Markov Chains for Programmable Active Matter

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Programmable Active Matter
as Self-Organizing Particle Systems (SOPS)

Active Matter: ensemble of self-organizing computational "particles"

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Programmable to change their collective physical properties

Algorithms: Devise the local, distributed rules that each particle runs in order to achieve the desired emergent, collective behavior

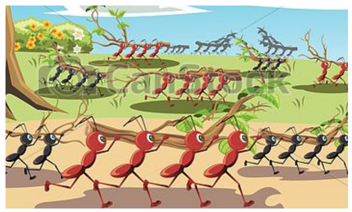
- No human intervention or central control
- Scalable
- Indistinguishable particles
- Oblivious to global properties

Self-Organization

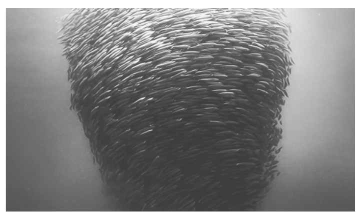
In Nature:

Compression

Separation



Flocking



Bridging

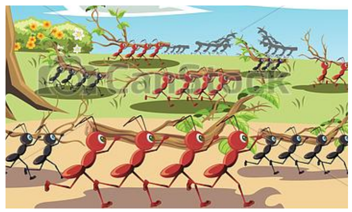
Locomotion

Self-Organization

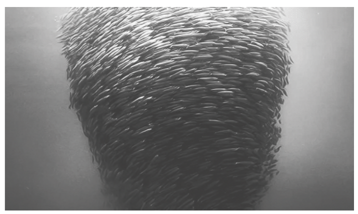
In Nature:

Compression

Separation



Flocking

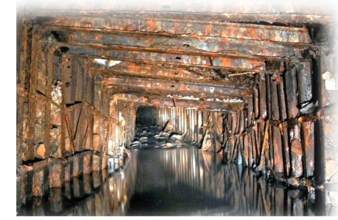


Bridging

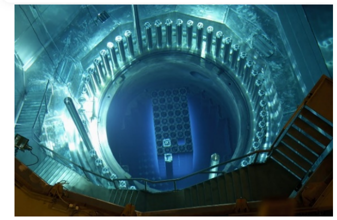
Locomotion

Applications:

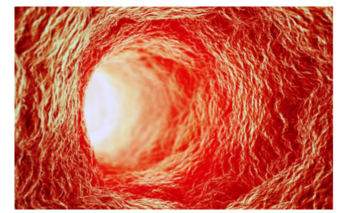
Sensing in materials



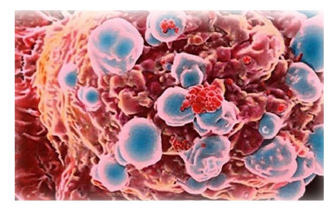
Self-regulation



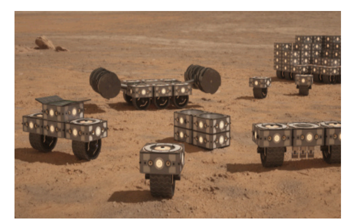
Monitoring health



Assisting surgeries



Exploring terrains

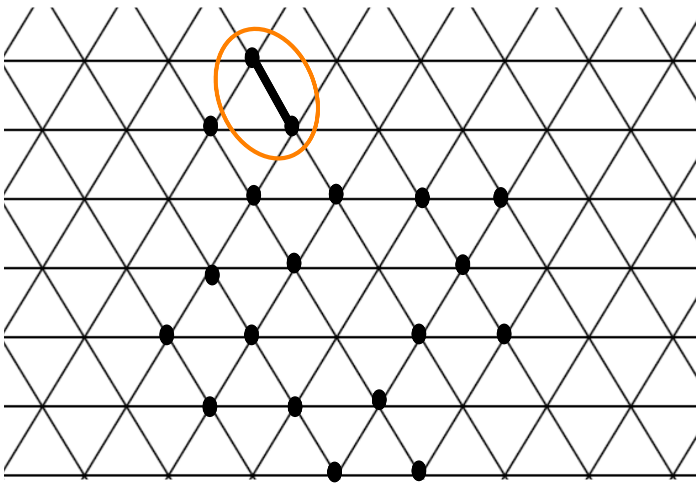


Self-Organizing Particle Systems

Abstraction of programmable matter as computational "particles" that use distributed, local algorithms to achieve system-level goals.

The Geometric Amoebot Model

[Derakhshandeh et al. '14]

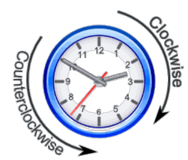


Particles:

anonymous

no global orientation

constant-size memory

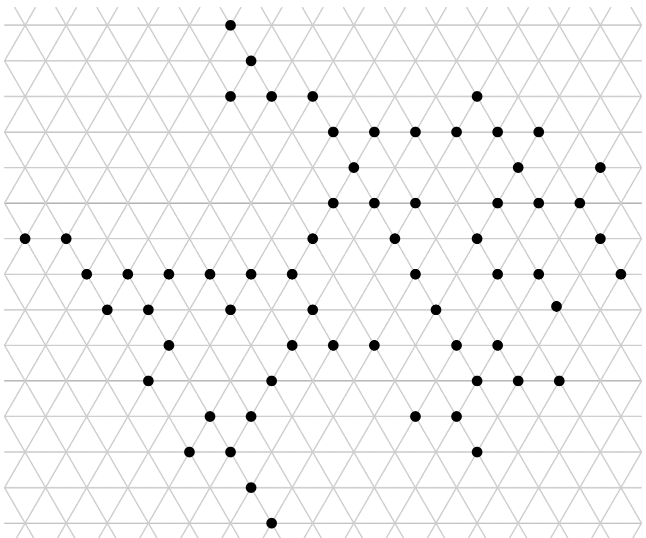


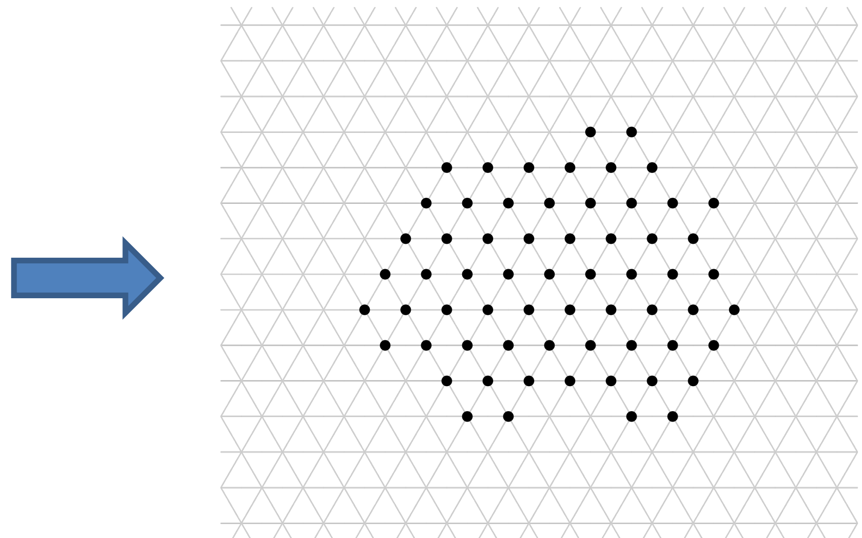
chirality

- Local communication: Exchange information via shared bonds.
- Actively move (via expansions and contractions)
- System progresses concurrently and asynchronously

Compression

Question: Using local, distributed rules, how can particles "compress" (or "aggregate")?





