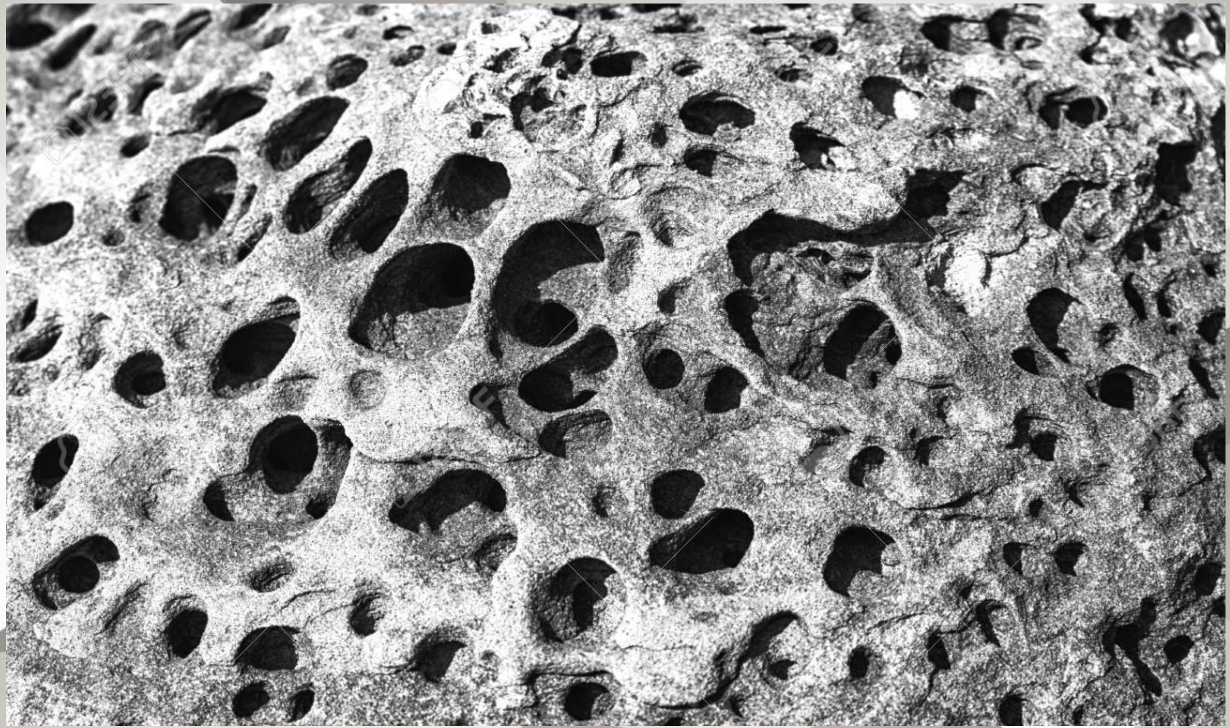
PERCOLATION Theory and Applications

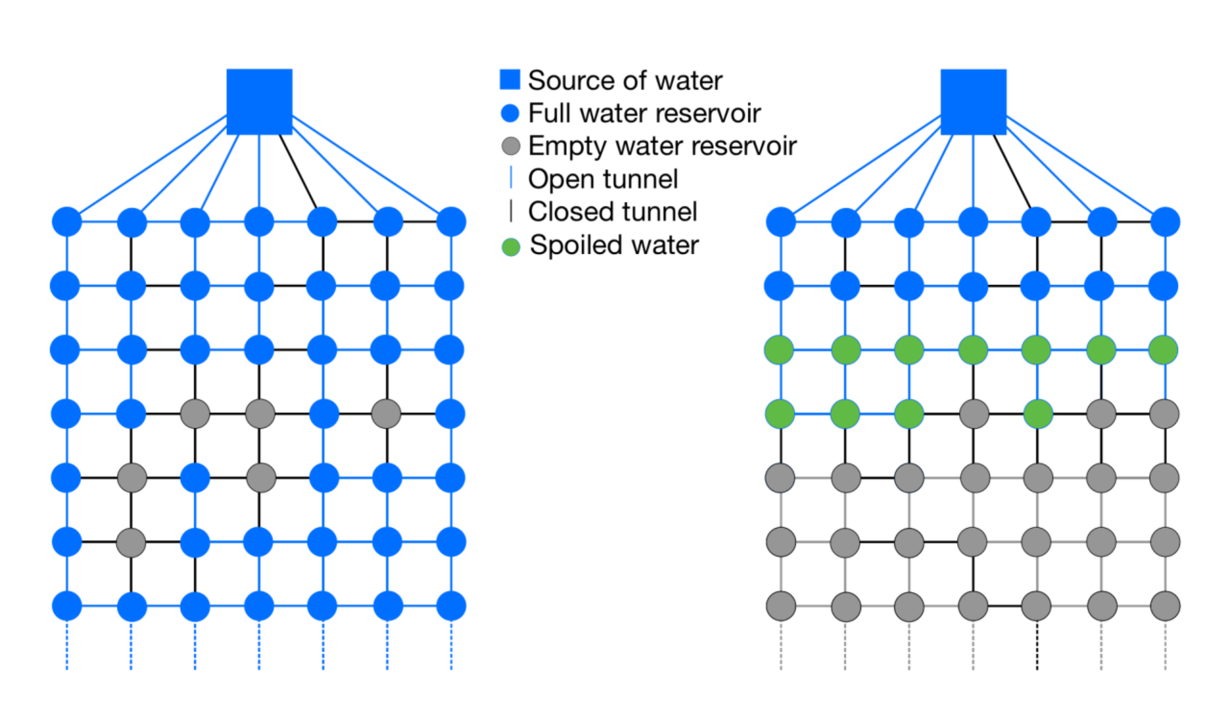
Student: Guglielmo Grillo

Course: Multi-scale methods in soft matter physics [145889]



Porous Stone

If a porous stone is immersed in water, which of its parts will get wet?

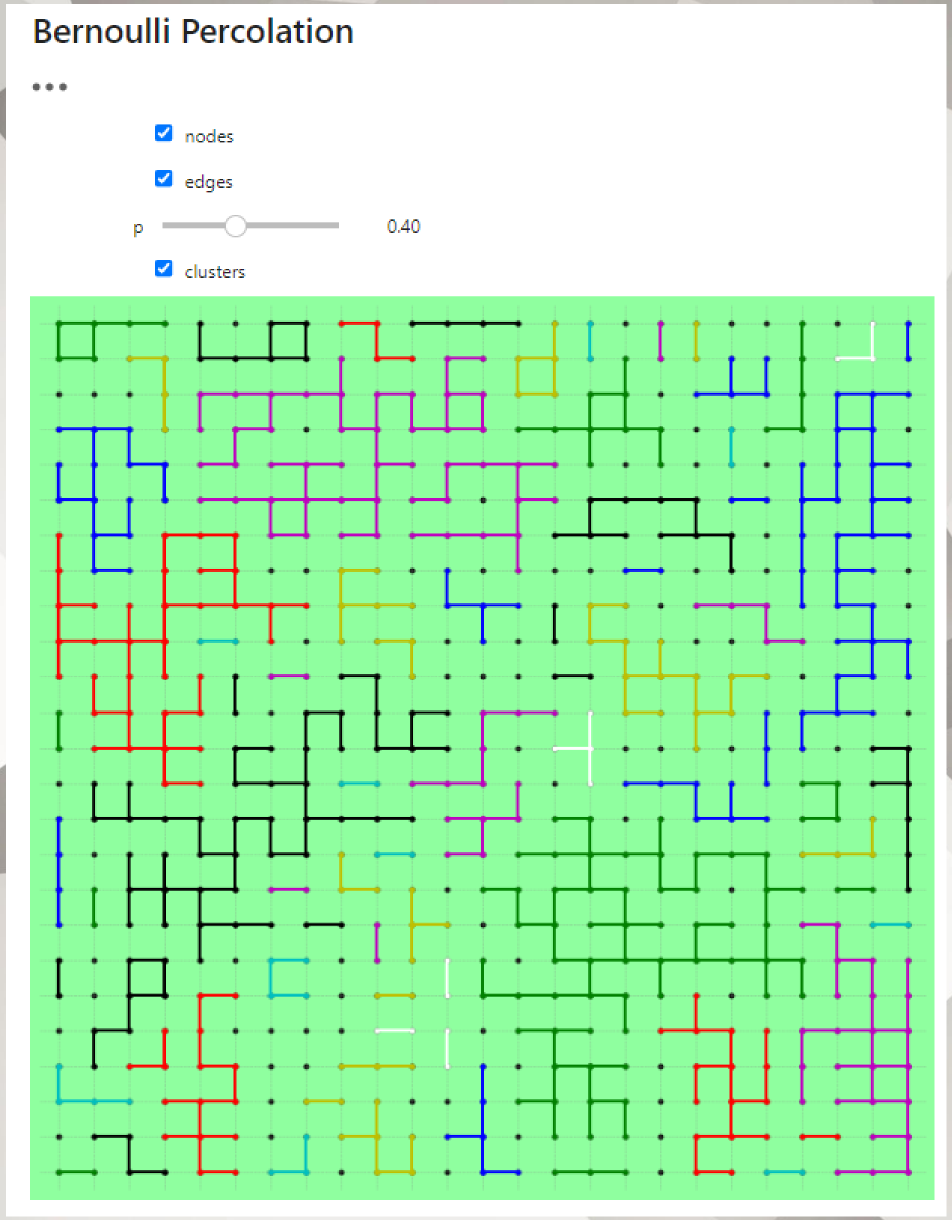


Porous City

What is the critical clog probability for which a constant maintenance of the sewers is needed?

