for some constant $\alpha > 1$ — to the weight of 480 configurations with minimum perimeter, p_{min} . The result is as follows. 481

Theorem 13. Consider algorithm \mathcal{M} when there are n total particles of two different colors. For c = 0.0001, when constants $\alpha > 1$, $\lambda > 1$, and $\gamma > 4^{5/4}$ satisfy

1,

$$-\frac{2(2+\sqrt{2})e^{3c}}{\lambda\gamma}\left(e^{3c}\lambda\gamma^{3/2}\right)^{1/\alpha}<$$

484 485

when n is sufficiently large then for \mathcal{M} with parameters λ and γ , configurations drawn from distribution π are α -compressed with probability at least $1 - \zeta^{\sqrt{n}}$ for some constant $\zeta < 1$.

One corollary is that if $\lambda > 1$ and $\gamma > 4^{5/4}$ such that $\lambda \gamma > 2(2 + \sqrt{2})e^{0.0003} \sim 6.83$, there exists a constant α such that a configuration drawn from the stationary distribution π of \mathcal{M} is α -compressed with high probability. (Recall, we say an event A occurs with high probability, or w.h.p., if $\Pr[A] \geq 1 - c^{n^{\delta}}$, where 0 < c < 1 and $\delta > 0$ are constants. Unless we explicitly state otherwise, it will always be the case that $\delta = 1/2$.) Conversely, for any $\alpha > 1$, there exist λ and γ such that \mathcal{M} with these parameter values achieves α -compression at stationarity w.h.p.

We next show, again when λ and γ are large enough, that separation provably occurs. 495 By the previous theorem, it suffices to show this among compressed configurations. We 496 use a technique known as *bridging* that was developed to analyze molecular mixtures called 497 colloids [28]. Adapting the bridging approach to our setting required several new innovations 498 to overcome obstacles such as the irregular shapes of particle system configurations, the 499 non-self-duality of the triangular lattice, the interchangeability between color classes, and 500 other technicalities related to interfaces between particles of different colors. The main result 501 of this section is the following theorem. Recall that for a fixed boundary \mathcal{P} , the probability 502 distribution $\pi_{\mathcal{P}}$ is over colored particle configurations with this boundary where $\pi_{\mathcal{P}}(\sigma)$ is 503 proportional to $\gamma^{-h(\sigma)}$. 504

▶ Theorem 14. Let \mathcal{P} be the boundary of n particles with $|\mathcal{P}| \leq \alpha p_{min}$. For any $\beta > 2\sqrt{3\alpha}$ 505 and any $\delta < 1/2$, if γ is large enough that 506

507
$$3^{\frac{2\alpha\sqrt{3}}{\beta}} 4^{\frac{1+3\delta}{4\delta}} \gamma^{-1+\frac{2\alpha\sqrt{3}}{\beta}} < 1$$

then for sufficiently large n a configuration drawn from $\pi_{\mathcal{P}}$ is (β, δ) -separated with probability 508 at least $1 - \zeta^{\sqrt{n}}$ for some constant $\zeta < 1$. 509

Combining this with the previous theorem, we see that for any $\lambda > 1$ and $\gamma > 4^{5/4} \sim 5.66$ 510 such that $\lambda \gamma > 2(2 + \sqrt{2})e^{0.0003} \sim 6.83$, there exist constants β and δ such that for large 511 enough n, \mathcal{M} provably achieves (β, δ) -separation at stationarity w.h.p. Furthermore, for any 512 $\beta > 2\sqrt{3}$ and any $\delta < 1/2$, there are values for λ and γ such that for large enough n, \mathcal{M} 513 provably achieves (β, δ) -separation at stationarity w.h.p. 514