Not compressed

Compressed

Def: A configuration is α-compressed if its perimeter is at most α times the minimum perimeter (for this number of particles).

Compression Algorithm

[Cannon, Daymude, R., Richa '16]

A distributed, stochastic algorithm for compression:

- Ensures system connectivity on the triangular lattice.
- Poisson clocks to activate particles (i.e., no synchronization).
- Metropolis probabilities to converge to $\pi(\sigma) \propto \lambda^{e(\sigma)}$, for $\lambda > 1$.

Fix $\lambda > 1$. Start in any connected configuration.

When a particle activates (according to its Poisson clock):

- Pick a random neighboring node.
- If the proposed node is unoccupied, and certain properties hold*,

  move with probability $\min\{\lambda^{\Delta e}, 1\}$.

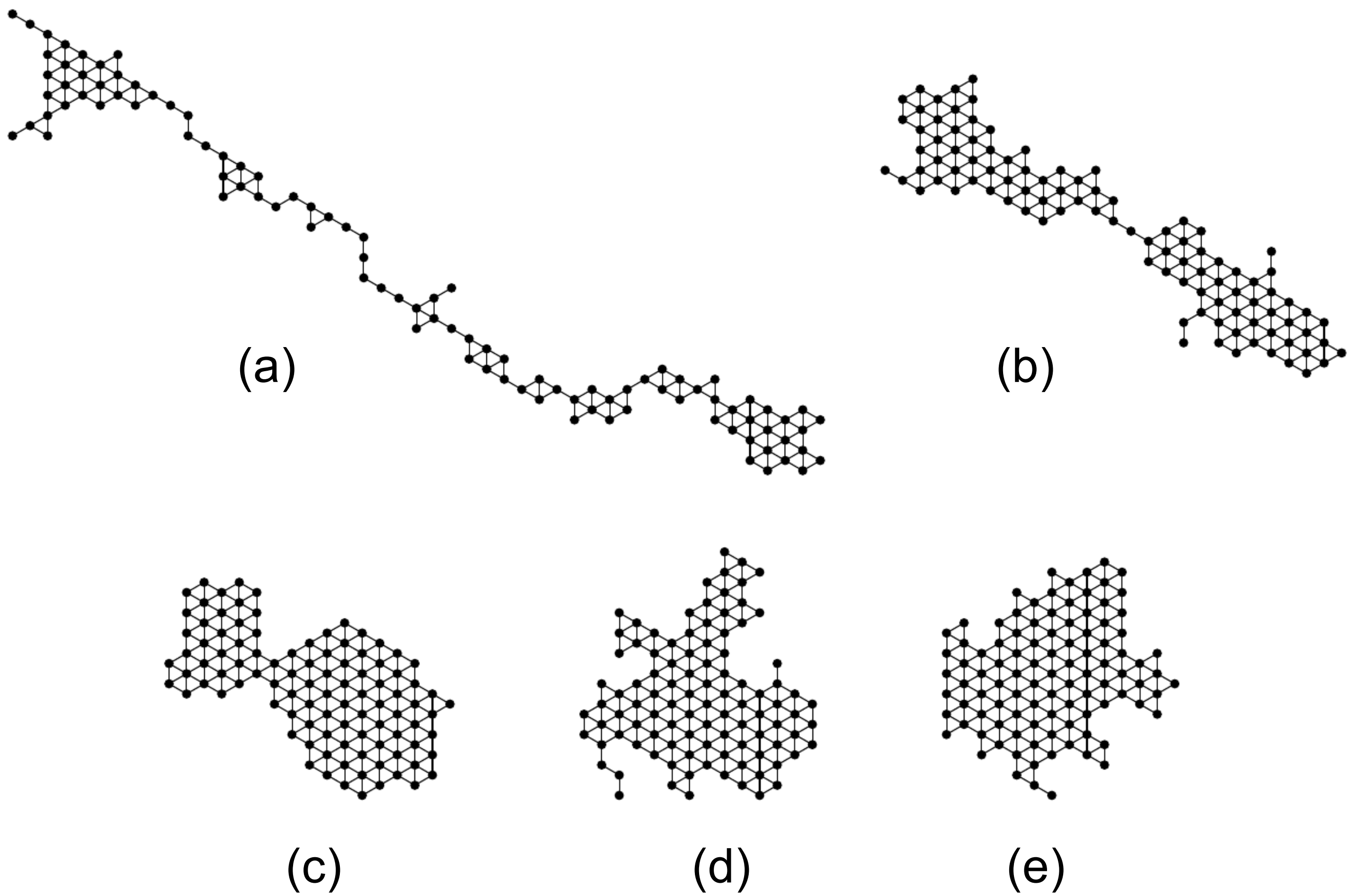
- Otherwise, do nothing.

*To maintain connectivity.

Compression Simulations

$\lambda = 4$

100 particles after:
a) 1 million
b) 2 million
c) 3 million
d) 4 million
e) 5 million
iterations.

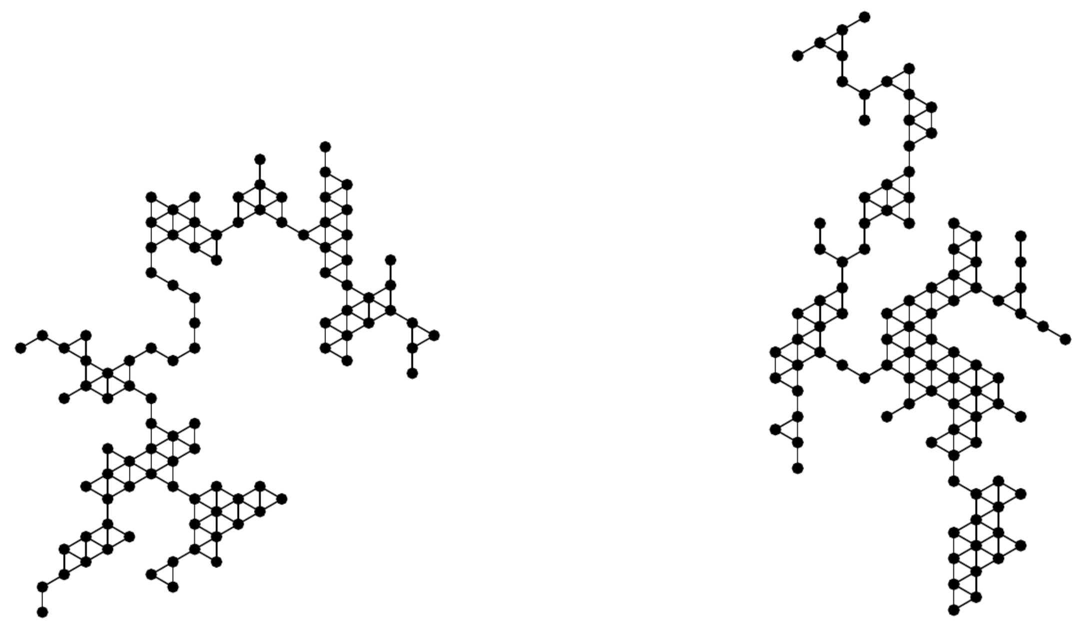


Compression Simulations

$\lambda = 2$

100 particles after:
a) 10 million
b) 20 million
iterations.

No compression.