Periodic maintenance: T

Clog probability: $p_{clog} = p_{clog}(T)$



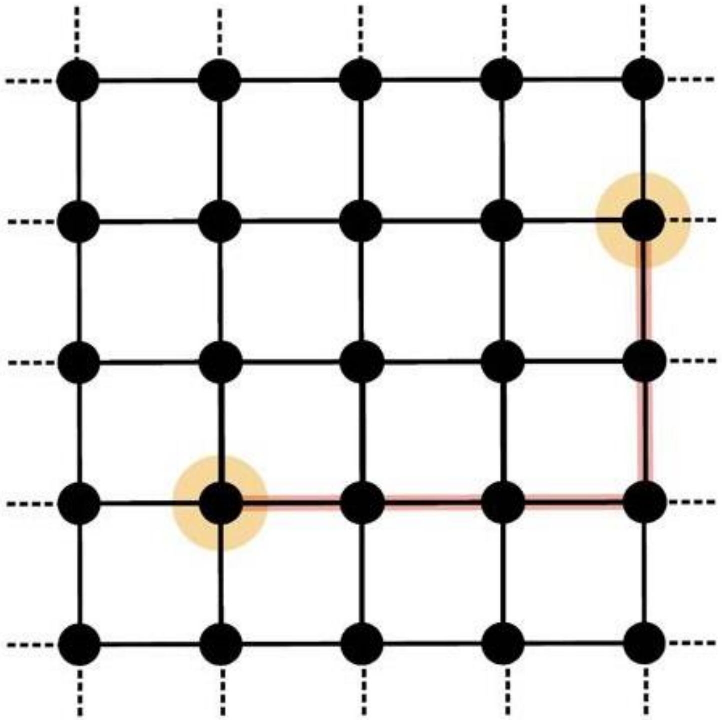
Bernoulli Percolation

Intuitive idea

- Square lattice
- Open and closed edges
- Clusters
- Two phases

Mathematical Fundaments

$$\delta(\vec{x}, \vec{y}) = \sum_{i=1}^{d} |x_i - y_i|$$

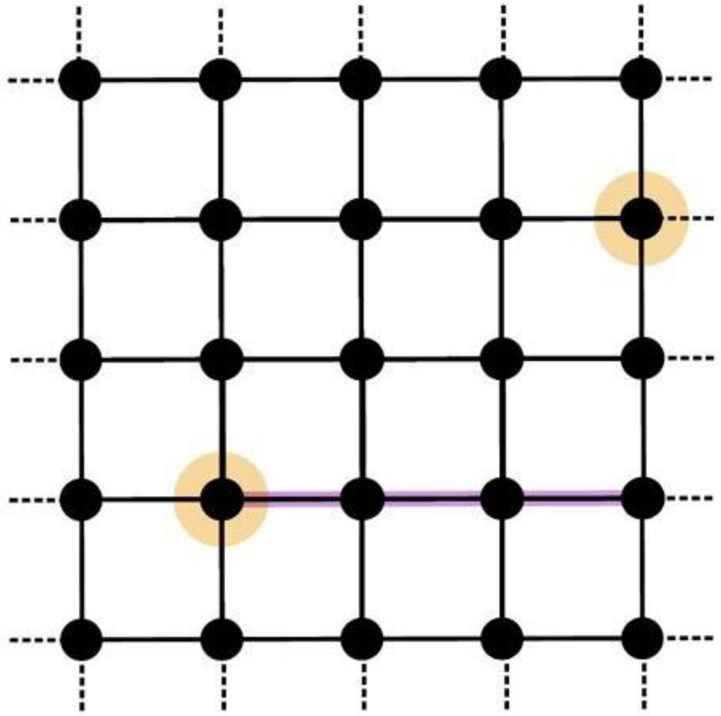


Mathematical Fundaments

Distance

- Taxicab distance

$$||\vec{x}|| = \max\{|x_i| : 1 \leq i \leq d\}$$

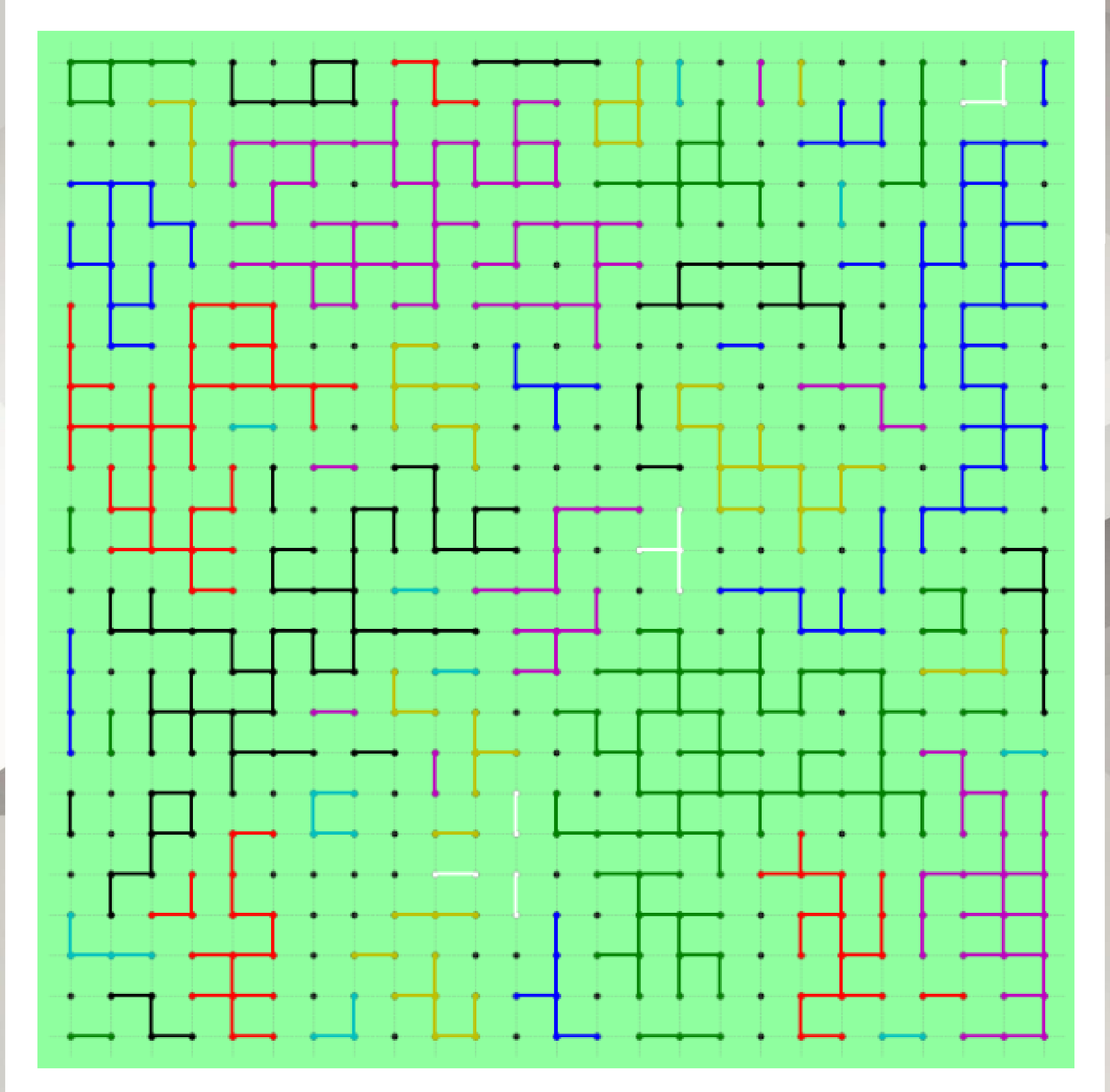


Mathematical Fundaments

Distance

Pseudodistance

- Chebyshev distance



Mathematical Fundaments