We are also able to show that there are some values of γ close to one for which separation 515 does not occur. This counterintuitively includes values where $\gamma > 1$ and particles have a 516 preference for being next to particles of the same color. As we did for large values of γ , we 517 first show that when λ is large and γ is close to one, compression provably occurs. The 518 polymer partition function $\Xi_{\mathcal{D}}^{\mathcal{L}}$ from above does not have a convergent cluster expansion when 519 γ is close to one, so we cannot use it to show compression. Instead, we carefully relate $Z_{\mathcal{P}}$ to 520 a different polymer partition function $\Xi_{\mathcal{P}}^{HT}$ by considering the high temperature expansion, 521 which rewrites a sum over configurations with a fixed boundary as a sum over even edge sets 522 within that boundary. The high-temperature expansion is well-studied for the Ising model 523 (see, e.g., [12], Section 3.7.3). We show $\Xi_{\mathcal{D}}^{HT}$ has a convergent cluster expansion when γ is 524 close to one. We then use the cluster expansion for this high temperature representation, 525 much the same as above, to show compression provably occurs. 526

Theorem 15. Consider algorithm \mathcal{M} when there are n total particles of two different 527 colors. For $a = 10^{-5}$, when constants $\alpha > 1$, $\lambda > 1$, and $\gamma \in (79/81, 81/79)$ satisfy 528

$$\sum_{529} \frac{2(2+\sqrt{2})e^{3a}}{\lambda(\gamma+1)} \left(\frac{\lambda(\gamma+1)}{2e^{-3a}\left(\frac{79}{81}\right)}\right)^{1/\alpha} < 1$$

5

when n is sufficiently large then for \mathcal{M} with parameters λ and γ , configurations drawn from 531 \mathcal{M} 's stationary distribution π are α -compressed with probability at least $1-\zeta^{\sqrt{n}}$ for some 532 constant $\zeta < 1$. 533

This theorem implies that for any $\lambda > 1$ and $\gamma \in (79/81, 81/79)$ such that $\lambda(\gamma + 1) > 1$ 534 $2(2+\sqrt{2})e^{0.0003} \sim 6.83$, there exists a constant α such that a configuration drawn from 535 the stationary distribution π of \mathcal{M} is α -compressed w.h.p. Conversely, for any $\alpha > 1$ and 536 any $\gamma \in (79/81, 81/79)$, for large enough λ algorithm \mathcal{M} with parameters λ and γ achieves 537 α -compression at stationarity w.h.p. 538

Once we have shown that compression occurs for large λ and γ near one, we show that 539 among these compressed configurations a large amount of separation between color classes 540 is very unlikely. We prove this with a probabilistic argument in which we find a set of 541 polynomially many events such that if separation occurs, then at least one of these events 542 occurs. We then show that each event occurs with probability at most $\zeta^{n^{1/2-\varepsilon}}$ for some $\zeta < 1$ 543 and arbitrarily small $\varepsilon > 0$, which via a union bound over the polynomial number of events 544 implies separation is very unlikely. 545

Theorem 16. Let \mathcal{P} be any α -compressed boundary. Let $\delta < 1/4$ and γ close enough to one such that there exists a $\mu \in (\delta/(1-2\delta), 1/2)$ where

548
$$\left(\frac{\mu}{1-\mu}\right)^{(\mu-\delta/(1-2\delta))/11} < \gamma < \left(\frac{1-\mu}{\mu}\right)^{(\mu-\delta/(1-2\delta))/11}$$

For any β and any c < 1/4, there is a constant $\zeta < 1$ such that the probability a particle configuration drawn at random from $\pi_{\mathcal{P}}$ is (β, δ) -separated is at most $\zeta^{n^{2c}}$.

⁵⁵² Combining this with the results above, we see that for $\lambda > 1$ and $\gamma \in (79/81, 81/79)$ such that ⁵⁵³ $\lambda(\gamma + 1) > 2(2 + \sqrt{2})e^{0.00003} \sim 6.83$, there are constants β and δ such that the probability ⁵⁵⁴ \mathcal{M} with parameters λ and γ achieves (β, δ) -separation at stationarity is at most $\zeta^{n^{1/2-\varepsilon}}$, ⁵⁵⁵ where $\varepsilon > 0$ and $\zeta < 1$. Conversely, for any $\beta > 0$ and any $\delta < 1/4$, there exists λ and γ such ⁵⁵⁶ that \mathcal{M} with these parameters achieves (β, δ) -separation at stationarity with probability at ⁵⁵⁷ most $\zeta^{n^{1/2-\varepsilon}}$ for $\varepsilon > 0$ and $\zeta < 1$.