(a) (b)

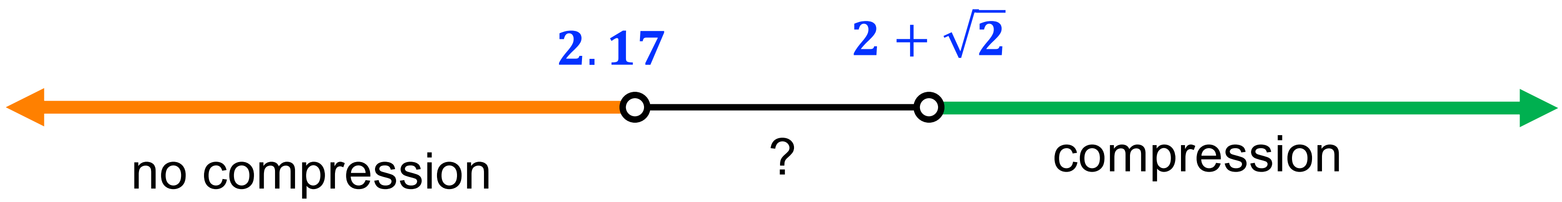
Compression: Theorems

[Cannon, Daymude, R., Richa '16]

Defn: A configuration is α-compressed if its perimeter is at most α times the minimum perimeter.

Thm: For all $\lambda > 2+\sqrt{2}$, there exists $\alpha = \alpha(\lambda)$ s.t. particles are α-compressed at stationarity almost surely.
(E.g., when $\lambda = 4$, $\alpha = 9$.)

Thm: When $\lambda < 2.17$, for *any* $\alpha > 1$, the probability particles are α-compressed at stationarity is exponentially small.



Note: Expansion works similarly for small λ.

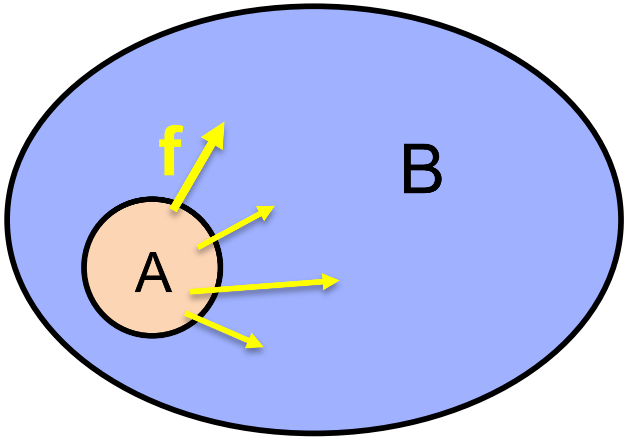
Main proof technique: Peierls Argument

To show that some subset has exponentially small probability:

Define f: $A \rightarrow B$ so that, for $c_1 > c_2$ such that:

- For all $a \in A$, $\pi(a) < \pi(f(a))\, e^{-c_1 n}$
- For all $b \in B$, $|\{f^{-1}(b)\}| < e^{c_2 n}$

Then: $\pi(A) < e^{(c_2 - c_1)\, n} << 1.$



Physics: Distinguish Gibbs states;

Comp Sci: Bound mixing times through identifying small cutsets;

Active Matter: Bound likelihood of (un)desirable ensemble behavior.

Proof Techniques

Thm: For all $\lambda > 2 + \sqrt{2}$, there exists $\alpha = \alpha(\lambda)$ s.t. particles are α-compressed at stationarity almost surely.

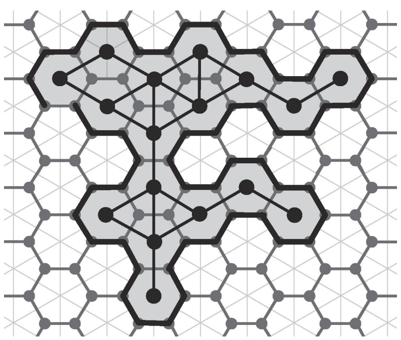
Pf: Note $p(\sigma) = 3n - e(\sigma) - 3$, so we can express the stat. dist'n as:

$$\pi(\sigma) \propto \lambda^{e(\sigma)} = \lambda^{-p(\sigma)}/Z\,.$$

Let S_α = configurations with perimeter > αp_{min}
m_k = number of configurations with perimeter k.

$$\pi(S_\alpha) = \sum_{k=\alpha\, p_{min}}^{p_{max}} m_k\, \lambda^{-k} \Big/ Z$$

The (# configs with perimeter k) < (# SAWs in the hexagonal lattice), i.e.,



$|\{\text{SAWs of length } t\}| \sim (\mu_{hex})^t = (2+\sqrt{2})^{t/2}$

[Duminil-Copin and Smirnov '12]

Proof Techniques

Thm: For all $\lambda > 2 + \sqrt{2}$, there exists $\alpha = \alpha(\lambda)$ s.t. particles are α-compressed at stationarity almost surely.

Pf: Let S_α = configurations with perimeter > αp_{min}
m_k = number of configurations with perimeter k.

$$\pi(S_\alpha) = \sum_{k=\alpha p_{min}}^{p_{max}} m_k \lambda^{-k} / Z \quad \lesssim \sum_{k=\alpha p_{min}}^{p_{max}} (2+\sqrt{2})^{k+5/2} \lambda^{-k} / Z$$

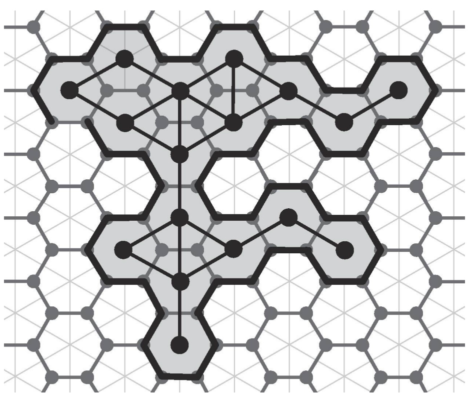
.... which is exponentially small for $\boldsymbol{\lambda} > \mathbf{2} + \sqrt{\mathbf{2}}$.

Proof Techniques

Thm: For all $\lambda > 2+\sqrt{2}$, there exists α s.t. particles are α-compressed at stationarity almost surely.

Thm: When $\lambda < 2.17$, for *any* $\alpha > 1$, the probability particles are α-compressed at stationarity is exponentially small.