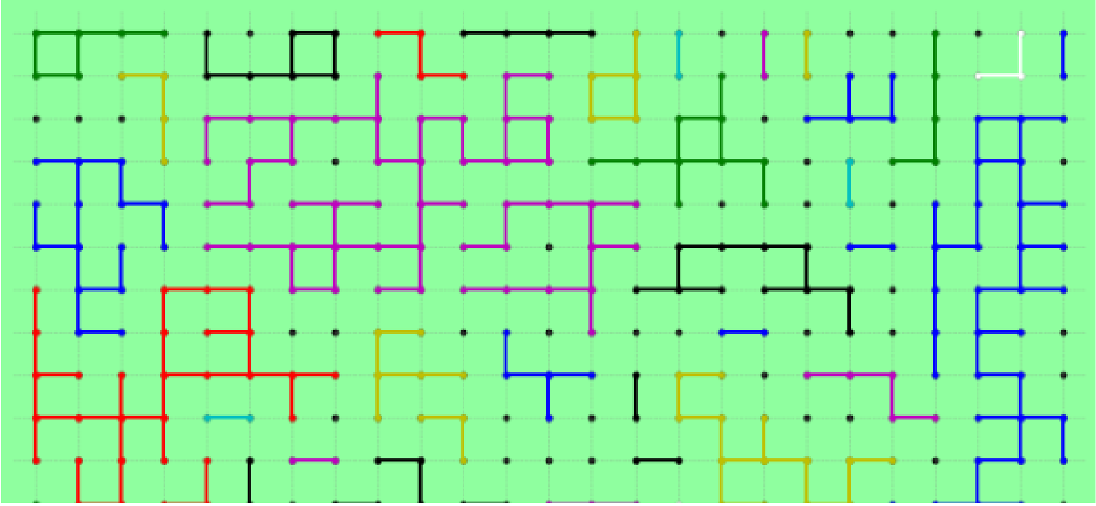
Distance

Pseudodistance

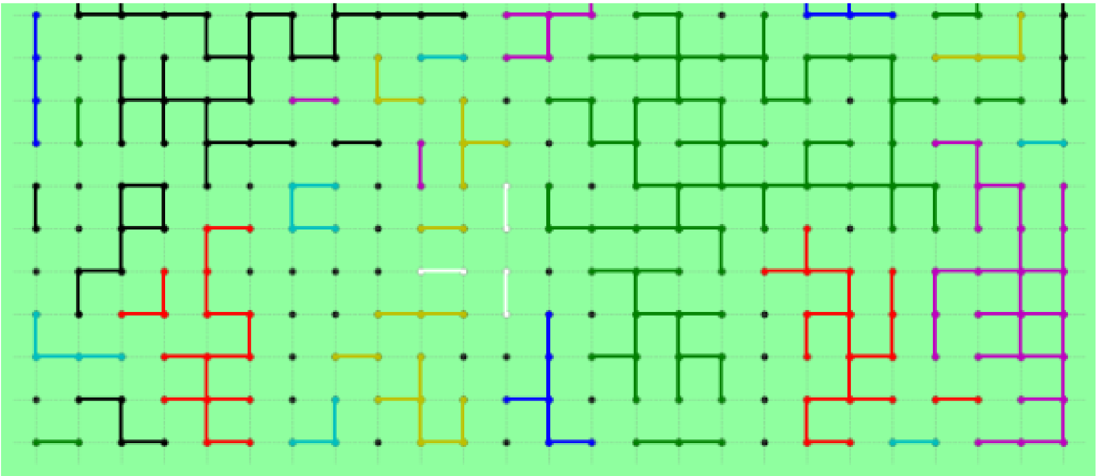
Clusters

- Connected components

Mathematical Fundaments



$$||C|| = \max\left\{||\vec{x}-\vec{y}|| : \vec{x},\vec{y}\in C\right\}$$



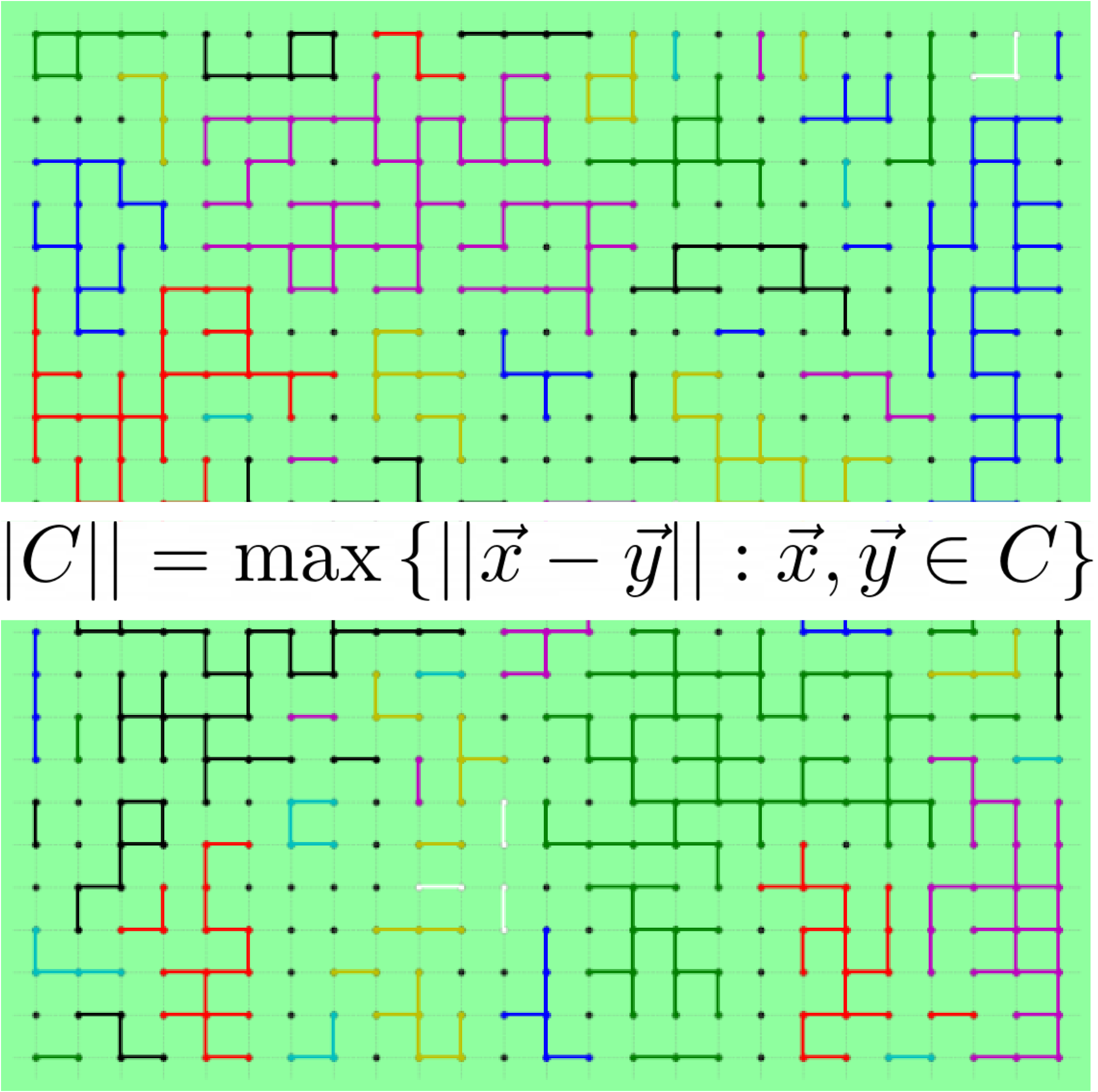
Distance

Pseudodistance

Clusters

- Connected components
- Length of a cluster

Mathematical Fundaments



$$||C|| = \max\{||\vec{x} - \vec{y}|| : \vec{x}, \vec{y} \in C\}$$

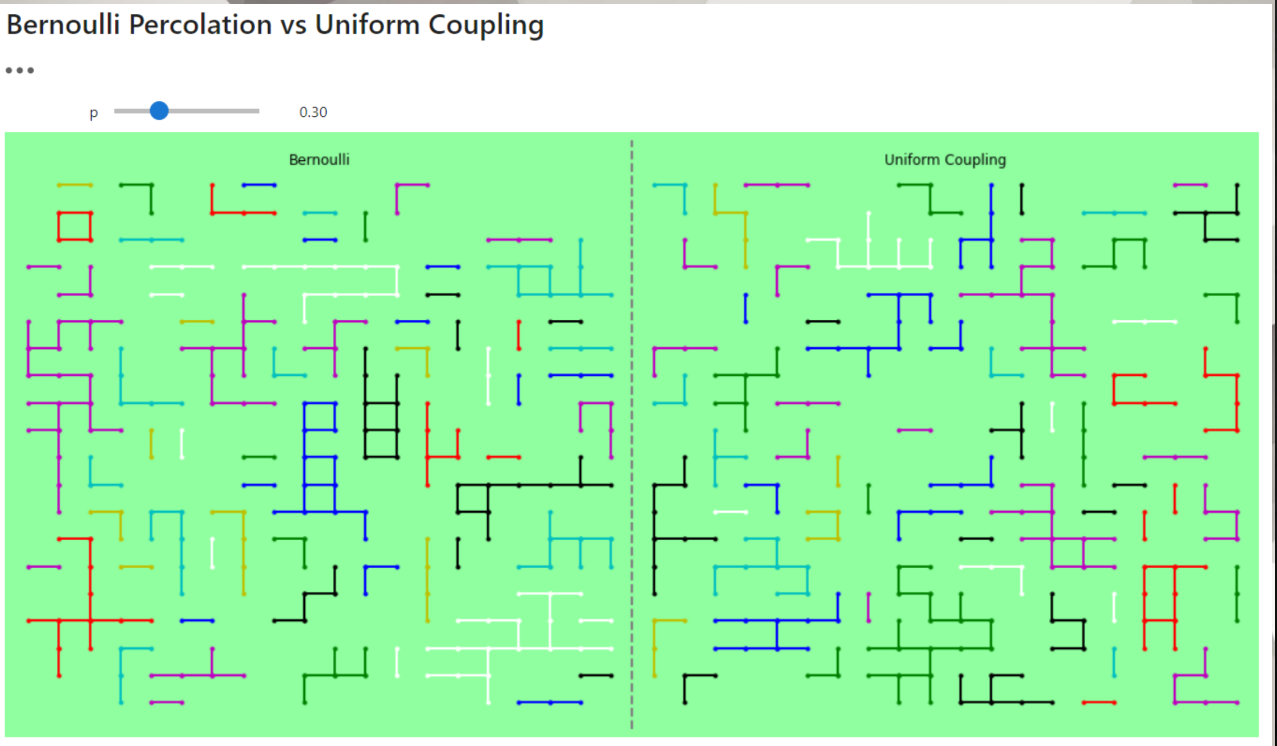
Distance

Pseudodistance

Clusters

- Connected components
