Clustering in Interfering Binary Mixtures

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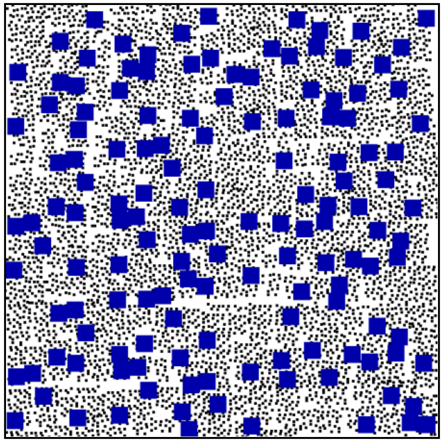
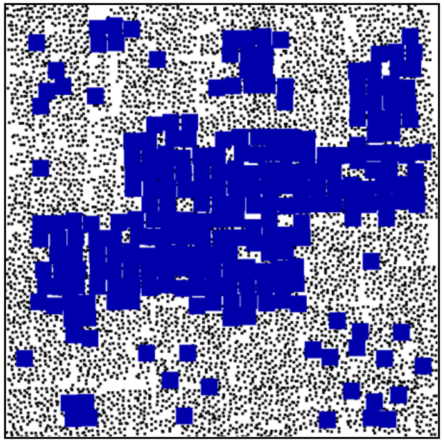
Colloids

Colloids are mixtures of 2 types of molecules
- one suspended in the other.



lower density



higher density

As the density increases, large particles cluster together.

* purely entropic *

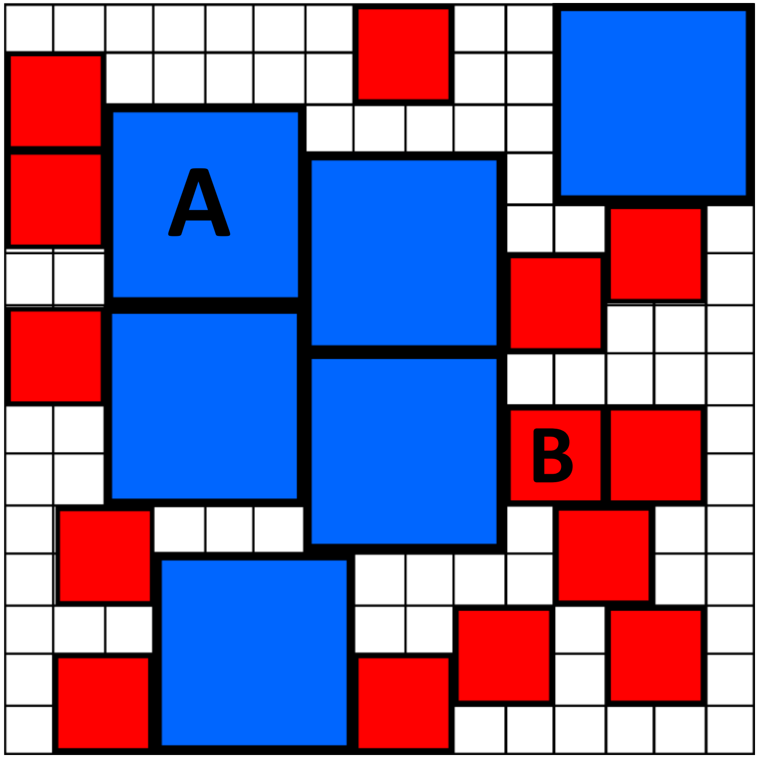
Folklore: A dense system of non-overlapping large and small tiles will exhibit “clumping”.

Framework for Colloid Models

Physicists study the model with fixed # of A-tiles and B-tiles, but it is often helpful to switch to a grand-canonical ensemble where the # of each type of tile is allowed to vary.

- α *A*-tiles and
- vary the # of *B*-tiles
- σ has weight:

