Cluster Algorithms for Discrete Models of Colloids

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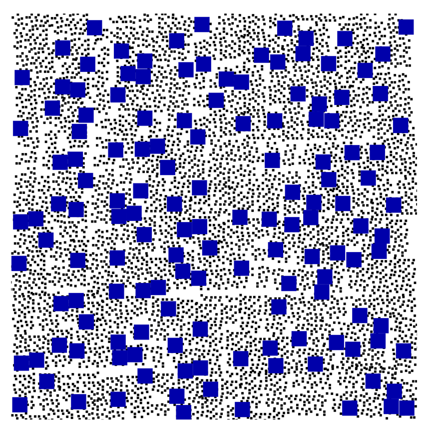
What are colloids?

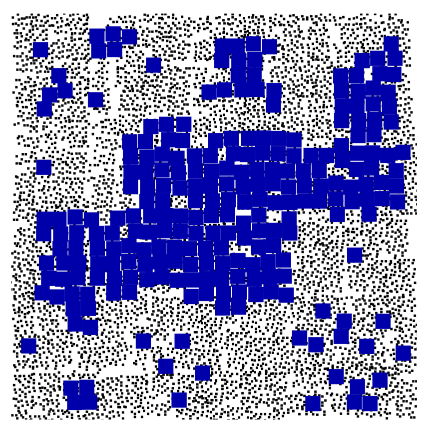
- Colloids are mixtures of two types of molecules in suspension. When the density of each type of molecule is low, the mixtures are homogeneous and consequently exhibit properties that make them suitable for many industrial applications, including fogs, gels, foods, paints and photographic emulsions. When the density is high, the two types of molecules seperate whereby one type appears to cluster together.
- Physicists have introduced various hard core models to show how this can be caused purely by entropy.

Squares Model:

$\Omega(\varphi) =$ the set of nonoverlapping packings of large squares and small squares of equal density φ in an $n \times n$ torus.



Lower density



Higher density

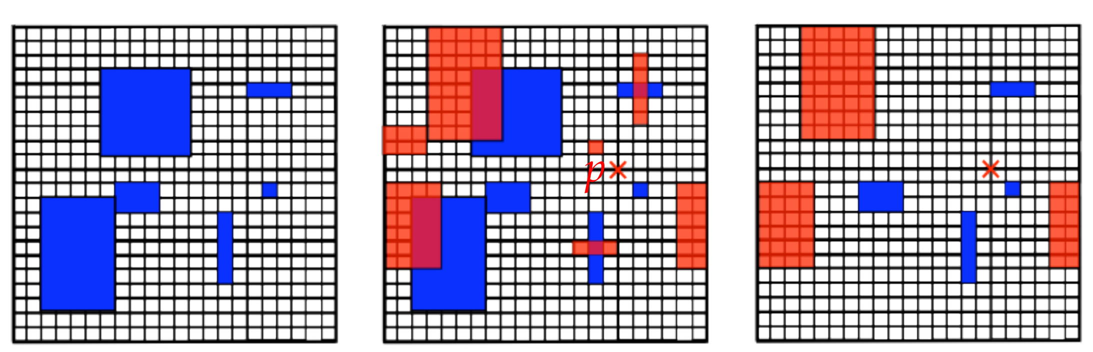
Physicists' Conjecture:

If the density φ is large enough then in a uniform sample from $\Omega(\varphi)$, the large squares will clump together.

How to verify? Local sampling algorithms fail when the density is high. A new nonlocal algorithm introduced by Buhot and Krauth (1) provided the first experimental evidence of the colloid effect.

The Dress-Krauth Algorithm

- Given $\sigma_i \in \Omega(\varphi)$, choose a pivot point p uniformly at random.
- Rotate σ_i 180° around p and superimpose on the original to obtain τ.
- For each pair of components independently choose red or blue to produce σ_{i+1}.

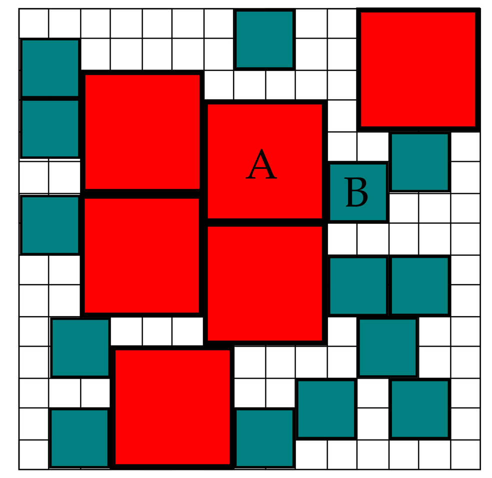


σ_i τ σ_{i+1}

Our Goals:

- Understand the stationary distribution.
- Analyze the Dress-Krauth algorithm.