- Length of a cluster
- Infinite cluster

Mathematical Fundaments

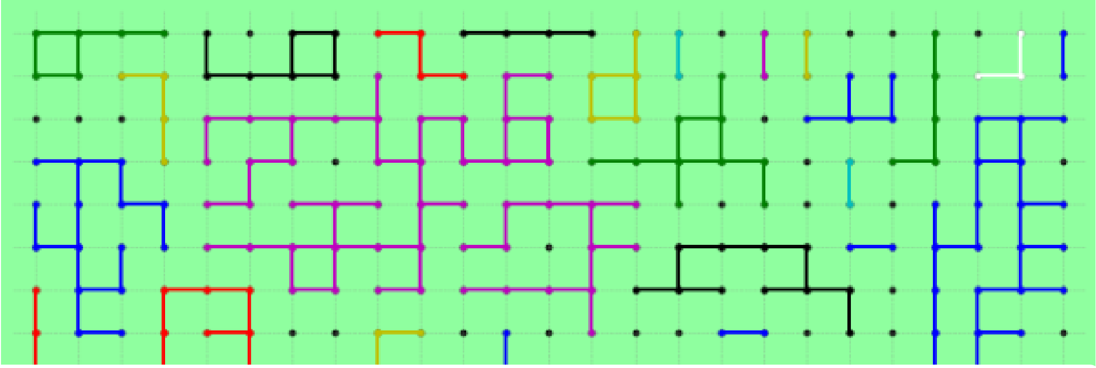


Distance

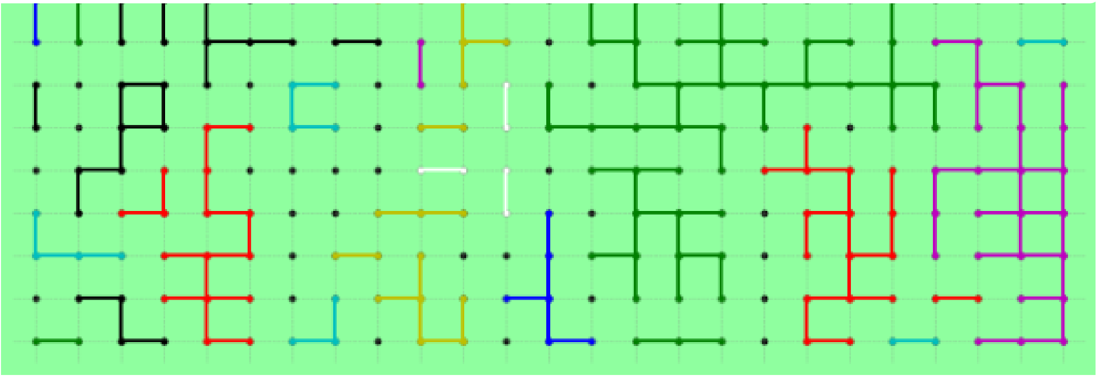
Pseudodistance

Clusters

Uniform Coupling



$$
\begin{aligned}
\theta(p) &= P_p\left(|C| = \infty\right) \\
&= 1 - \sum_{n=1}^{\infty} P_p\left(|C| = n\right)
\end{aligned}
$$



Mathematical Fundaments

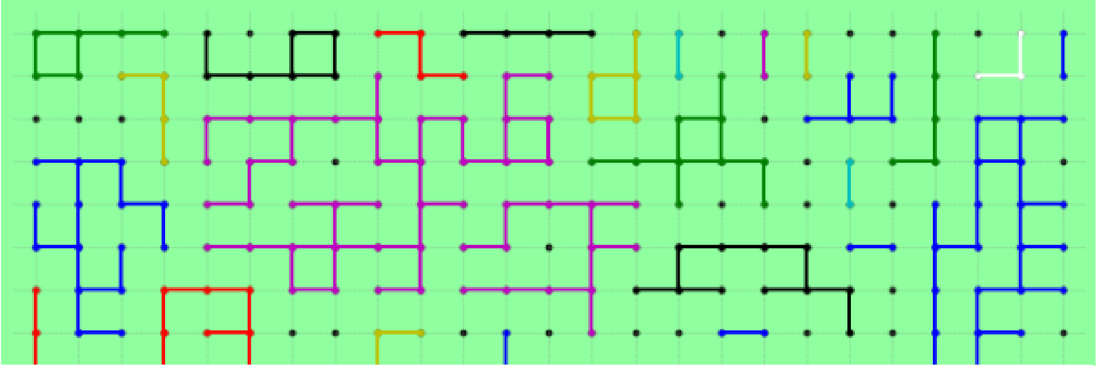
Distance

Pseudodistance

Clusters

Uniform Coupling

Percolation Probability



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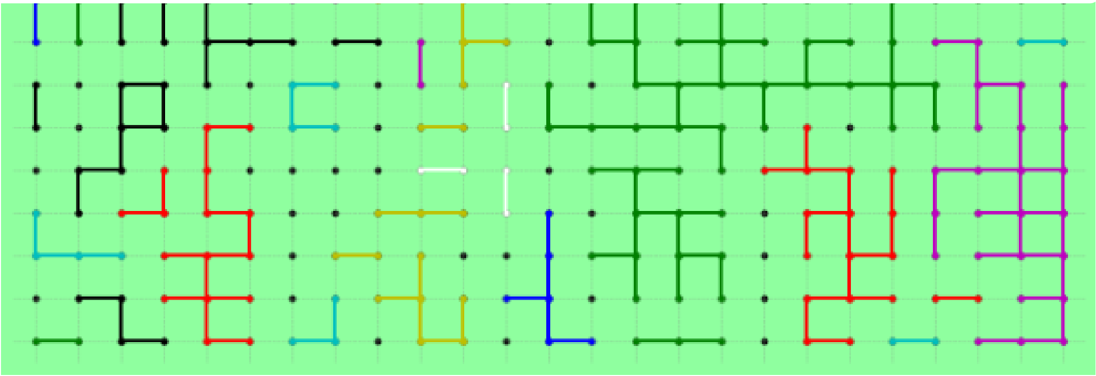