558 **5** Conclusion

We considered separation with two colors, but expect our proofs to generalize in a straight-559 forward way to heterogeneous systems with more colors using insights that generalize cluster 560 expansion polymers from the Ising model to the Potts model (see the notion of a *contour* in 561 Pirogov-Sinai theory, e.g., in Chapter 7 of [12]). The proofs would follow the same strategy 562 for two colors, requiring little additional insight but a fairly large amount of technical detail. 563 We note that, as with previous papers using stochastic, distributed algorithms for 564 programmable matter, we are unable to give any nontrivial bounds on the mixing time of our 565 Markov chain \mathcal{M} . The difficulties in proving polynomial upper bounds on the mixing time 566 are unsurprising, given similarities between \mathcal{M} and a well-studied open problem in statistical 567 physics about the mixing time of Glauber dynamics of the Ising model on \mathbb{Z}^2 with plus 568 boundary conditions starting from the all minus state [26, 24] (see remarks concluding [6]). 569 However, the mixing time may not be the best bound for characterizing when compression 570 and separation occur. Simulations show that both compression and separation occur fairly 571 quickly (Figure 2), although the algorithm continues to gradually achieve more compression 572

and separation, confirming we likely achieve these goals well before converging to stationarity. 573 We believe the stochastic approach to self-organizing particle systems, used here to develop 574 a distributed algorithm for separation and integration in programmable matter, is much 575 more broadly applicable. This approach can potentially be applied to any objective described 576 by a global energy function (where the desirable configurations have low energy values), 577 provided changes in energy due to particle movements can be calculated with only local 578 information. Choosing the correct global energy function is the key; translating the energy 579 function into a Markov chain and then into a distributed algorithm is, by now, fairly routine 580 (see [6, 2]). However, proving that the stationary distribution has our desired properties with 581 high probability remains challenging, requiring application-specific proof techniques. 582

Last, we believe the proof techniques developed here extend beyond our current work. 583 For separation and integration, the key ingredient is the cluster expansion, used recently to 584 develop efficient low-temperature approximations and sampling algorithms, and the related 585 Pirogov-Sinai theory, used to show slow mixing of certain Markov chains. Here, however, we 586 used a completely different aspect of the cluster expansion by separating partition functions 587 into surface and volume terms. The cluster expansion and Pirogov-Sinai theory have been 588 widely used in statistical physics for many purposes, and we believe there are many more 589 ways a thorough understanding of these methods can benefit computer science. 590

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692 **A** Appendix

⁶⁹³ Here we include the proofs of some of our claims that were omitted from the main body of ⁶⁹⁴ this paper for conciseness and clarity. We do not include any detailed proofs of our technical ⁶⁹⁵ results due to length constraints.

696 A.1 Proof of Lemma 2

Recall that Lemma 2 states that for any $n \ge 1$, there is a connected, hole-free particle configuration of n particles with perimeter at most $2\sqrt{3}\sqrt{n}$. That is, $p_{min}(n) \le 2\sqrt{3}\sqrt{n}$.

⁶⁹⁹ **Proof.** The lemma can easily be verified for $n \leq 6$. For $n \geq 7$, we begin with the case ⁷⁰⁰ where $n = 3\ell^2 + 3\ell + 1$ for some integer $\ell \geq 1$. A regular hexagon with side length ℓ can be ⁷⁰¹ decomposed into six triangles, each with $\ell(\ell + 1)/2$ particles, and a single center vertex, for ⁷⁰² $3\ell^2 + 3\ell + 1$ total particles; see Figure 4a. Such a hexagon has perimeter 6ℓ . We see that

703
$$p_{min}(3\ell^2 + 3\ell + 1) \le 6\ell \le 2\sqrt{3}\sqrt{3\ell(\ell+1)} \le 2\sqrt{3}\sqrt{n-1} \le 2\sqrt{3}\sqrt{n}.$$