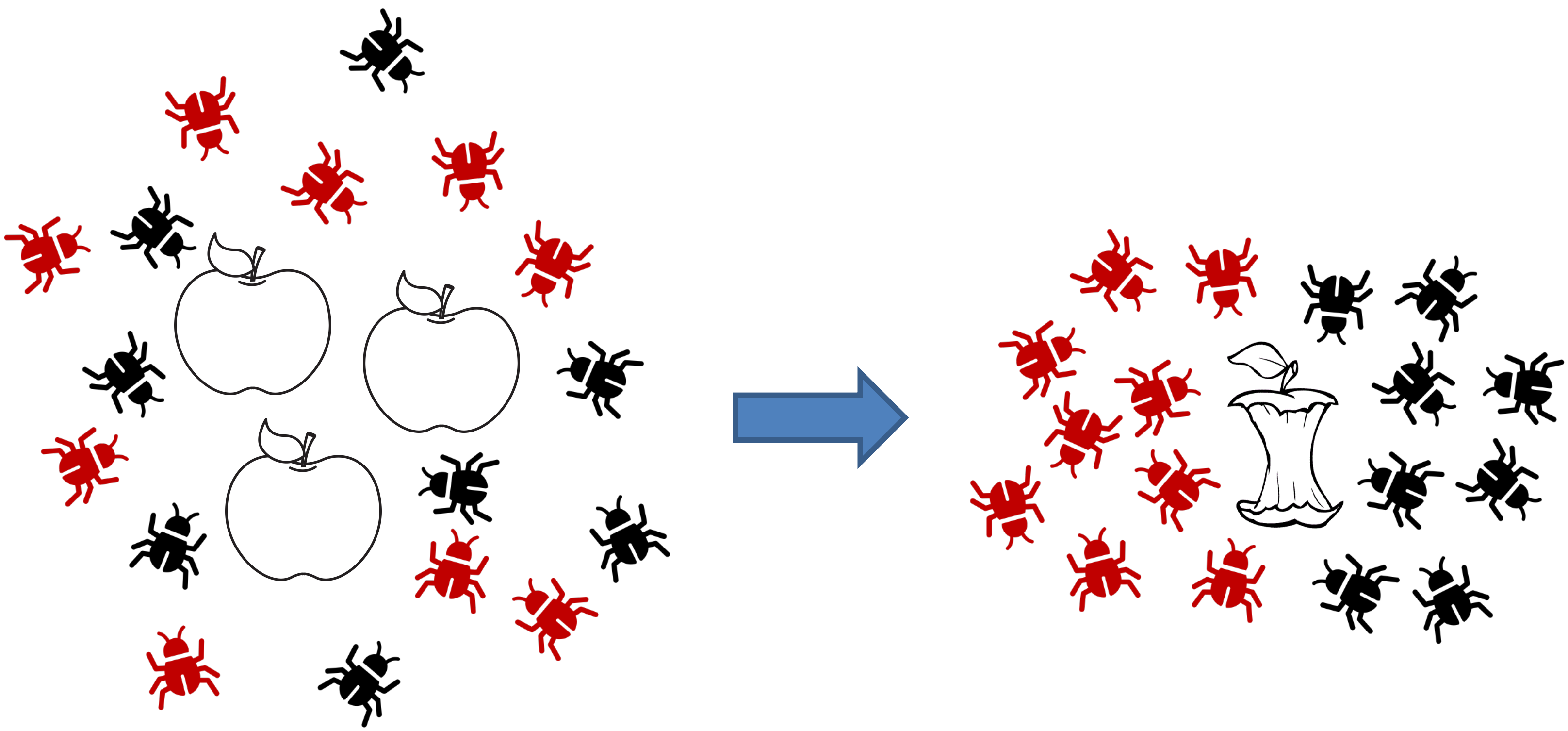
Pf: Another Peierls argument to show non-compression with high prob.
Bijection between configurations and hydrocarbons (or "animals" on the hexagonal lattice).



The normalizing constant Z satisfies:

$$Z = \sum_{\sigma} \lambda^{e(\sigma)} \geq 0.13\left(\frac{2.17}{\lambda}\right)^{2n-2}$$

Separation (or Speciation)

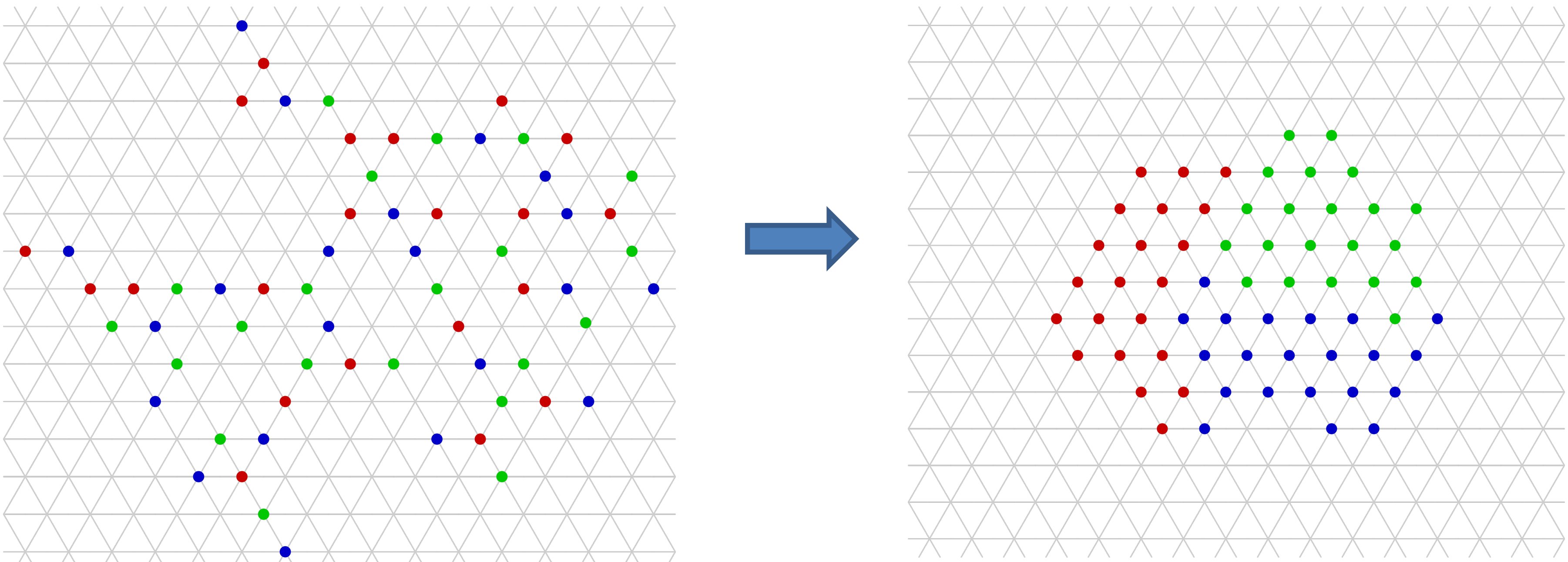


"Integrated"

"Separated"

Separation

Question: Using local, distributed rules, how can heterogeneous particles "compress" overall while also "separating" into (mostly) monochromatic groups?

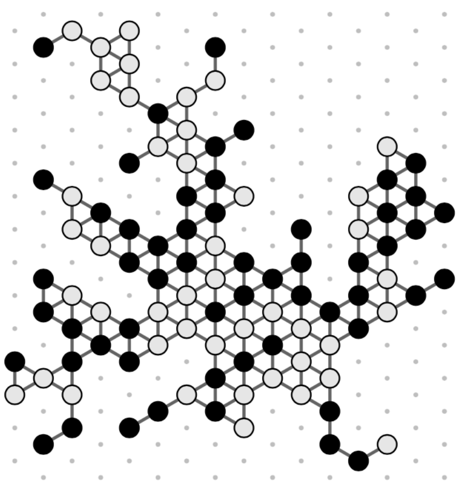


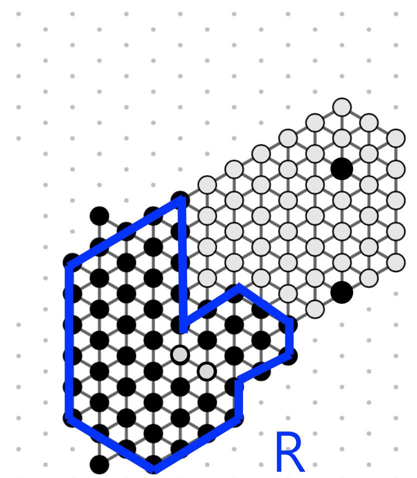
Neither compressed nor separated   compressed and separated

Definition of Separated

Defn: A configuration is (β,δ)-separated if there is a subset of particles R s.t.:

1. There are at most $\beta\sqrt{n}$ particles with exactly one endpoint in R;
2. The density of particles of color c_1 *inside* R is at least $1-\delta$;
3. The density of particles with color c_1 *outside* R is at most δ.