Mathematical Fundaments

Distance

Pseudodistance

Clusters

Uniform Coupling

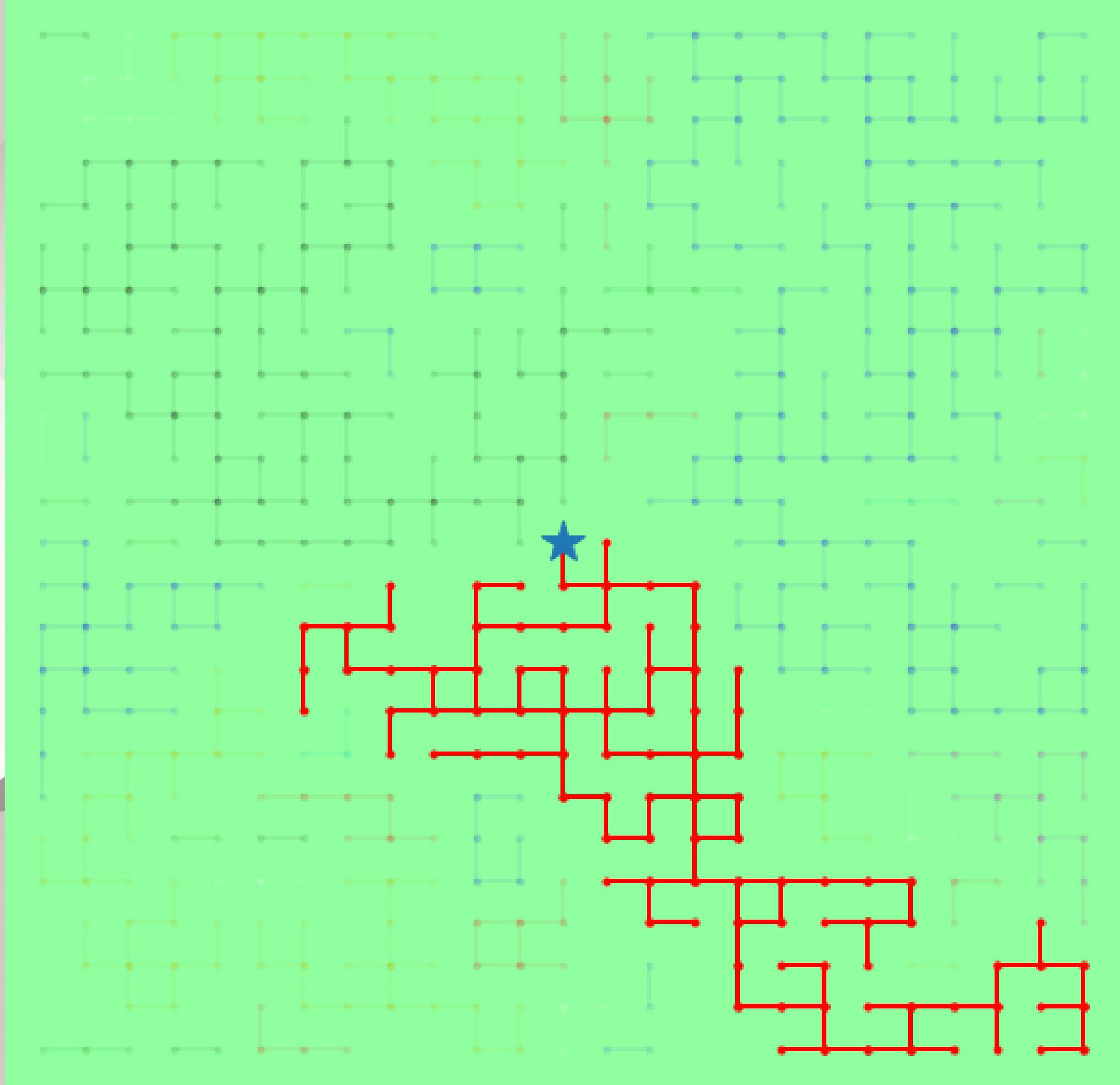
Percolation Probability

Critical Probability

$$p_c = \sup\{p : \theta(p) = 0\}$$

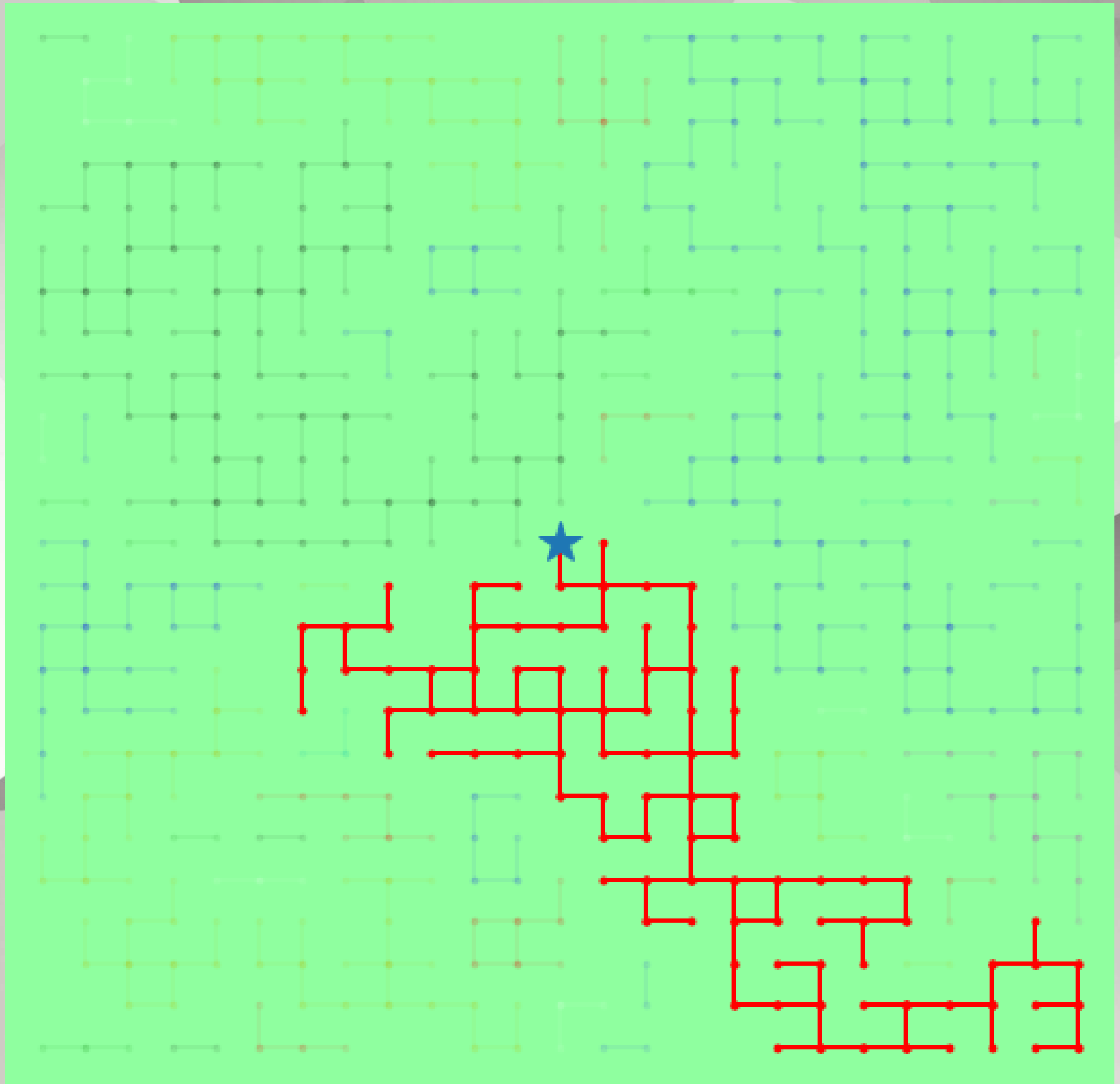
Lower Bound for p_c

Peierls argument



Lower Bound for p_c

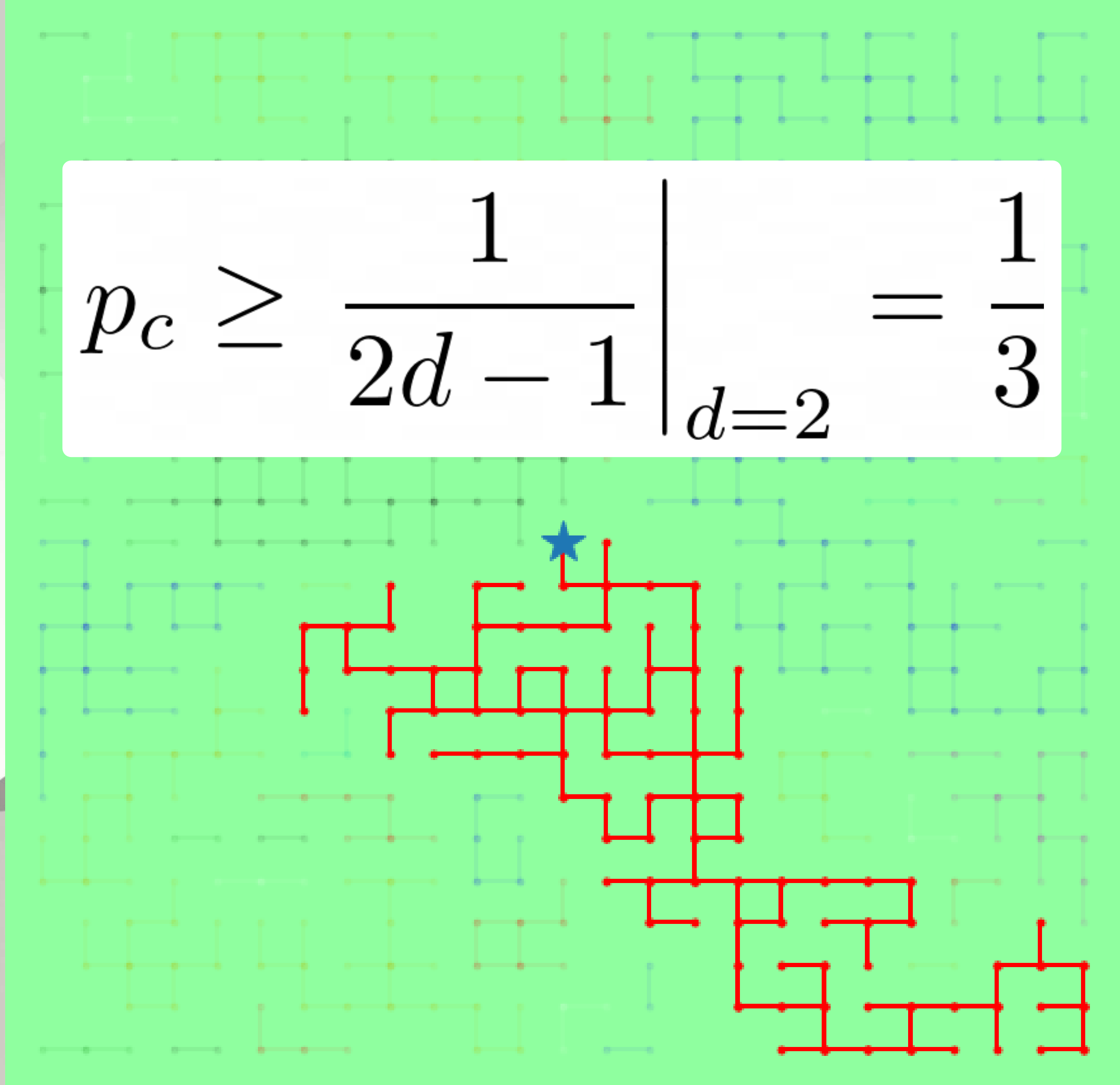
Peierls argument



Lower Bound for p_c

Peierls argument

$$\begin{aligned}
\theta(p) &\leq P_p\left(|C| = l\right) \\
&\leq p^l \cdot \#\left\{\text{of paths of length l}\right\} \\
&\leq p^l 2d(2d-1)^{l-1} \\
&= \frac{2d}{2d-1}\left[p(2d-1)\right]^l \\
&= \frac{4}{3}\left[3p\right]^l \quad \text{if} \quad d = 2
\end{aligned}$$