Now we consider $n = 3\ell^2 + 3\ell + 1 + k$, for integers ℓ and k, where $k \in [1, 6\ell + 6)$. As 704 $(3\ell^2 + 3\ell + 1) + 6\ell + 6 = 3(\ell + 1)^2 + 3(\ell + 1) + 1$, this covers all possible values of n. We 705 construct a particle configuration on $n = 3\ell^2 + 3\ell + 1 + k$ particles by first constructing 706 a regular hexagon of side length ℓ and then adding the remaining k particles around the 707 outside of this hexagon in a single layer, completing one side before beginning the next; see 708 Figure 4b, where $\ell = 3$ and k = 6. For $k \leq \ell$, the perimeter of this configuration is $6\ell + 1$. 709 More generally, the perimeter increases by one when particles begin to be added to a new side 710 of the hexagon, and so for i = 2, 3, 4, 5, 6, for $(i-1)\ell + (i-2) < k \le i\ell + (i-1)$ the perimeter 711 of this configuration is $6\ell + i$. We see that (using $i \leq 6$ and $\ell \geq 1$), for any i = 1, 2, 3, 4, 5, 6, 712

$$p_{min}(3\ell^2 + 3\ell + 1 + k) \le 6\ell + i \le 2\sqrt{3}\sqrt{\left(\sqrt{3\ell} + \frac{i}{2\sqrt{3}}\right)^2} = 2\sqrt{3}\sqrt{3\ell^2 + \frac{i^2}{12} + i} \le 2\sqrt{3}\sqrt{3\ell^2 + 3 + i}$$

$$\leq 2\sqrt{3}\sqrt{3\ell^2 + 3\ell + 1 + i - 1}$$

$$\leq 2\sqrt{3}\sqrt{3\ell^2 + 3\ell + 1 + k} = 2\sqrt{3}\sqrt{n}.$$

718 This concludes our proof.



Figure 4 (a) The regular hexagon with side length $\ell = 3$ with $3\ell^2 + 3\ell + 1$ total particles. (b) A configuration with $n = 3\ell^2 + 3\ell + 1 + k$ particles for $\ell = 3$ and k = 6 with perimeter $20 < 2\sqrt{3}\sqrt{n}$.

A.2 Detailed Balance Proof that π is the Stationary Distribution of \mathcal{M} 719

Recall that Lemma 9 states that the stationary distribution of \mathcal{M} is given by $\pi(\sigma) = 0$ 720 if σ is disconnected or has holes, and by $\pi(\sigma) = (\lambda \gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}/Z$ otherwise, where 721 $Z = \sum_{\sigma} (\lambda \gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}$. Here, we analyze the necessary cases to verify this with detailed 722 balance. 723

Proof. We first verify that $\pi(\sigma) = \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}/Z_e$ — where $e(\sigma)$ is the number of edges of σ , 724 $a(\sigma)$ is the number of homogeneous edges of σ , and $Z_e = \sum_{\sigma} \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}$ — is the stationary 725 distribution by detailed balance. We then show that this form of π can be rewritten as in 726 the lemma. 727

Consider any two connected, hole-free configurations σ, τ that differ by one move of some 728 particle from location ℓ in σ to a neighboring location ℓ' in τ . By examining \mathcal{M} , we see that 729 the probability of transitioning from σ to τ is: 730

$$_{^{731}} \qquad M(\sigma,\tau) = \min\left\{1, \lambda^{|N(\ell')| - |N(\ell)|} \cdot \gamma^{|N_i(\ell')| - |N_i(\ell)|}\right\} / 6n.$$

A similar analysis shows: 732

733
$$M(\tau,\sigma) = \min\left\{1, \lambda^{|N(\ell)| - |N(\ell')|} \cdot \gamma^{|N_i(\ell)| - |N_i(\ell')|}\right\} / 6n.$$