Compressed and separated

MC for Separation

Distributed algorithm for separation:

- Ensures global connectivity and is not synchronized.
- Uses Metropolis probabilities to converge to:

$$\pi(\sigma) \propto \lambda^{e(\sigma)} \cdot \gamma^{m(\sigma)},$$

for bias parameters λ (for compression) and γ (for separation),

where $m(\sigma)$ is the # of monochromatic edges.

Fix λ and γ. Start in any connected configuration.

When a particle activates (according to its Poisson clock):

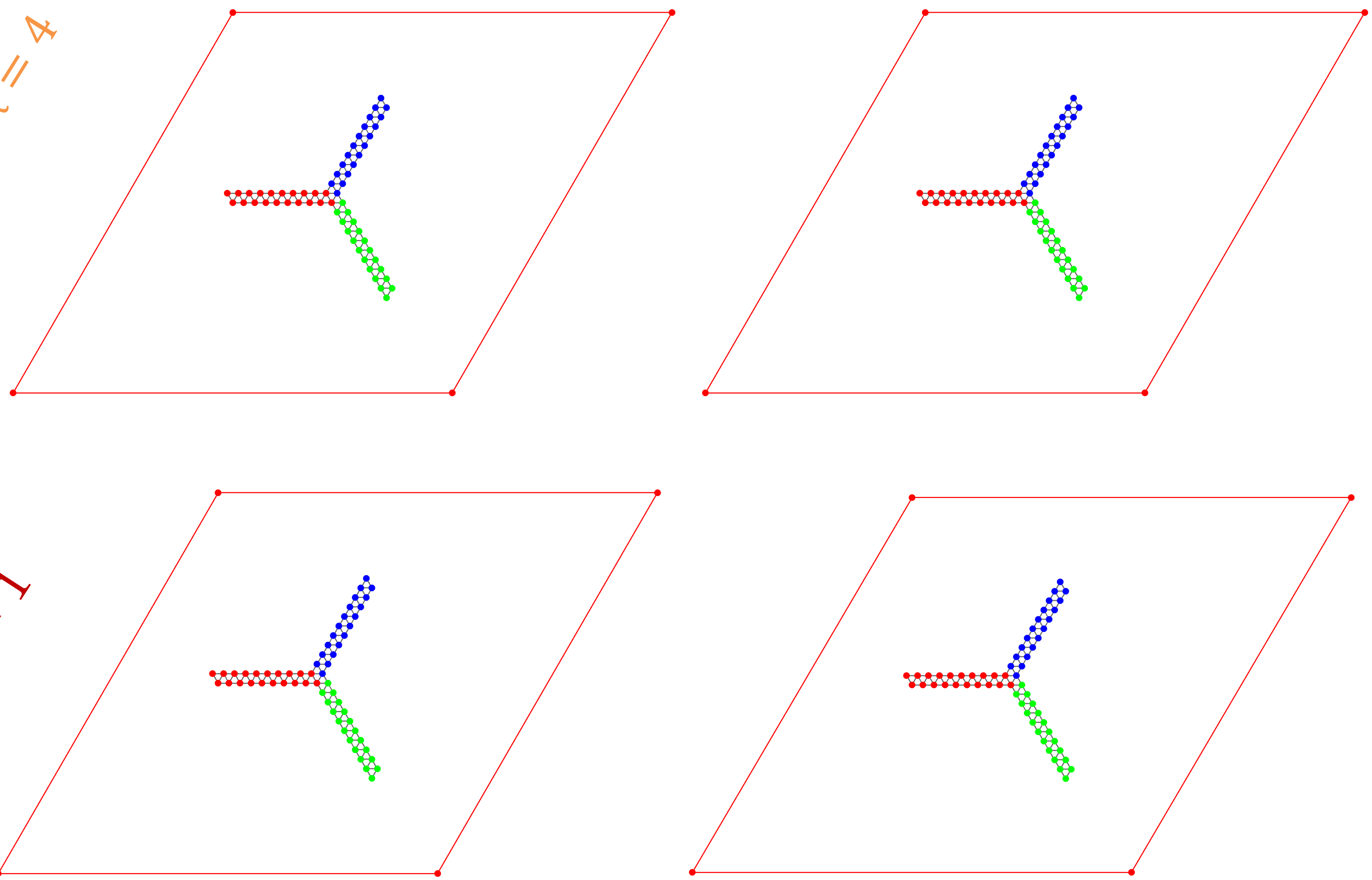
- Pick a random neighbor.
- Move with probability $\min\{(\lambda^{e'} \cdot \gamma^{m'} / \lambda^{e} \cdot \gamma^{m}), 1\}$.
- Otherwise, do nothing.

Separation: Simulations

Integration: $\gamma = 0.25$ Separation: $\gamma = 4$

Compression: $\lambda = 4$

Expansion: $\lambda = 1$



(simulations by Cem Gokmen)

Separation for large γ

Stationary distribution: $\pi(\sigma) \propto \lambda^{e(\sigma)} \cdot \gamma^{m(\sigma)} = (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}$.

Thm: When $\lambda\gamma > 6.83$ and $\gamma > 5.66$, there exists α s.t. the particle system is α-compressed and separated at stationarity a.s.

(Now have to account for both *monochromatic* / *heterogenous* edges!)

Pf: The stationary distribution $\pi(\sigma) = (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}/Z$.

Let S_α be the non-α-compressed configurations. *(Need $\pi(S_\alpha)$ small.)*

Partition S_α into sets of configurations A_k with perimeter k. Then:

$$\pi(A_k) = \sum_{\sigma \in A_k} (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}/Z$$

$$= (\lambda\gamma)^{-k} \cdot \sum_{\sigma \in A_k} \gamma^{-h(\sigma)}/Z$$

Separation for large γ

Thm: When $\lambda\gamma > 6.83$ and $\gamma > 5.66$, there exists α s.t. the particle system will be α-compressed and separated a.s.

Pf: $\pi(A_k) = (\lambda\gamma)^{-k} \cdot \sum_{\sigma \in A_k} \gamma^{-h(\sigma)}/Z.$

If we had $\sum_{\sigma \in A_k} \gamma^{-h(\sigma)} \leq b^k$ for some $b > 1$, then:

$$\pi(S_\alpha) = \sum_{k=\alpha \cdot p_{min}}^{p_{max}} \pi(A_k) = \sum_{k=\alpha \cdot p_{min}}^{p_{max}} (\lambda\gamma)^{-k} \cdot \sum_{\sigma \in A_k} \gamma^{-h(\sigma)}/Z$$

$$\leq \sum_{k=\alpha \cdot p_{min}}^{p_{max}} (\lambda\gamma)^{-k} \cdot \frac{b^k}{Z}$$

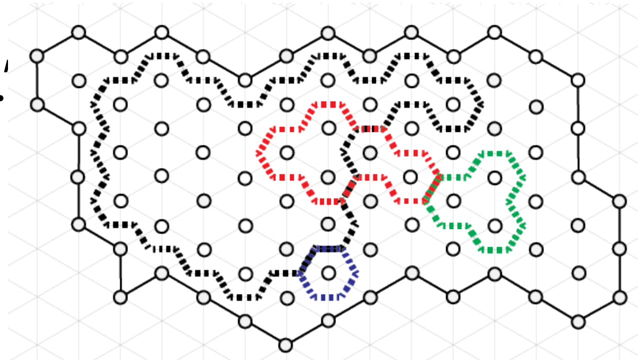
as before.

But not true for our heterogeneous setting!