$$p_c \geq \left.\frac{1}{2d-1}\right|_{d=2} = \frac{1}{3}$$

Lower Bound for p_c

Peierls argument

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Upper Bound for p_c

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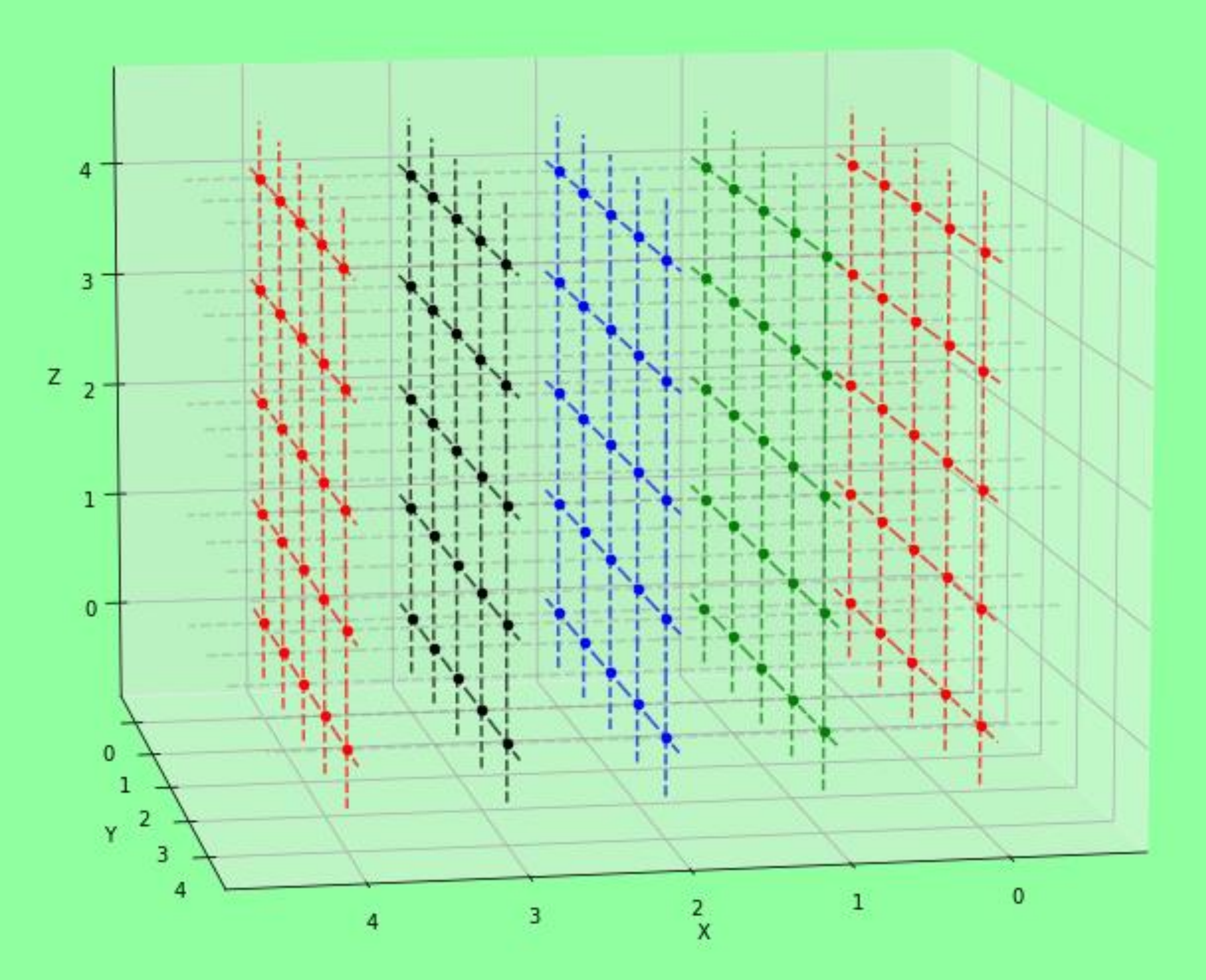
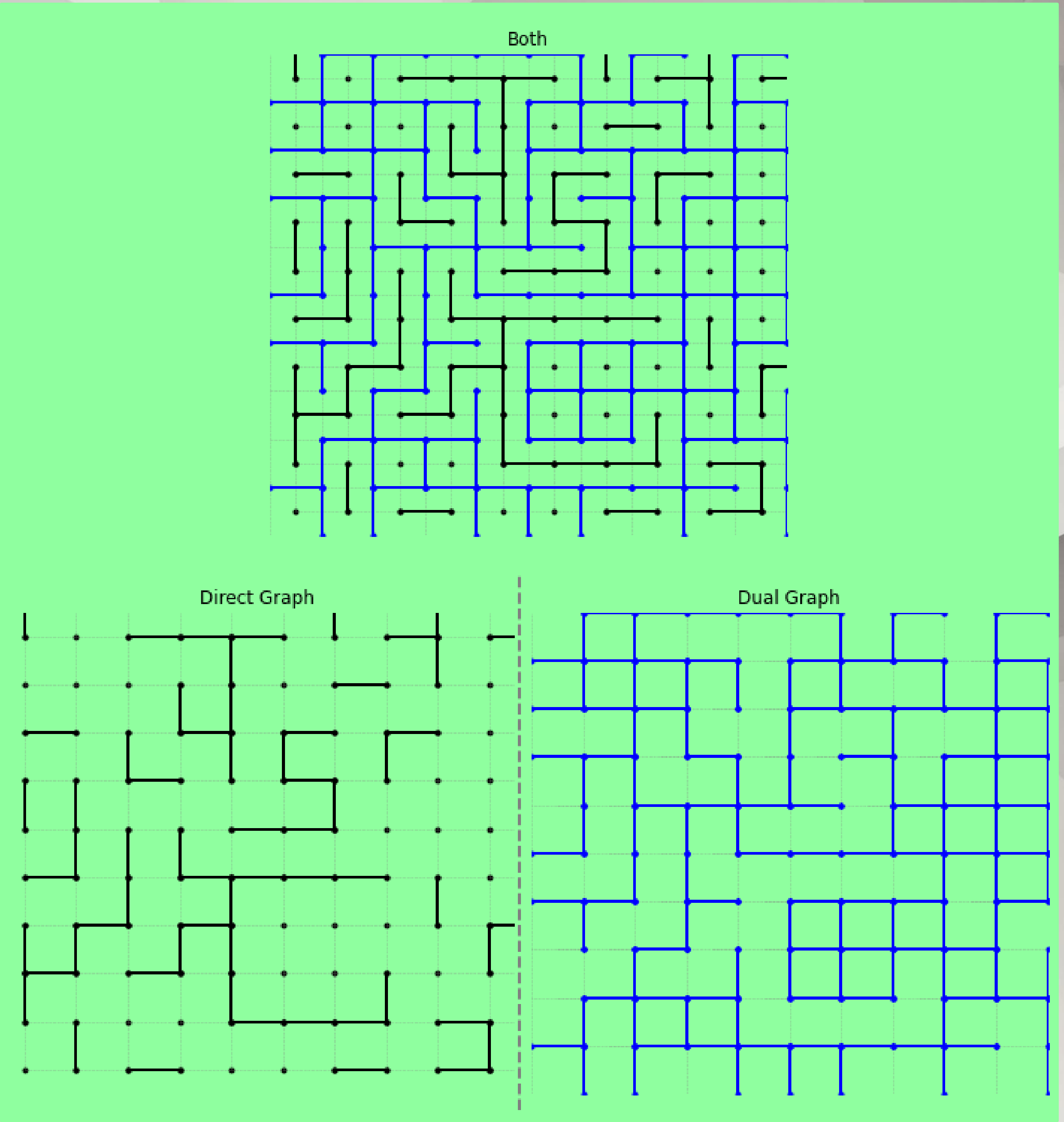