$$\pi(\sigma) = \frac{\lambda^{\#B\text{–}tiles}}{Z}$$

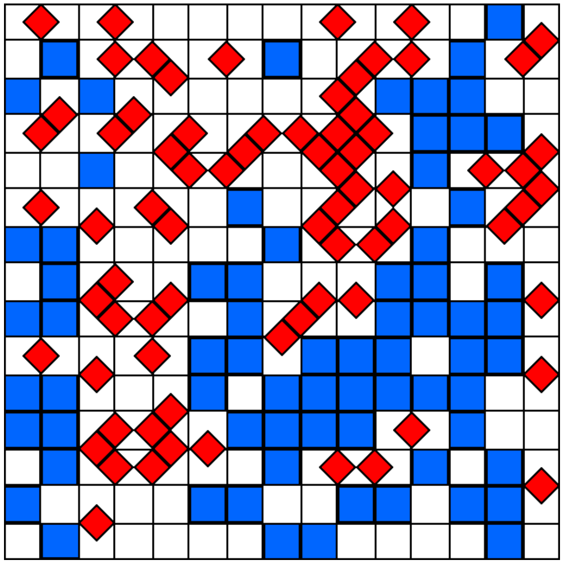


Examples of Colloid Models

Model 1

A-tiles: squares on faces

B-tiles: diamonds on edges

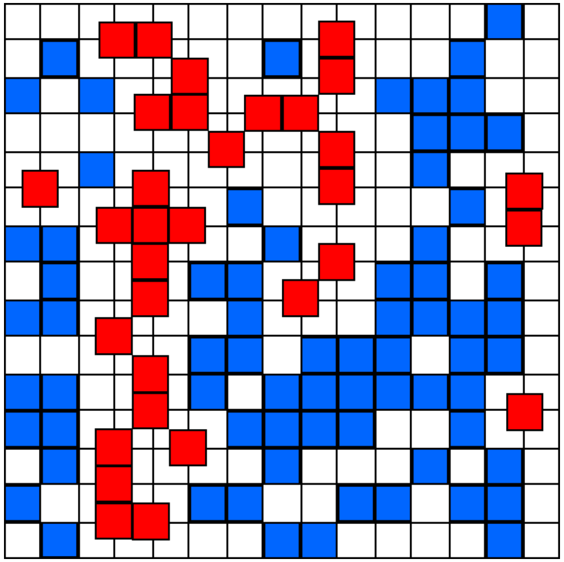


Ising Model

Model 2

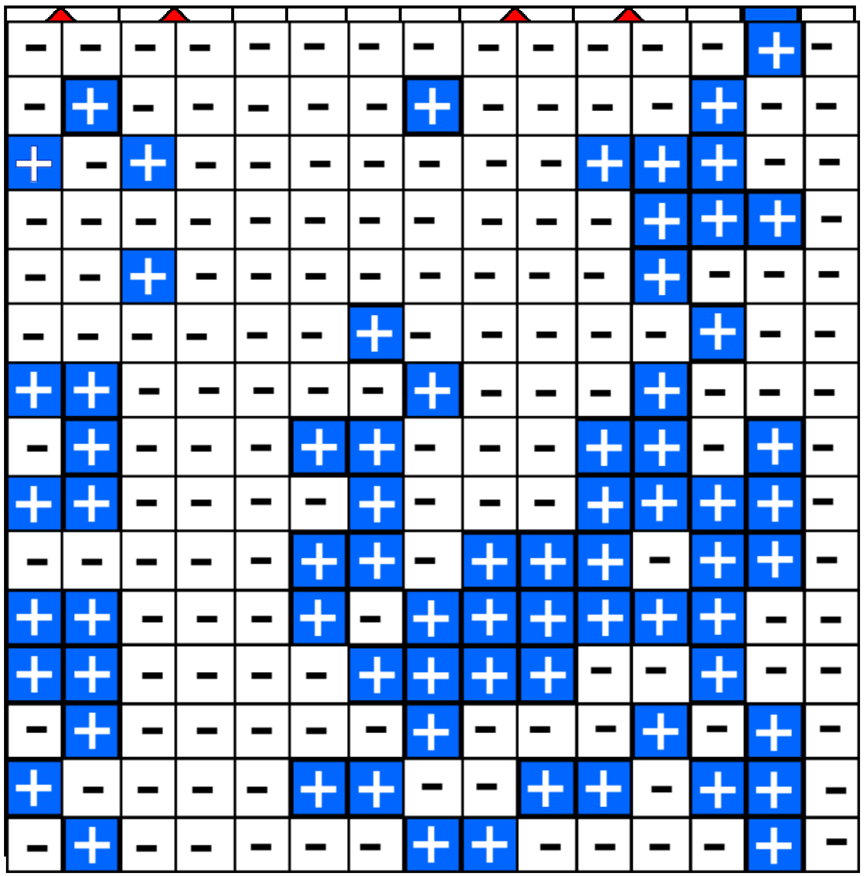
A-tiles: squares on faces

B-tiles: squares on vertices



Independent Sets

Model 1 – Ising Model



Ising Model

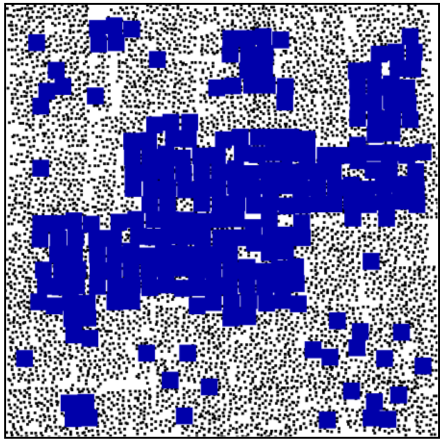
Model 1

$$P_\pi(X) = \sum_{\sigma : X(\sigma) = X} \pi(\sigma) = \sum_{\sigma : X(\sigma) = X} \frac{\lambda^{\#B\text{-tiles}}}{Z} = \frac{(1+\lambda)^{\#\text{open edges}}}{Z} = \frac{\mu^{\text{perimeter of A-tiles}}}{Z}$$

$$\pi(\sigma) = \frac{\mu^{\text{disagree}}}{Z} = \frac{\mu^{\text{perimeter}}}{Z}$$

Goal: Identify Clustering

What does a typical configuration look like?