Separation for large γ

Thm: When $\lambda\gamma > 6.83$ and $\gamma > 5.66$, there exists α s.t. the particle system will be α-compressed and separated a.s.

Pf (cont): $\pi(A_k) = (\lambda\gamma)^{-k} \cdot \sum_{\sigma \in A_k} \gamma^{-h(\sigma)}/Z.$



Instead, express $\sum_{\sigma \in \Omega_\Lambda} \gamma^{-h(\sigma)}$ as a "polymer model."

An interface I between two color classes is a loop.

Let Γ_Λ be the set of all interfaces in Λ. Then:

$$\sum_{\sigma \in \Omega_\Lambda} \gamma^{-h(\sigma)} = \sum_{\text{pairwise disjoint } \Gamma' \in \Gamma_\Lambda} \prod_{I \in \Gamma'} \gamma^{-|I|}.$$

A cluster is a multiset $X \subseteq \Gamma_\Lambda$ of connected interfaces.

The "cluster expansion" is: $\ln\left(\sum_{\sigma \in \Omega_\Lambda} \gamma^{-h(\sigma)}\right) = \sum_{X \subseteq \Gamma_\Lambda} \phi(X) \prod_{I \in X} \gamma^{-|I|}$.

When $\gamma > 5.66$, we have convergence (of the formal series) and:

$$a^n \cdot e^{-ck} \leq \sum_{\sigma \in \Omega_\Lambda} \gamma^{-h(\sigma)} \leq a^n \cdot e^{ck},$$

which shows compression.

Integration for small γ (close to 1)

Stationary distribution: $\pi(\sigma) \propto \lambda^{e(\sigma)} \cdot \gamma^{m(\sigma)} = (\lambda\gamma)^{-p(\sigma)} \cdot \gamma^{-h(\sigma)}$.

<u>Thm</u>: When $\lambda(\gamma+1) > 6.83$ and $0.98 \leq \gamma \leq 1.02$, there exists $\alpha(\lambda, \gamma)$ s.t. the particle system will be α-compressed and integrated (i.e., <u>not</u> separated) at stationarity a.s.

Here we use the "high temperature expansion" (to express Z as a weighted sum over even degree subgraphs):

$$\sum_{\sigma \in \Omega_\Lambda} \gamma^{-h(\sigma)} = (\ldots) \sum_{\text{even } E \subseteq E(\Lambda)} \left(\frac{\gamma - 1}{\gamma + 1}\right)^{|E|}$$

+ a similar strategy as before with the cluster expansion + a Peierls arg.

Programmable Matter in the "Real World"

[Dutta, Li, Cannon, Daymude, Aydin, Richa, Goldman, R. '20]

- Relax the connectivity requirement.
- Self-organizing particles system algorithms without look-ahead.

Compression Algorithm (without the connectivity requirement):

Fix $\lambda > 1$. Start in any ~~connected~~ configuration.

When a particle activates (according to its Poisson clock):

- Pick a random neighboring node v.
- If unoccupied, ~~and certain properties hold,~~ move with

probability $\cancel{\min\{\lambda^{\Delta e}, 1\}} \propto \lambda^{-\deg(v)}$.

- Otherwise, do nothing.

(A variant on Metropo... just depends on *current position*)

Can be implemented *mechanically* !!

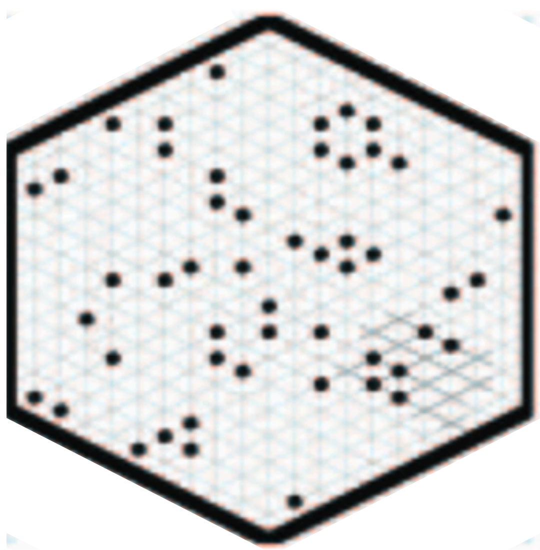
- Proving connectivity of the state space is much easier.
- Proving aggregation (or compression) is trickier,
  but just Peierls + cluster expansion as for separation.

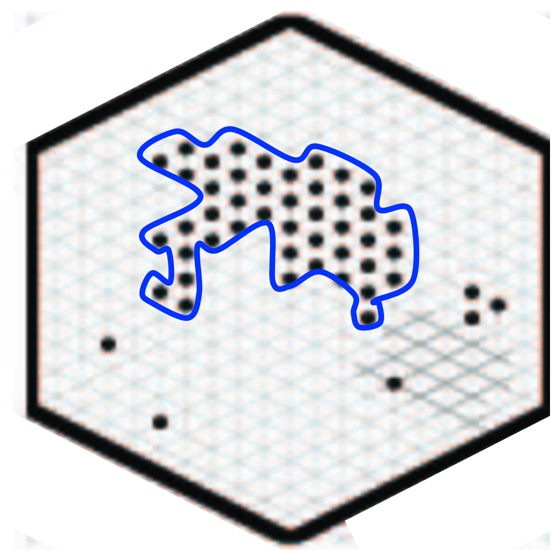
Compression without Connectivity

What does it mean for a configuration to "aggregate"?

- There is a "region" with large area and small perimeter
- that is dense with particles
- and the complement of the region is sparsely occupied