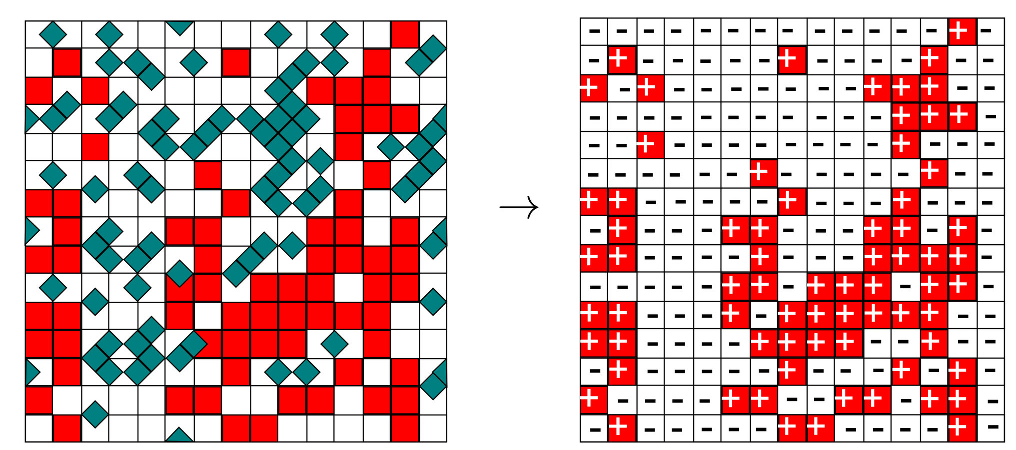
Discrete Colloid Models



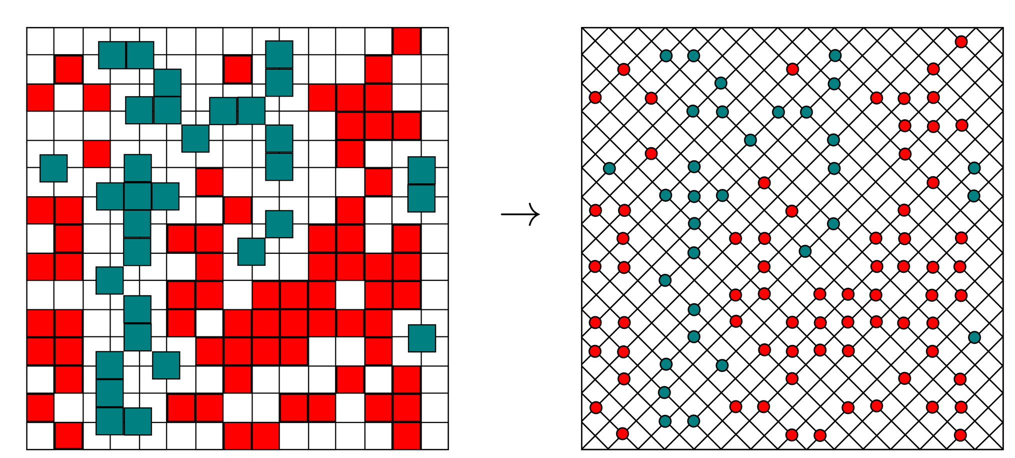
Consider Ω, the set of non-overlapping embeddings on a $n \times n$ torus of:
- α type A-tiles
- a variable number of B-tiles

where β is the number of B-tiles and each configuration σ has weight $\pi(\sigma) = \lambda^\beta / Z$.

Examples:

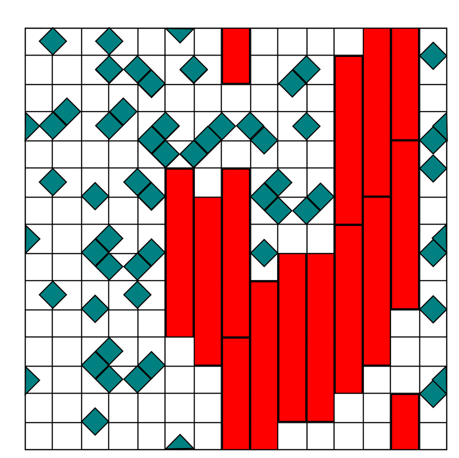


A-**tiles:** squares on faces; B-**tiles:** diamonds on edges



A-**tiles:** squares on faces; B-**tiles:** squares on vertices

Bar Model:



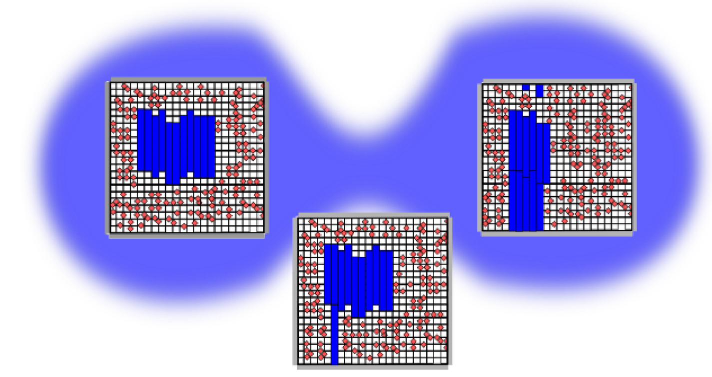
A-**tiles:** $L \times 1$ bars, where $L = cn$; B-**tiles:** diamonds on edges

Analyzing Cluster Algorithms

- A Markov chain **Mixes Rapidly** if it converges to the stationary distribution in time polynomial in n.
- A Markov chain **Mixes Slowly** if it takes time exponential in n to converge to the stationary distribution.

Slow Mixing for the Bar Model:

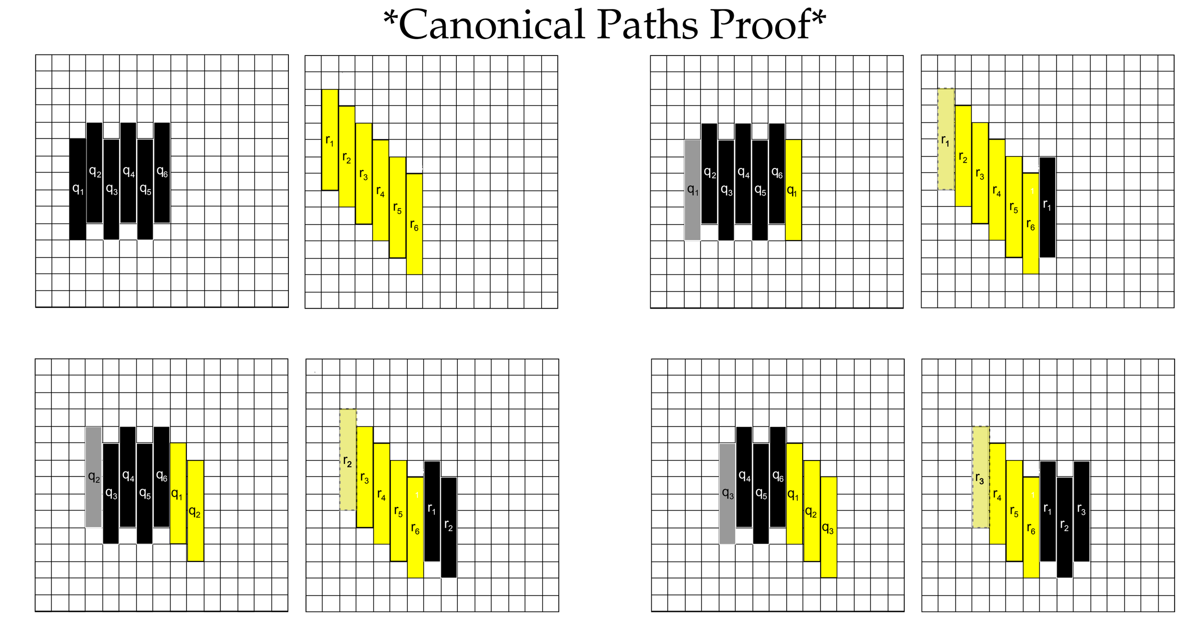
Theorem: If $L = cn$, $L < n/2$, then the Dress-Krauth algorithm is slow mixing.



Rapid Mixing for the Bar Model:

Theorem: If $L > n/2$ (at most one bar per column), then the Dress-Krauth algorithm is rapidly mixing.

Canonical Paths Proof



Related DOE Office of Science Research Program Areas:

- Advanced Scientific Computing Research - Applied Mathematics
- Advanced Scientific Computing Research - Computer Science

References

[1] A. Buhot, W. Krauth. Phase Separation in Two-Dimensional Additive Mixtures. Phys. Rev. E 59(1990) pp. 2939-2941.

[2] C. Dress and W. Krauth. Cluster Algorithm for Hard Spheres and Rlated Systems. J. Phys. A: Math. Gen. L597 (1995).