2 approaches:

(1) Sampling

- Local algorithms are inefficient at high densities
- [Buhot and Krauth '99] Using algorithm from Dress and Krauth, provided experimental evidence of clustering in a colloid model consisting of different sized squares
- [M., Randall and Streib '11] Showed that the Dress and Krauth algorithm can take exponential time to converge

(2) Counting

Previous Work

[Frenkel and Louis '92]

Introduced Model 1, constructed so that its behavior could be inferred from the Ising Model.

→ Model 1 inherits clustering from Ising Model

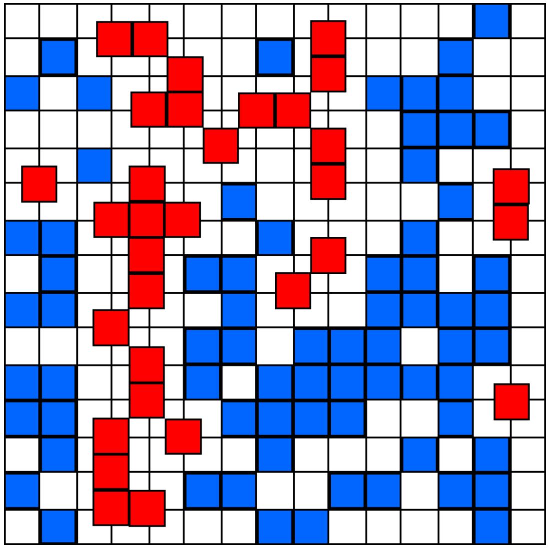
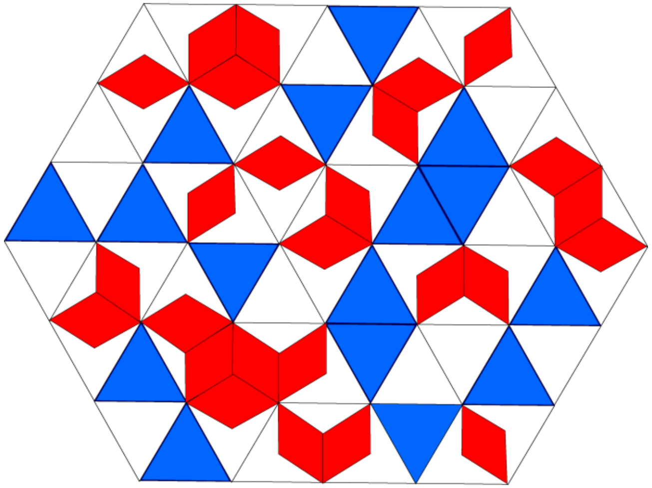
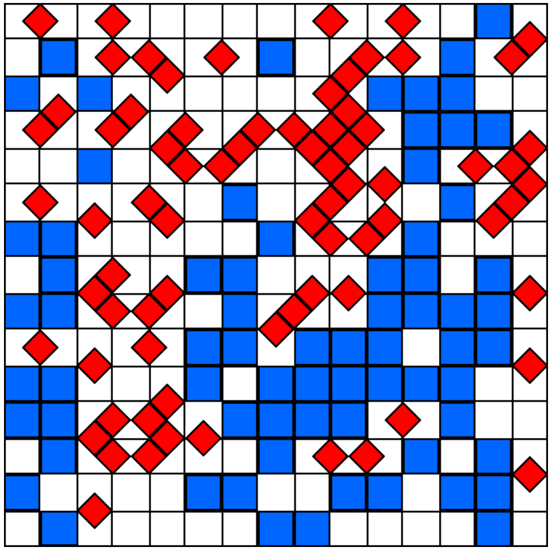
[Dobrushin, Kotecký and Shlosman '92]

In the Ising Model, the exact limiting shape is the Wulff shape.

We prove clustering directly for Interfering Binary Mixtures

- Uses elementary methods
- Applies broad class of colloid models
- Direct proof in terms of parameters natural for clustering