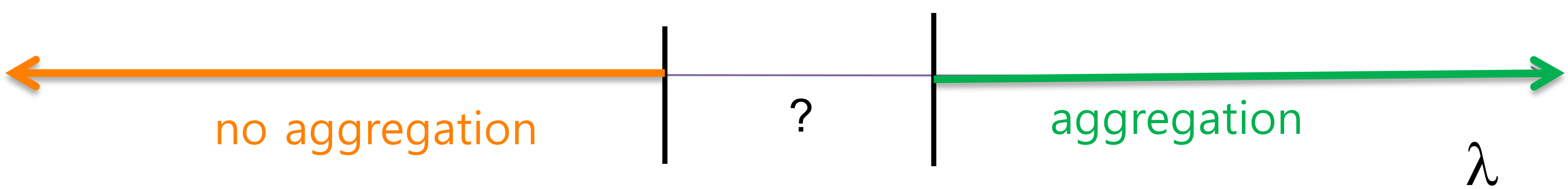
No Aggregation





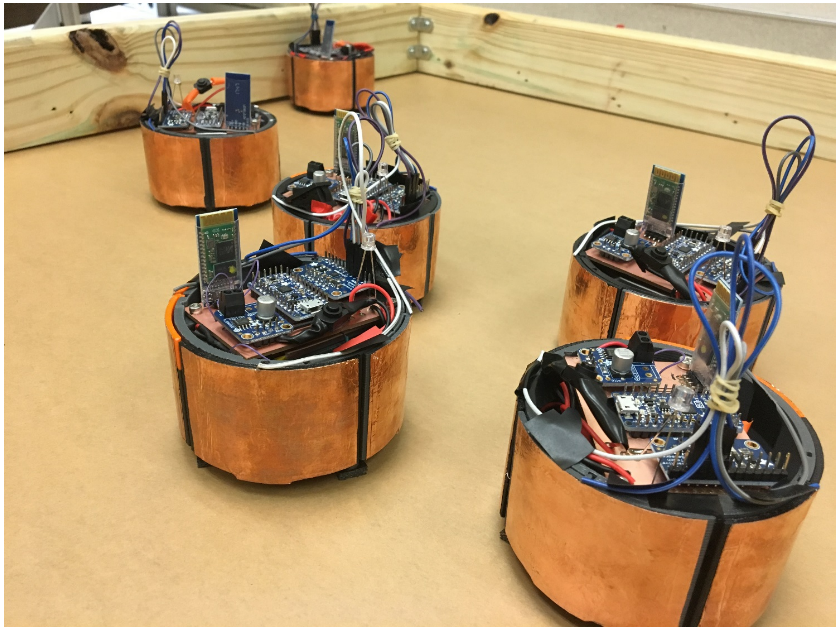
Aggregation

We provably get a similar phase change



Theory to Practice: Experiments with robots

Collections of "Dumb" Robots



BOBbots

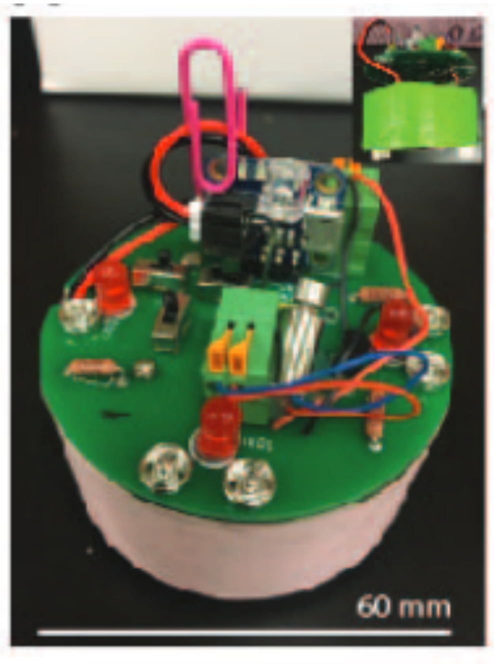
Daniel Goldman, GT

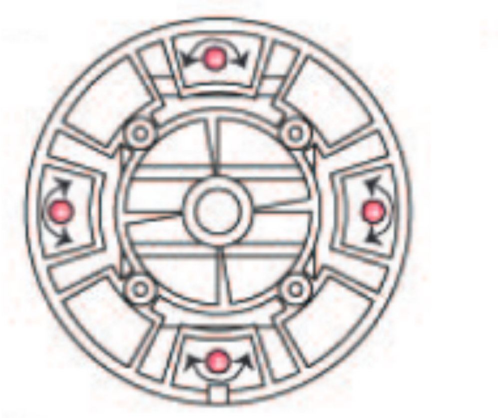
Cell-sized Colloidal "Robots"

Syncells

Michael Strano, MIT

BOBbots: *"Behaving, Oscillating, Buzzing Bots"*



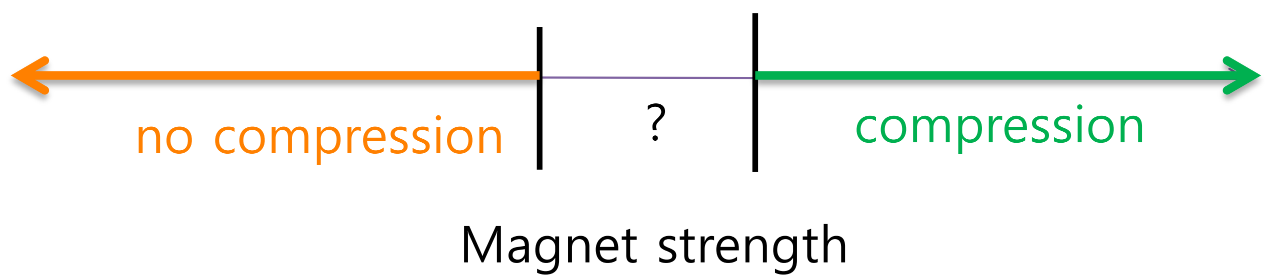


- A motor to create "random" motion
- Peripheral magnets to dampen detachment

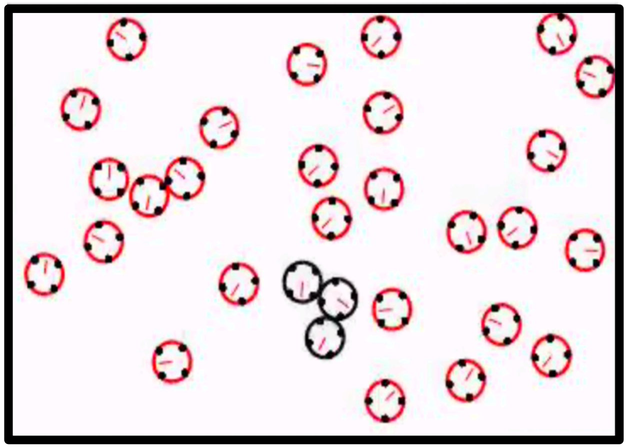
NO computational capacity; NO memory!

More magnets engaged = Smaller probability of detaching = Preference for more neighbors

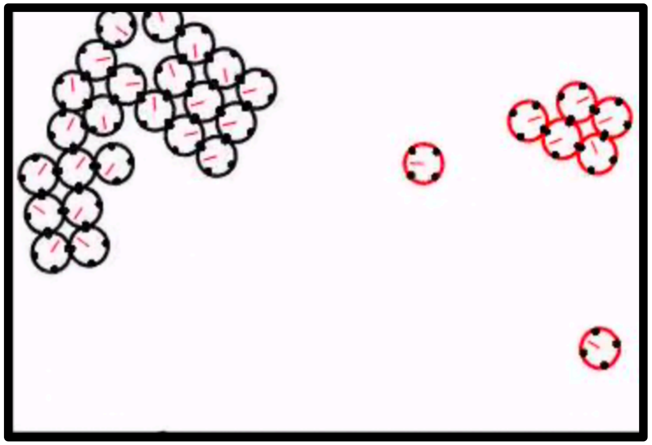
Prediction:



Varying Magnetic Strength

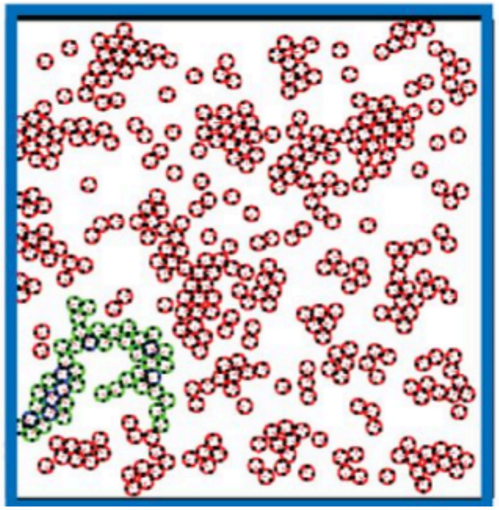


Experiments

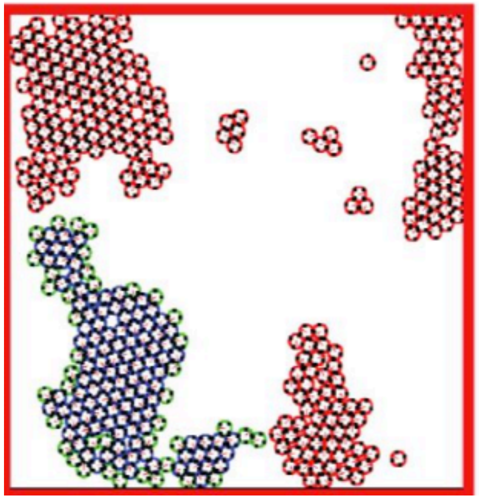


Weaker Magnets

Stronger Magnets



Simulations

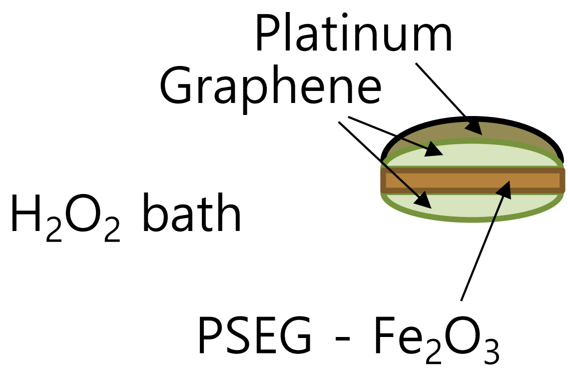


Compression for a Clearing Task

Low magnetization

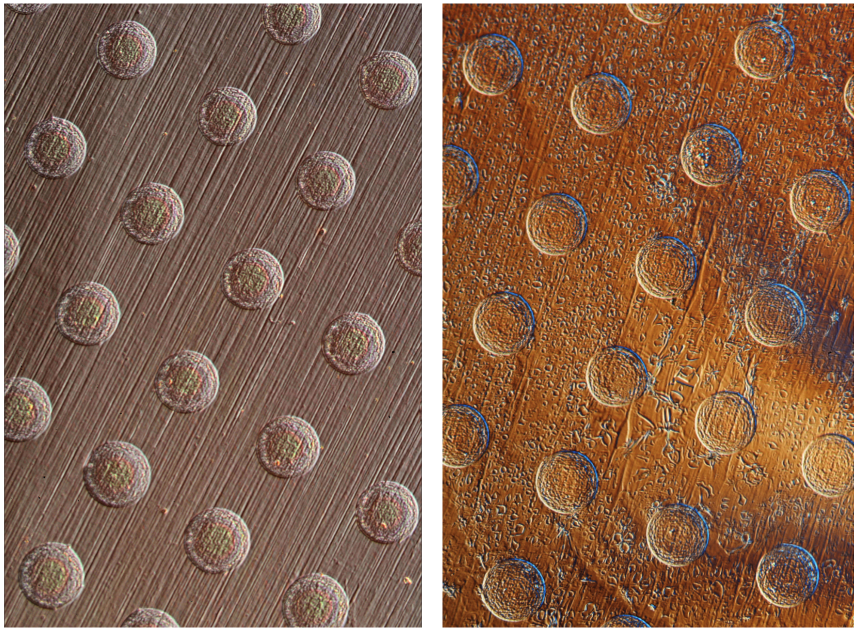
High magnetization

Theory to Practice: Syncells



- Interparticle interaction
- Dispersion potential

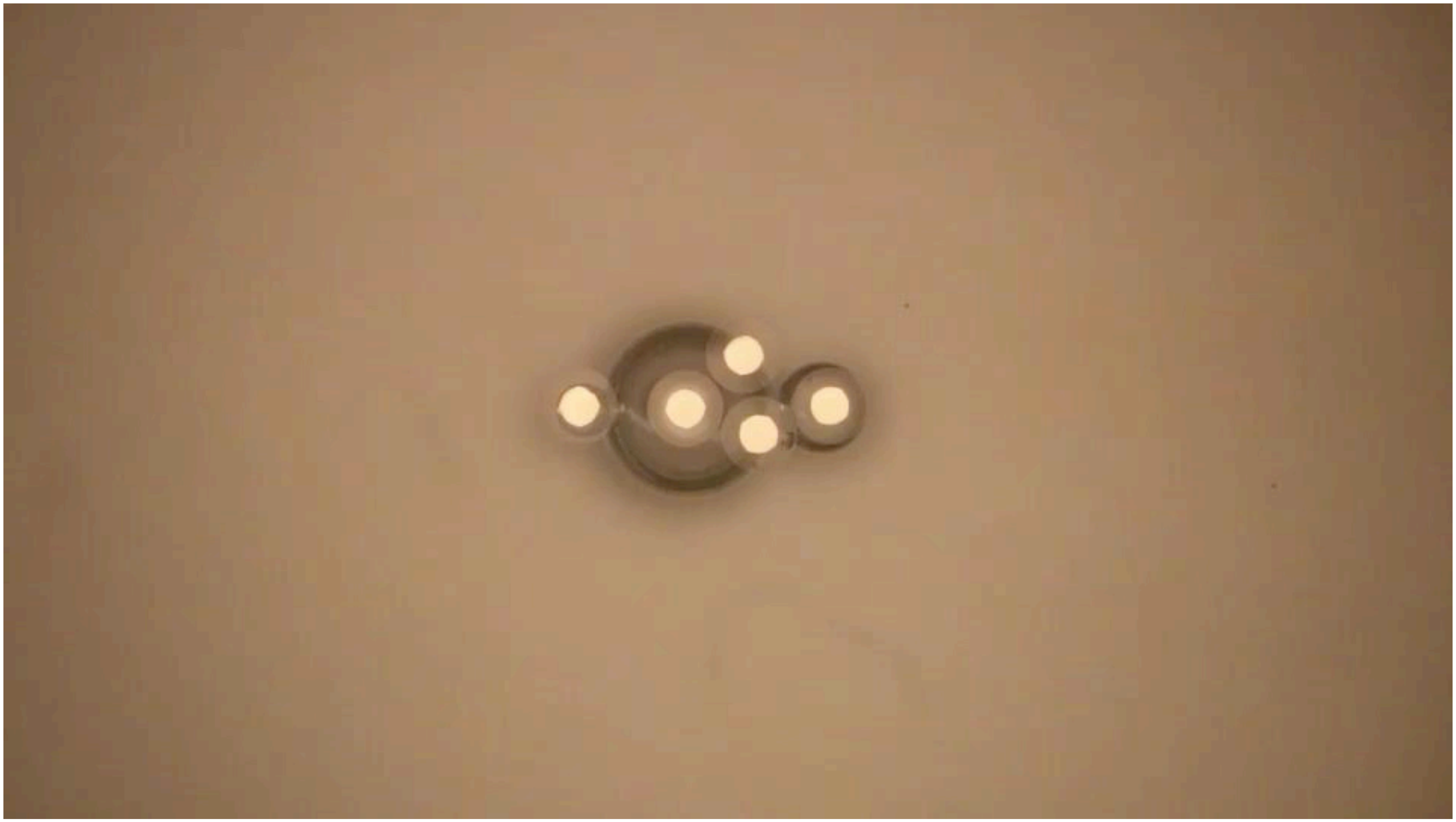
Cell-sized Colloidal "Robots"



Syncells

Michael Strano, MIT

Oscillation in Colloidal System



Advantages of Stochastic SOPS Algorithms

- Simpler than previous SOPS algorithms for active matter
- Robust to particle failures
- No central controller (or leader) necessary
- Can be made to be self-regulating

Open Questions

1. What is the running time of our algorithms?

   Emergent behavior occurs at low temperatures, and can take exponential time to reach stationarity, but emergence occurs much earlier.

2. When do our predictions about equilibrium behavior hold in nonequilibrium driven physical systems?

3. What other emergent behavior can we design for simple models of programmable active matter?

   Alignment? Locomotion? Beating? Transport? …

Thank you !

Questions?