Without loss of generality, suppose $\lambda^{|N(\ell')|-|N(\ell)|} \cdot \gamma^{|N_i(\ell')|-|N_i(\ell)|} < 1$, meaning $M(\sigma, \tau)$ is 734 this value over 6n and $M(\tau, \sigma) = 1/6n$. Because the only edges that differ in σ and τ are 735 incident to ℓ or ℓ' , 736

$$\pi(\sigma)M(\sigma,\tau) = \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \cdot \frac{1}{n} \cdot \frac{1}{6} \cdot \lambda^{|N(\ell')| - |N(\ell)|} \cdot \gamma^{|N_i(\ell')| - |N_i(\ell)|}$$

$$= \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \cdot \frac{1}{2} \cdot \frac{1}{2} \cdot \lambda^{e(\tau) - e(\sigma)} \cdot \gamma^{a(\tau) - a(\sigma)}$$

$$= \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \cdot \frac{1}{n} \cdot \frac{1}{6} \cdot \lambda^{e(\tau) - e(\sigma)} \cdot \gamma^{a(\tau) - e(\sigma)} \cdot \gamma^{a(\tau) - e(\sigma)}$$
$$= \frac{\lambda^{e(\tau)} \cdot \gamma^{a(\tau)}}{Z_e} \cdot \frac{1}{n} \cdot \frac{1}{6} \cdot 1 = \pi(\tau) M(\tau, \sigma)$$

739 740

751

Thus, detailed balance is satisfied for particle moves that are not swaps. 741

Suppose instead that σ and τ differ by a swap move of particle P with color c_i at location 742 ℓ in σ and particle Q with color c_i at neighboring location ℓ' in σ . This move could occur if 743 P or Q is chosen in Step 1 of \mathcal{M} , so: 744

⁷⁴⁵
$$M(\sigma,\tau) = \min\left\{1, \gamma^{|N_i(\ell') \setminus \{P\}| - |N_i(\ell)| + |N_j(\ell) \setminus \{Q\}| - |N_j(\ell')|}\right\} / 3n.$$

Similarly, because τ has P at location ℓ' and Q at location ℓ , we have: 746

747
$$M(\tau,\sigma) = \min\left\{1, \gamma^{|N_i(\ell) \setminus \{P\}| - |N_i(\ell')| + |N_j(\ell') \setminus \{Q\}| - |N_j(\ell)|}\right\} / 3n.$$

Without loss of generality, suppose that $\gamma^{|N_i(\ell')\setminus\{P\}|-|N_i(\ell)|+|N_j(\ell)\setminus\{Q\}|-|N_j(\ell')|} < 1$, so 748 $M(\sigma, \tau)$ is this value over 3n and $M(\tau, \sigma) = 1/3n$. Then,

$$\pi(\sigma)M(\sigma,\tau) = \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \cdot \frac{2}{n} \cdot \frac{1}{6} \cdot \gamma^{|N_i(\ell') \setminus \{P\}| - |N_i(\ell)| + |N_j(\ell) \setminus \{Q\}| - |N_j(\ell')|}}{\lambda^{e(\sigma)} \cdot 2}$$

$$=\frac{\lambda^{e(\sigma)}\cdot\gamma^{a(\sigma)}}{Z_e}\cdot\frac{2}{n}\cdot\frac{1}{6}\cdot\gamma^{(|N_i(\ell')\setminus\{P\}|+|N_j(\ell)\setminus\{Q\}|)-(|N_i(\ell)|+|N_j(\ell')|)}$$

$$_{^{752}} \qquad \qquad = \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \cdot \frac{2}{n} \cdot \frac{1}{6} \cdot \gamma^{a(\tau)-a(\sigma)}$$

$$\lambda^{e(au)}\cdot\gamma^{a(au)}=2$$

⁷⁵³₇₅₄ =
$$\frac{7}{Z_e} \cdot \frac{1}{2} \cdot \frac{1}{6} \cdot 1 = \pi(\tau) M(\tau, \sigma)$$

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In both cases, detailed balance is satisfied, so we conclude the stationary distribution π (which 755 is only non-zero over connected, hole-free configurations) is given by $\pi(\sigma) = \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}/Z_e$. 756 Since every edge of σ is either homogeneous or heterogeneous, we have $e(\sigma) = a(\sigma) + h(\sigma)$. 757 From [6], we have $e(\sigma) = 3n - p(\sigma) - 3$, where n is the number of particles in the system. 758