Examples of
Interfering Binary Mixtures

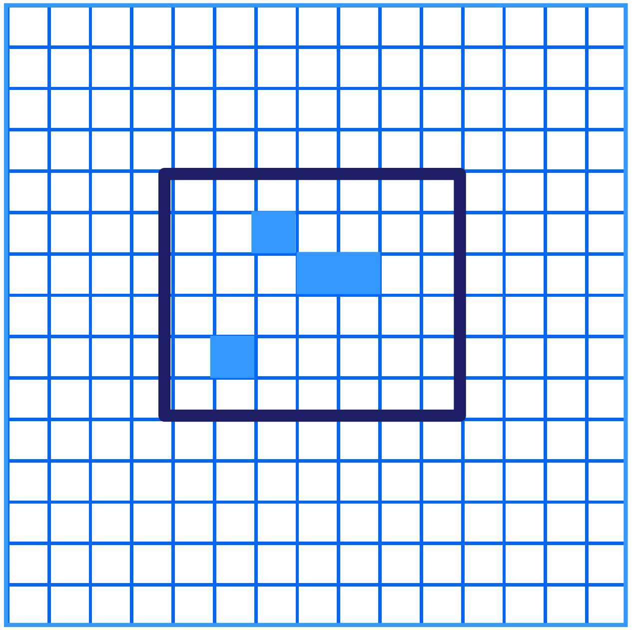




Interfering Binary Mixtures

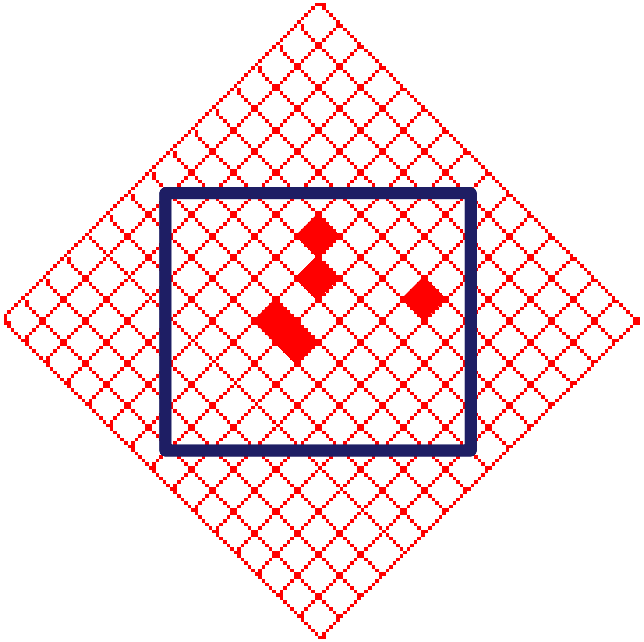
Take two planar lattices Λ_A,Λ_B.

- *A*-tiles lie on the faces of Λ_A
- *B*-tiles lie on the faces of Λ_B

Take their intersection with some finite region.



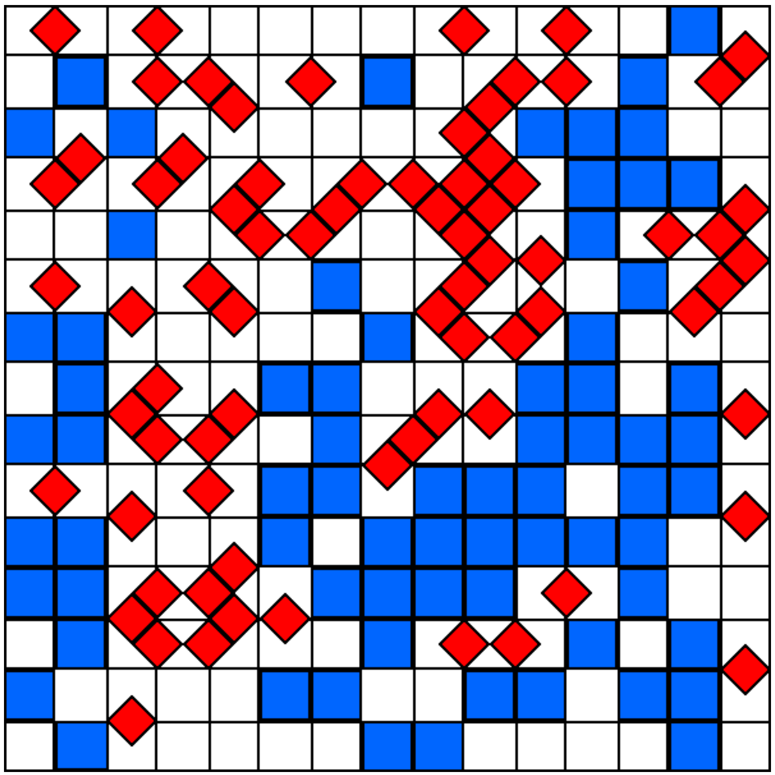
Λ_A



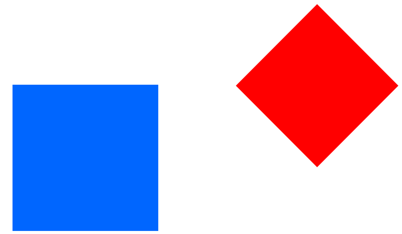
Λ_B

Interfering Binary Mixtures

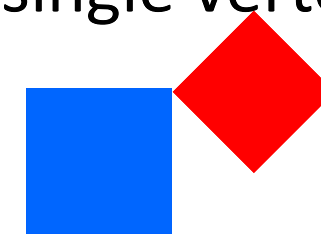
Require that the faces of Λ_A and Λ_B are either