Upper Bound for p_c

Peierls argument

Lattice Embedding

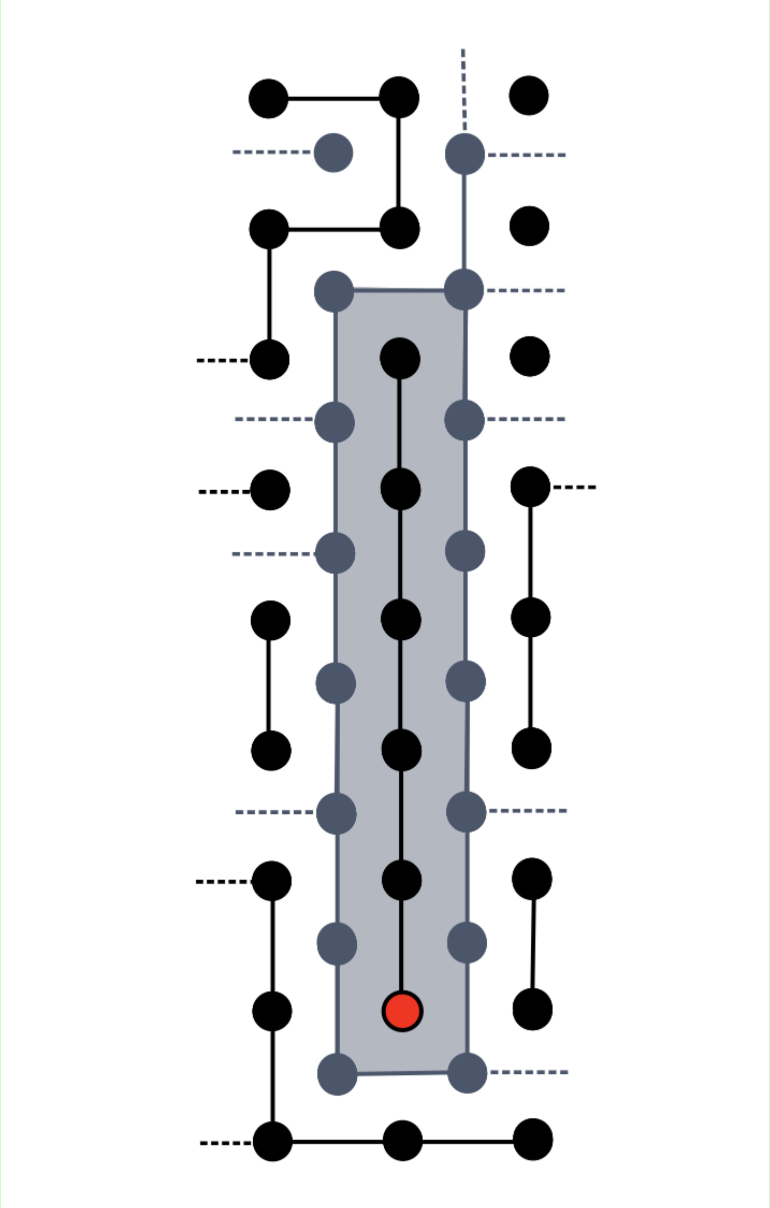


Upper Bound for p_c

Peierls argument

Lattice Embedding

Dual Graph



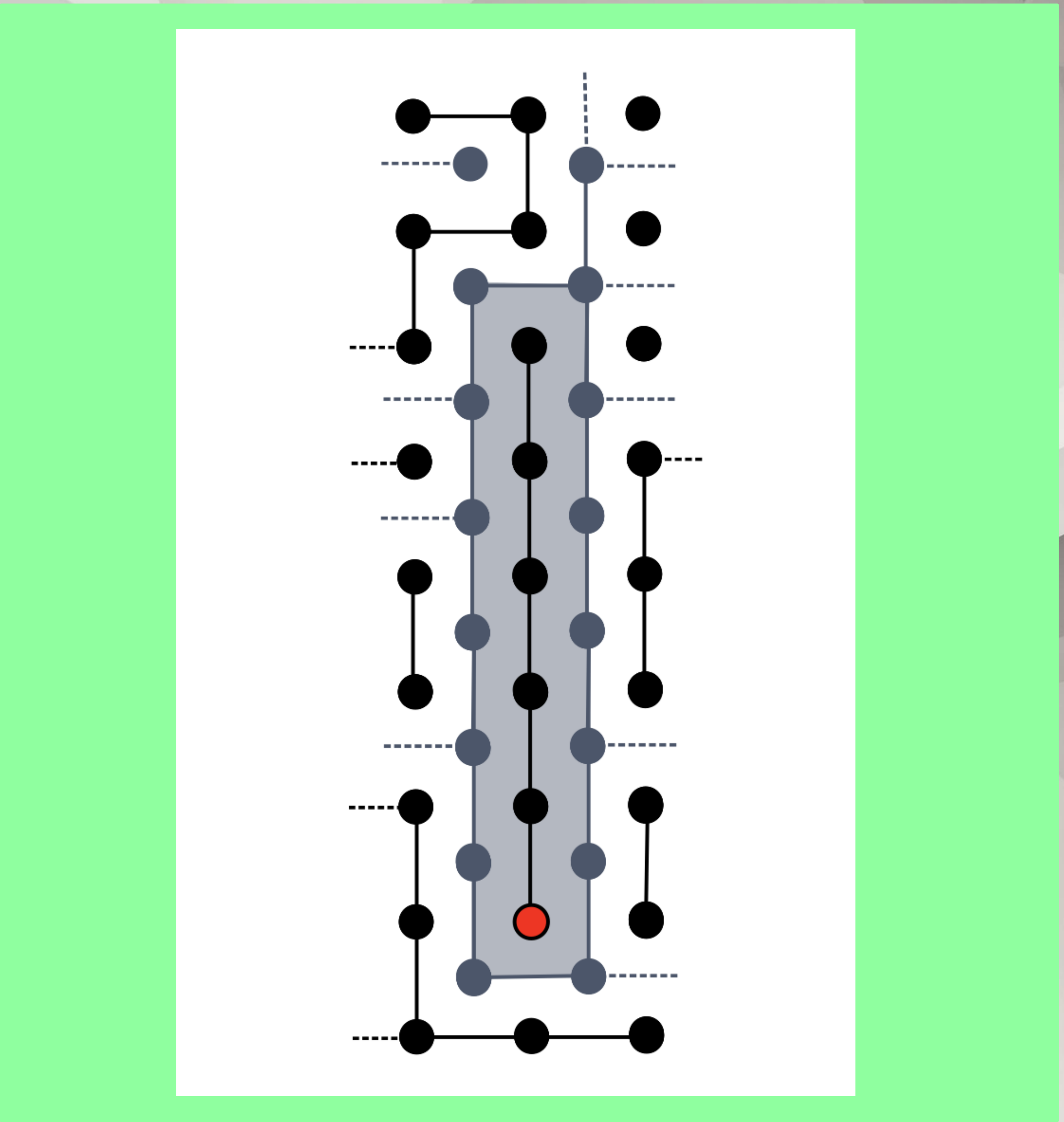
Upper Bound for p_c

Peierls argument

Lattice Embedding

Dual Graph

Upper Bound



Upper Bound for p_c

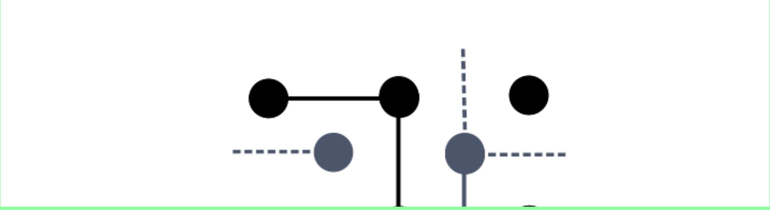
Peierls argument

Lattice Embedding

Dual Graph

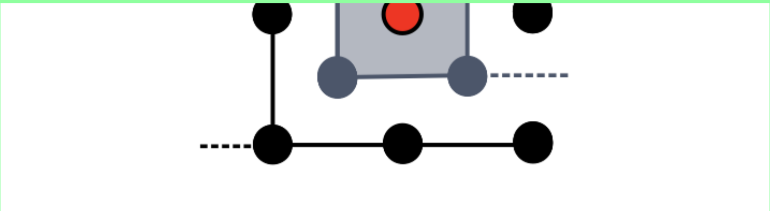
Upper Bound

$$
\begin{aligned}
&P\left(\{\text{path of length l encircling the origin}\}\right)\\
&\quad \leq P\left(\{\text{any path of length l}\}\right)\\
&\quad \leq p_{dual}^{l} \cdot \#\{\text{of paths of length l}\}\\
&\quad \leq p_{dual}^{l}\ 4 \cdot 3^{l-1} = \frac{4}{3}\left(3p_{dual}\right)^{l}
\end{aligned}
$$



No infinite path surrounding the origin can exist if

$$p_{dual} < \frac{1}{3} \implies p_{primal} > \frac{2}{3}$$



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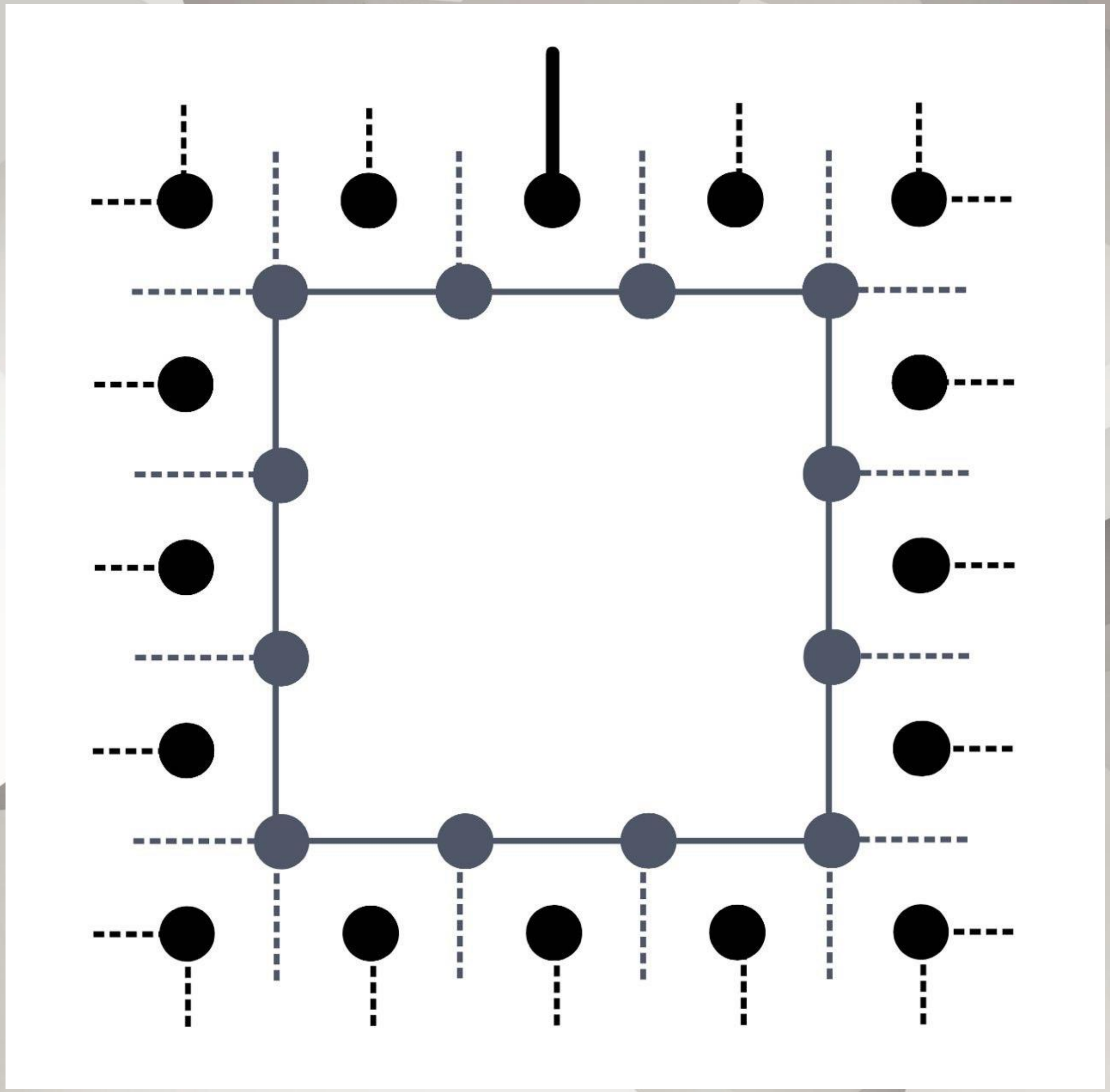