Thus, we can rewrite this unique stationary distribution as follows: 759

761

$$\pi(\sigma) = \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{Z_e} \\ \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}$$

$$= \frac{\lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}{\sum \lambda^{e(\sigma)} \cdot \gamma^{a(\sigma)}}$$

$$= \frac{(\lambda\gamma)^{-3n+3} \cdot (\lambda\gamma)^{e(\sigma)} \cdot \gamma^{a(\sigma)-e(\sigma)}}{(\lambda\gamma)^{-3n+3} \cdot \sum_{\sigma} (\lambda\gamma)^{e(\sigma)} \cdot \gamma^{a(\sigma)-e(\sigma)}}$$

$$= \frac{(\lambda\gamma)^{e(\sigma)-3n+3} \cdot \gamma^{a(\sigma)-e(\sigma)}}{\sum_{\sigma} (\lambda\gamma)^{e(\sigma)-3n+3} \cdot \gamma^{a(\sigma)-e(\sigma)}}$$
$$= \frac{(\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}}{(\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}}$$

763

$$= \frac{(\chi\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\gamma)}}{\sum_{\sigma} (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\gamma)}}$$

This concludes our proof. 766

Proof of Boundary-Volume Decomposition of Cluster Expansion A.3 767

In this section we provide the proof of Theorem 11, which is our decomposition of a polymer 768 partition function into boundary and volume terms via the cluster expansion. For the sake 769 of clarity we restate this theorem here, including all of its hypotheses and assumptions. 770

Theorem 11. Let Γ be an infinite set of polymers $\xi \subseteq E(G_{\Delta})$ that is closed under 771 translation and rotation, and let $\Lambda \subseteq E(G_{\Delta})$ be finite. If there is a constant c such that for 772 any edge $e \in E(G_{\Delta})$, 773

$$\sum_{\substack{\xi \in \Gamma:\\e \in \xi}} |w(\xi)| e^{c|[\xi]|} \le c, \tag{3}$$

then for any Λ the partition function 776

$$\pi \pi \qquad \Xi_{\Lambda} := \sum_{\substack{\Gamma' \subseteq \Gamma_{\Lambda} \\ compatible}} \prod_{\xi \in \Gamma'} w(\xi)$$

satisfies 778

$$e^{\psi|\Lambda|-c|\partial\Lambda|} \le \Xi_{\Lambda} \le e^{\psi|\Lambda|+c|\partial\Lambda|}$$

for some constant $\psi \in [-c, c]$ that is independent of Λ . 780

Proof. We follow the same outline as the proof of the same fact for the Ising model in Section 781 5.7.1 of [12]. 782

Let \mathcal{X} be all clusters comprised of polymers from Γ , and let \mathcal{X}_{Λ} be all clusters of polymers 783 in Γ_{Λ} . Note that Equation 3 implies the hypothesis of Theorem 10 (Equation 1) is satisfied, 784 with function $a: \Gamma \to \mathbb{R}$ given by $a(\xi) = c|[\xi]|$: 785

786
$$\sum_{\substack{\xi \in \Gamma: \\ \xi, \xi^* \text{ incompatible}}} |w(\xi)| e^{a(\xi)} \le \sum_{e \in [\xi^*]} \sum_{\substack{\xi \in \Gamma: \\ e \in \xi}} |w(\xi)| e^{c|[\xi]|} \le c|[\xi^*]|.$$

Because this hypothesis is satisfied for all $\xi^* \in \Gamma$, it certainly holds when we restrict our 787 attention to polymers in Γ_{Λ} . By Theorem 10, because Γ_{Λ} is a finite set, this means the 788 cluster expansion for Ξ_{Λ} converges: 789

⁷⁹⁰
$$\ln \Xi_{\Lambda} = \sum_{X \in \mathcal{X}_{\Lambda}} \Psi(X)$$

Let $\overline{X} = \bigcup_{\xi \in X} \xi$ be the support of cluster X and $|\overline{X}|$ the size of this support. Using 791 Equation 3 and standard techniques (see [12], the proof of Theorem 5.4 and Equation (5.29)), 792 the translation and rotation invariance of Γ imply that for any edge $e \in E(G_{\Delta})$, 793

$$\sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}}} |\Psi(X)| \le c.$$
(4)