- Disjoint,

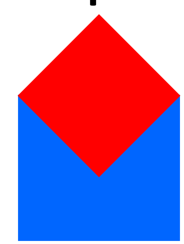


- Intersect at a single vertex



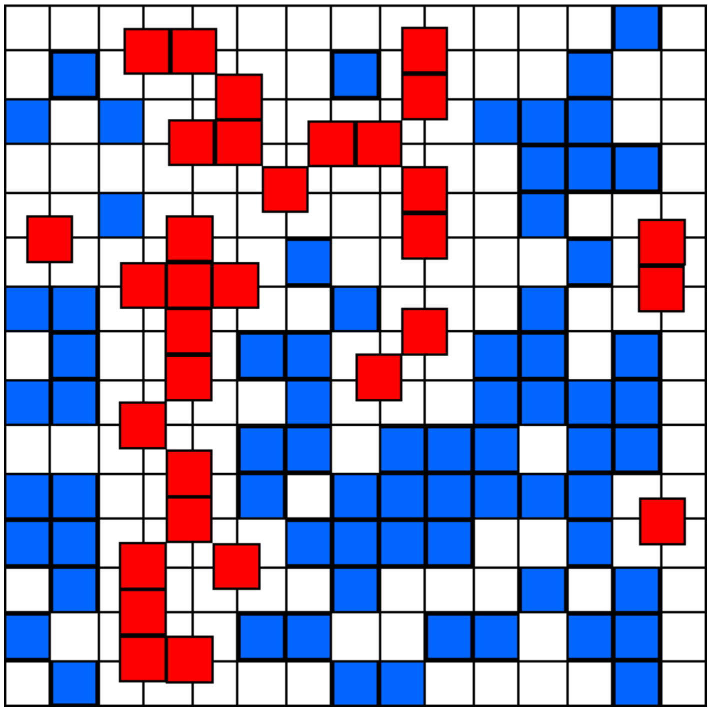
- Intersect at a fixed shape S with positive area

S

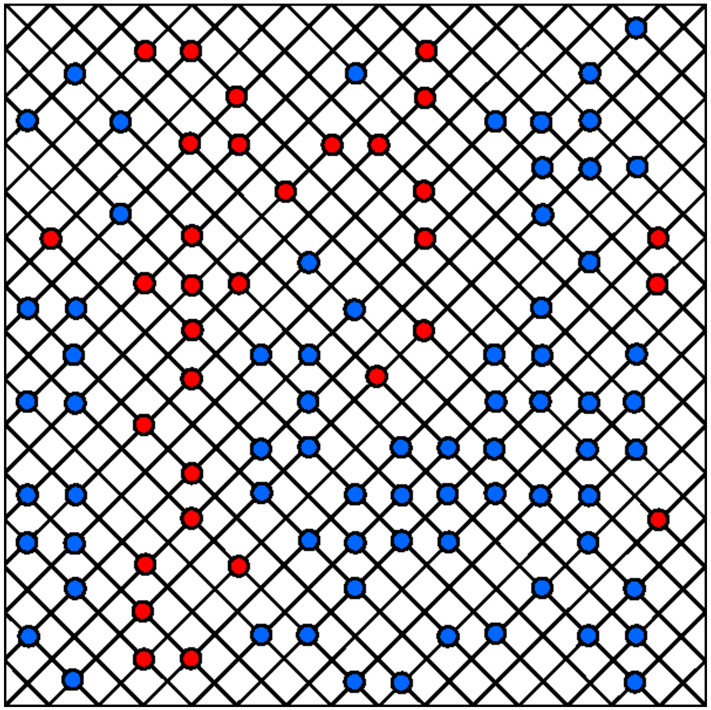


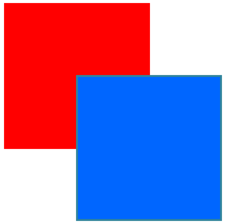
Interfering Binary Mixtures

Model 2



Independent Sets





$S =$

Main Theorems

Model 1 on an $n \times n$ region with bn^2 A-tiles

Theorem 1:

For $0 < b \leq 1/2$, there exist constants $\lambda^* = \lambda^*(b) > 1$, $\Upsilon_1 < 1$ and $n_1 = n_1(b)$ such that for all $n > n_1$, $\lambda \geq \lambda^*$ a random sample from Ω will have the *clustering property* with probability at least $(1\text{-}\Upsilon_1{}^n)$.

Theorem 2:

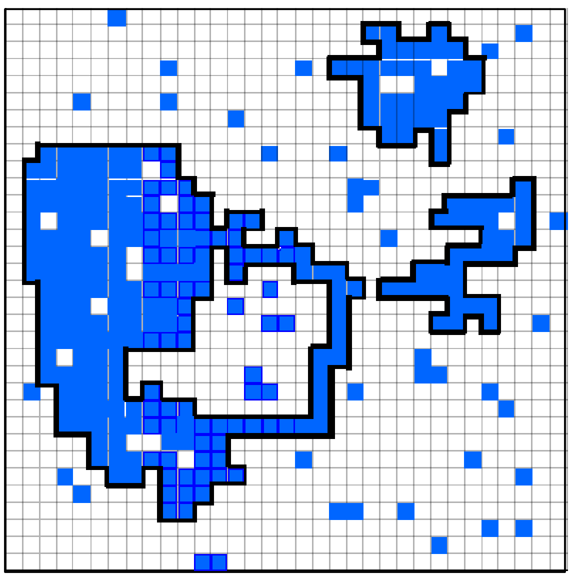
For $0 < b < ½$, there exist constants $\lambda_* = \lambda_*(b) > 0$, $\Upsilon_2 < 1$ and $n_2 = n_2(b)$ such that for all $n > n_2$, $\lambda \leq \lambda_*$ a random sample from Ω will not have the *clustering property* with probability at least $(1\text{-}\Upsilon_2{}^n)$.

Thms 1 and 2 hold for all Interfering Binary Mixtures

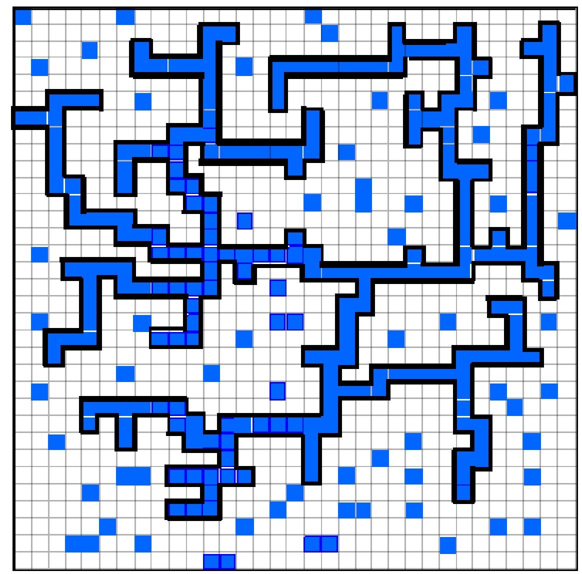
Our Results: The Cluster Property

What does it mean for a config. to "cluster"?

- has large, very dense region
- tightly packed (small perimeter:area ratio)
- the rest of the config. is very sparse



Clustering



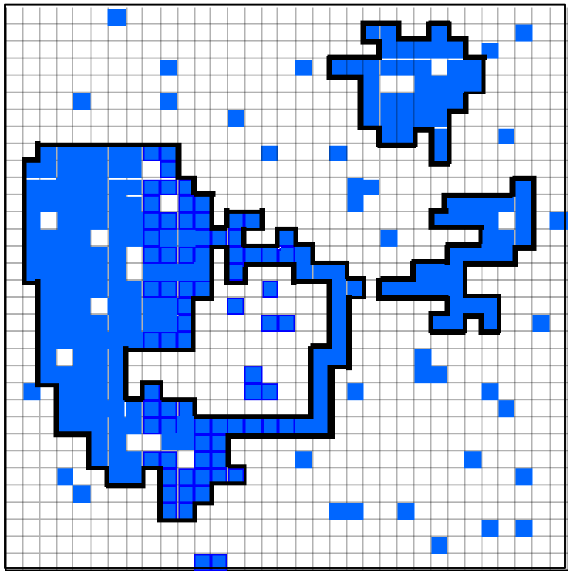
No Clustering

Formal Definition of Clustering

A configuration has the clustering property if it contains a region R such that:

1. R contains at least $(b-c)n^2$ *A*-tiles
2. Perimeter of R is at most $8\sqrt{b}n$
3. Density of *A*-tiles in R is at least

   1-c and in $\overline{R}$ is at most c.