The proof of this fact is the reason we need a slightly stronger hypothesis (Equation 3) than 796 is needed to guarantee the cluster expansion converges (Equation 1). 797

For any cluster $X \in \mathcal{X}_{\Lambda}$, it trivially holds that $1 = (\sum_{e \in \Lambda} \mathbf{1}_{e \in \overline{X}})/\overline{X}$. We can use this fact 798 to rewrite the cluster expansion for Ξ_{Λ} : 799

$$\ln \Xi_{\Lambda} = \sum_{X \in \mathcal{X}_{\Lambda}} \Psi(X) = \sum_{\substack{X \in \mathcal{X}: \\ \overline{X} \subseteq \Lambda}} \Psi(X) = \sum_{\substack{e \in \Lambda \\ e \in \overline{X}, \\ \overline{X} \subseteq \Lambda}} \sum_{\substack{X \in \mathcal{X}: \\ \overline{X} \subseteq \Lambda}} \frac{1}{|\overline{X}|} \Psi(X)$$

$$= \sum_{e \in \Lambda} \left(\sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}}} \frac{1}{|\overline{X}|} \Psi(X) - \sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}, \\ \overline{X} \subseteq \Lambda}} \frac{1}{|\overline{X}|} \Psi(X) \right)$$

$$= \left(\sum_{e \in \Lambda} \sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}}} \frac{1}{|\overline{X}|} \Psi(X) \right) - \left(\sum_{\substack{e \in \Lambda \\ X \in \mathcal{X}: \\ \overline{X} \subseteq \Lambda}} \frac{1}{|\overline{X}|} \Psi(X) \right).$$
(5)

The two infinite sums in parentheses above are absolutely convergent by Equation 4, so this 804 difference is well-defined. 805

To analyze the first term of Equation 5, we note that by the translation and rotation 806 invariance of Γ , the sum 807

$$\psi := \sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}}} \frac{1}{|\overline{X}|} \Psi(X)$$

is independent of e and of Λ and only depends on our particular polymer model; this is 810 the value ψ that appears in the statement of the theorem, and by Equation 4, $|\psi| < c$. We 811 conclude the first term of Equation 5 is $\psi|\Lambda|$. 812

To analyze the second term of Equation 5, recall if cluster X satisfies both $e \in \overline{X}$ for 813 some $e \in \Lambda$ and $\overline{X} \not\subseteq \Lambda$, then \overline{X} must contain some edge $f \in \partial \Lambda$. We rewrite the absolute 814

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⁸¹⁵ value of this second sum as

$$\sum_{\substack{e \in \Lambda \\ e \in \overline{X}, \\ \overline{X} \not\subseteq \Lambda}} \sum_{\substack{X \in \mathcal{X}: \\ e \in \overline{X}, \\ \overline{X} \not\subseteq \Lambda}} \frac{1}{|\overline{X}|} \Psi(X) \left| \leq \sum_{\substack{e \in \Lambda \\ e \in \overline{X}, \\ \overline{X} \not\subseteq \Lambda}} \sum_{\substack{X \in \mathcal{X}: \\ \overline{X} \not\subseteq \Lambda}} \frac{1}{|\overline{X}|} |\Psi(X)| \right|$$

$$\leq \sum_{\substack{f \in \partial \Lambda \\ f \in \overline{X}}} \sum_{\substack{X \in \mathcal{X}: \\ f \in \overline{X}}} |\Psi(X)| \leq c |\partial\Lambda|.$$

$$\leq \sum_{\substack{F \in \partial \Lambda \\ F \in \overline{X}}} \sum_{\substack{X \in \mathcal{X}: \\ F \in \overline{X}}} |\Psi(X)| \leq c |\partial\Lambda|.$$

819

The last inequality above follows from Equation 4 and the translation and rotation invariance 820 of Λ . 821

We conclude that Equation 5 implies 822

$$\psi|\Lambda| - c|\partial\Lambda| \le \ln \Xi_{\Lambda} \le \psi|\Lambda| + c|\partial\Lambda|.$$

Exponentiation proves the theorem. 825