$$c = \min\left\{{}^{b}/_{2}, {}^{1}/_{100}\right\}$$

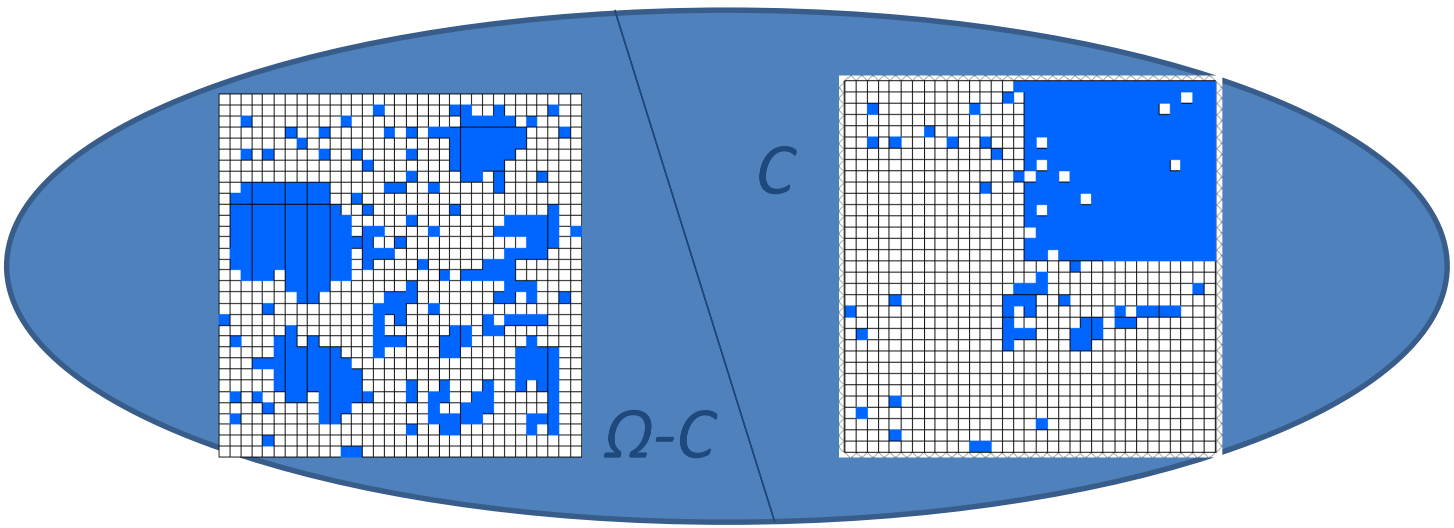
Thm 1 (high density): Proof Sketch

C: configurations that have the clustering property

Want to show: $\pi(\Omega - C) \leq \gamma^{-n}\pi(C)$

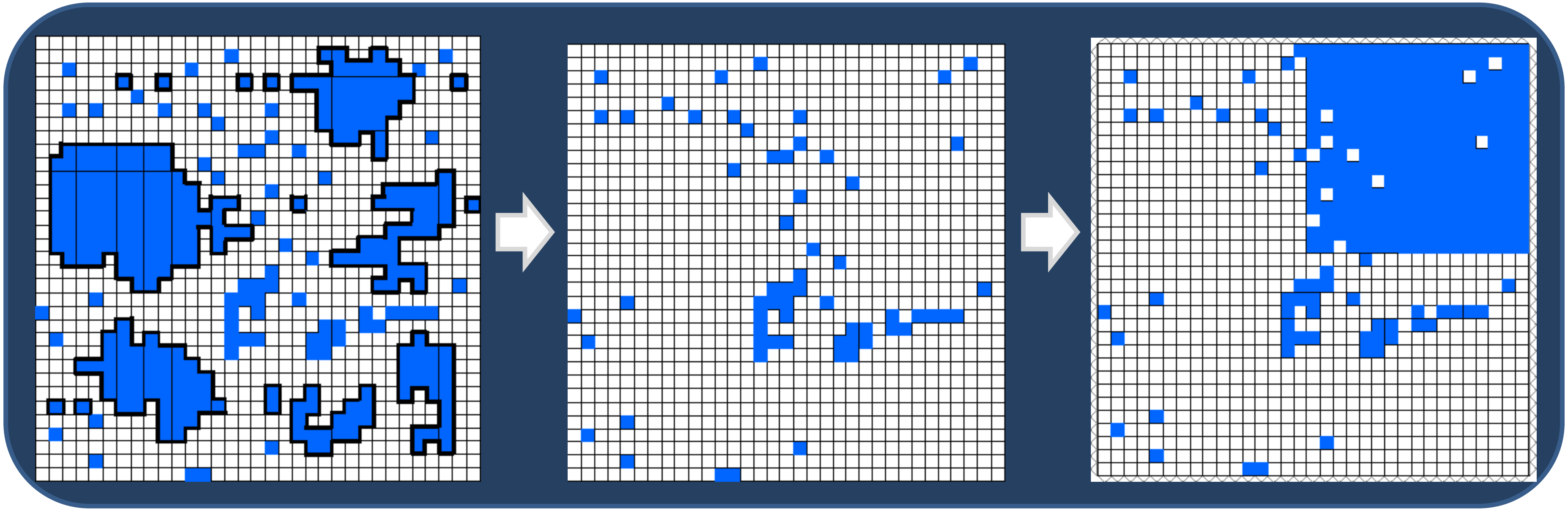
Define $f\colon \Omega - C \to C$ such that for every $\tau \epsilon C$,

$$\sum_{\sigma \epsilon f^{-1}(\tau)} \pi(\sigma) \leq \gamma^{-n}\pi(\tau)$$



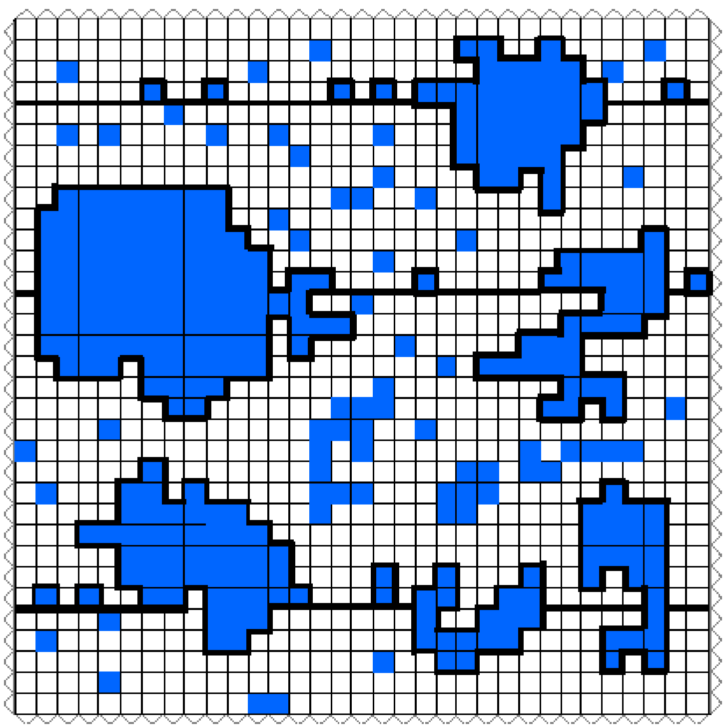
Thm 1 (high density): Proof Sketch

1. Identify a set of components to remove.
2. Remove selected components to obtain a “bank” of tiles
3. Use bank of tiles to create a large square component



Thm 1 (high density): Proof Sketch

To bound $|f^{-1}(\tau)|$: Record where the components were and what they looked like



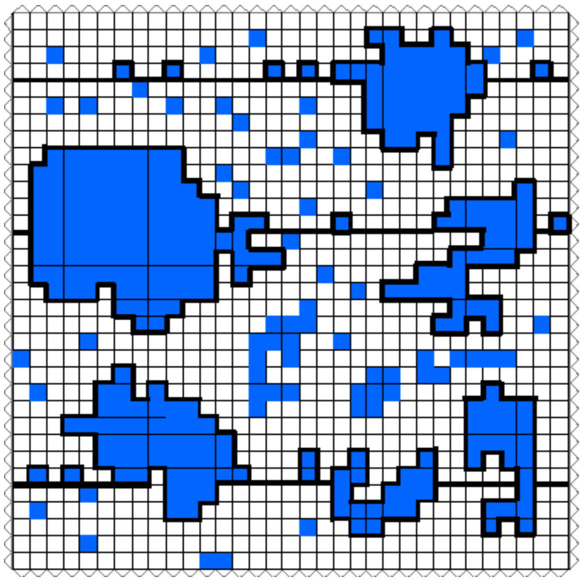
Plan: Find a set B of edges (**bridges**) that connect several components to the boundary of the region.

Use those bridges to encode the location and perimeter of the components removed.

→ # preimages is at most $6^{\#edges\ encoded}$

Thm 1 (high density): Proof Sketch

Plan: Find a set B of edges (**bridges**) that connect several components to the boundary of the region.



Properties of bridges:

- # edges < c * perimeter of components we remove
- Perimeter of components removed is large $\theta(n^2)$

preimages is at most $6^{\#edges\ encoded} \leq 6^{t\Delta perim}$

and $\pi(\sigma) \leq \mu^{-\Delta perim}\pi(\tau)$

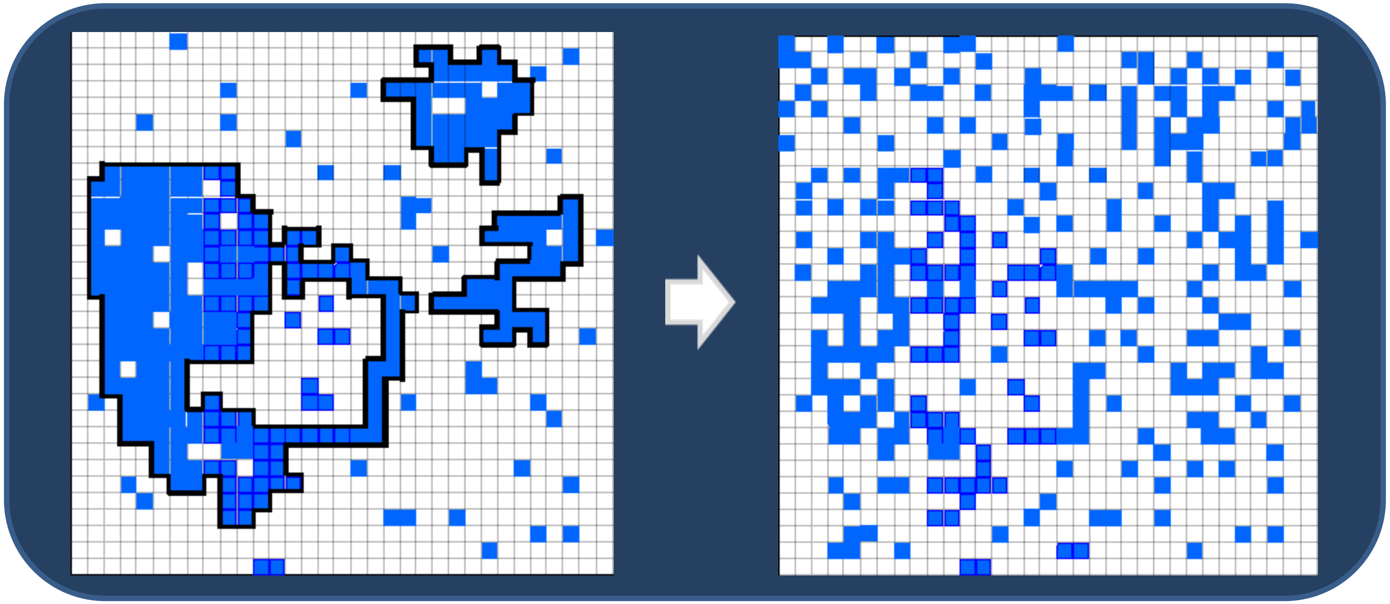
So: $\sum_{\sigma\in f^{-1}(\tau)} \pi(\sigma) \leq \left(\frac{6^t}{\mu}\right)^{\Delta perim} \pi(\tau) \leq \mu^{-n}\pi(\tau)$

Thm 2 (low density): Proof Sketch

Want to show if λ is small enough: $\pi(C) \leq \gamma^{-n}\pi(\Omega - C)$

Proof idea:

1. Define bridges as before.
2. Remove big components – t tiles.
3. Redistribute the t tiles uniformly: $\binom{n^2 - an^2}{t}$ ways



Open Problems

- Prove clustering occurs in other discrete models where the overlap between lattice faces is not a fixed shape.
- Generalize to higher dimensions
- Other algorithms for sampling