Upper Bound for p_c

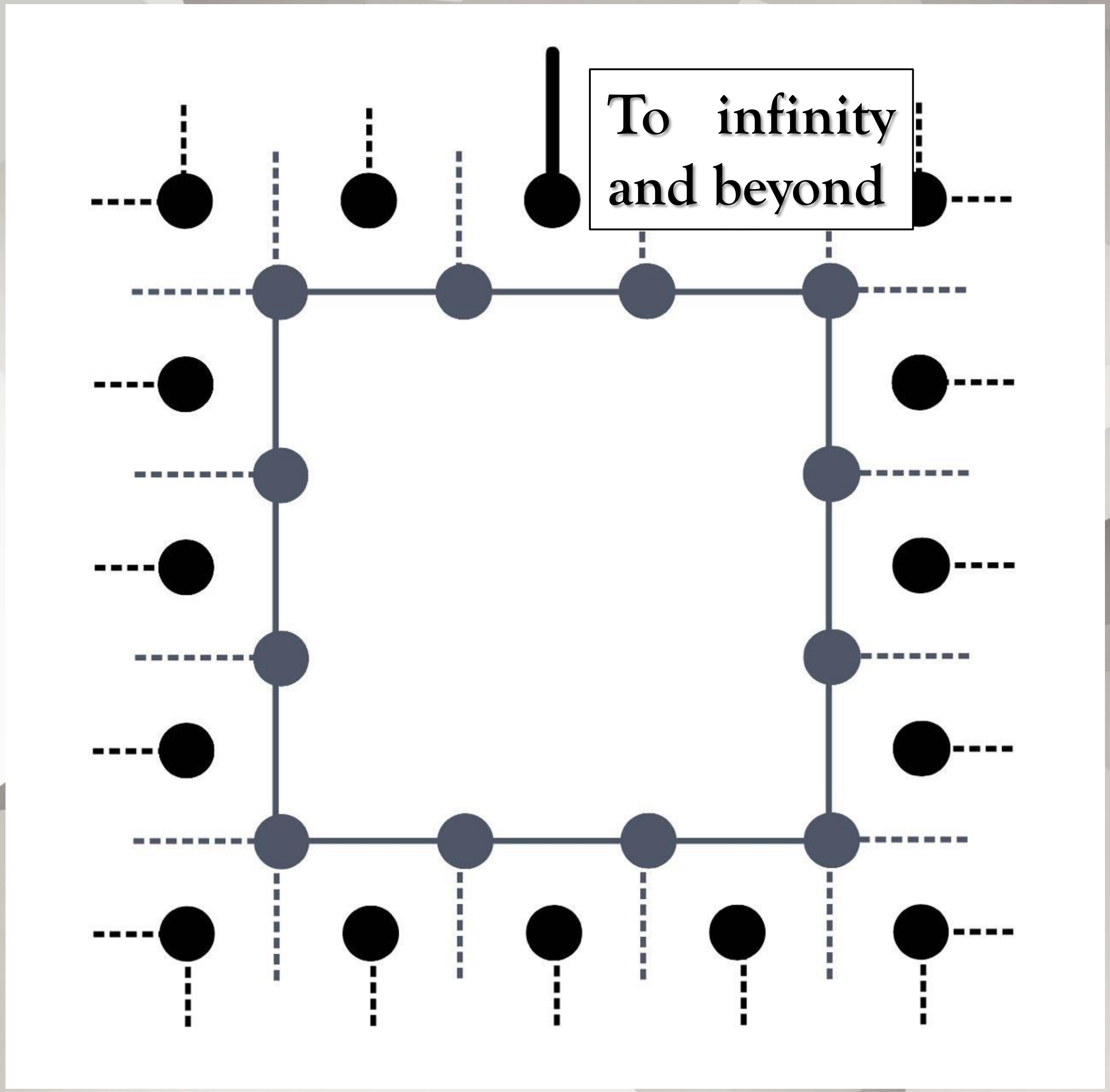
Peierls argument

Lattice Embedding

Dual Graph

Upper Bound

Finite Length Path



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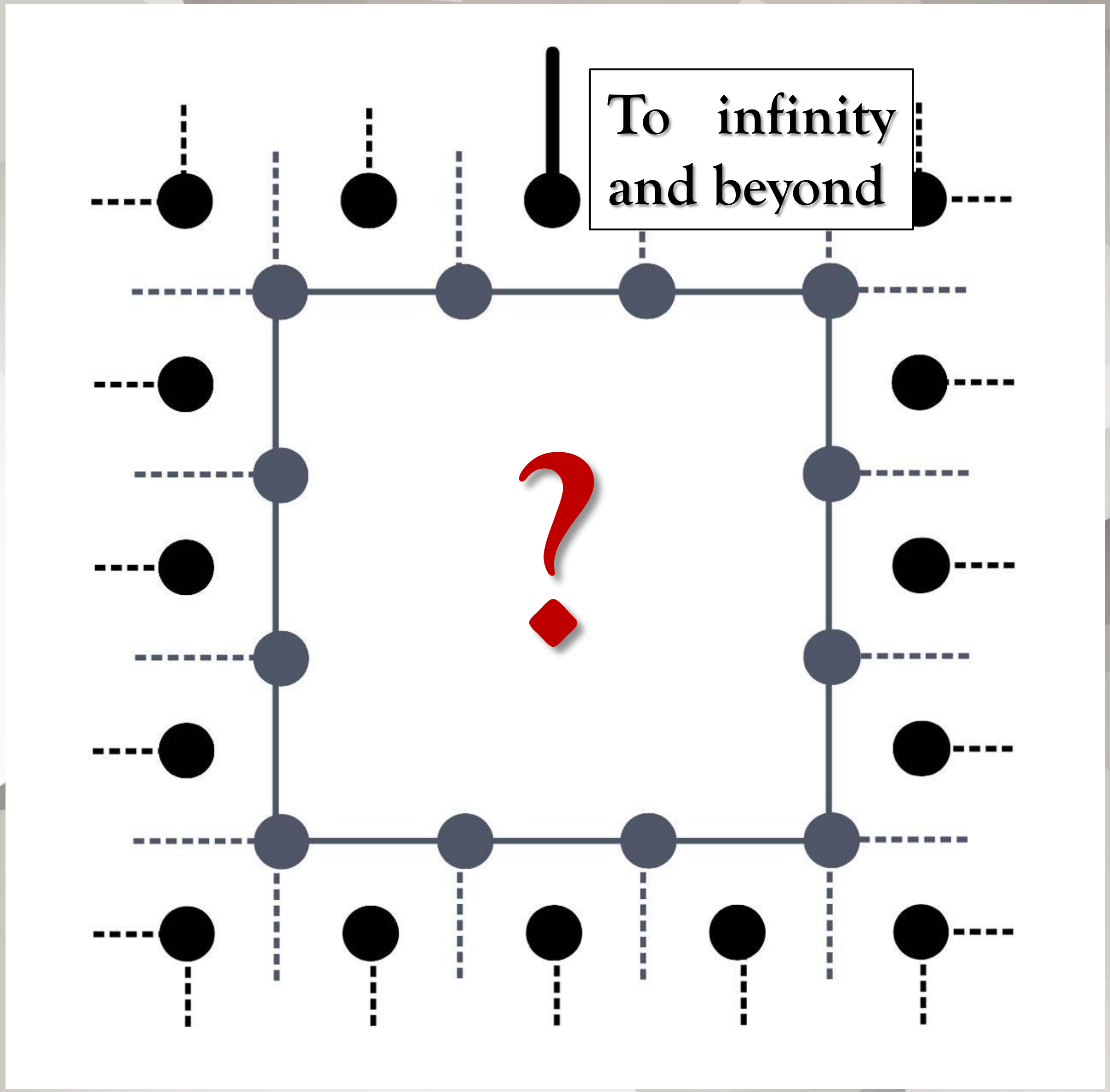

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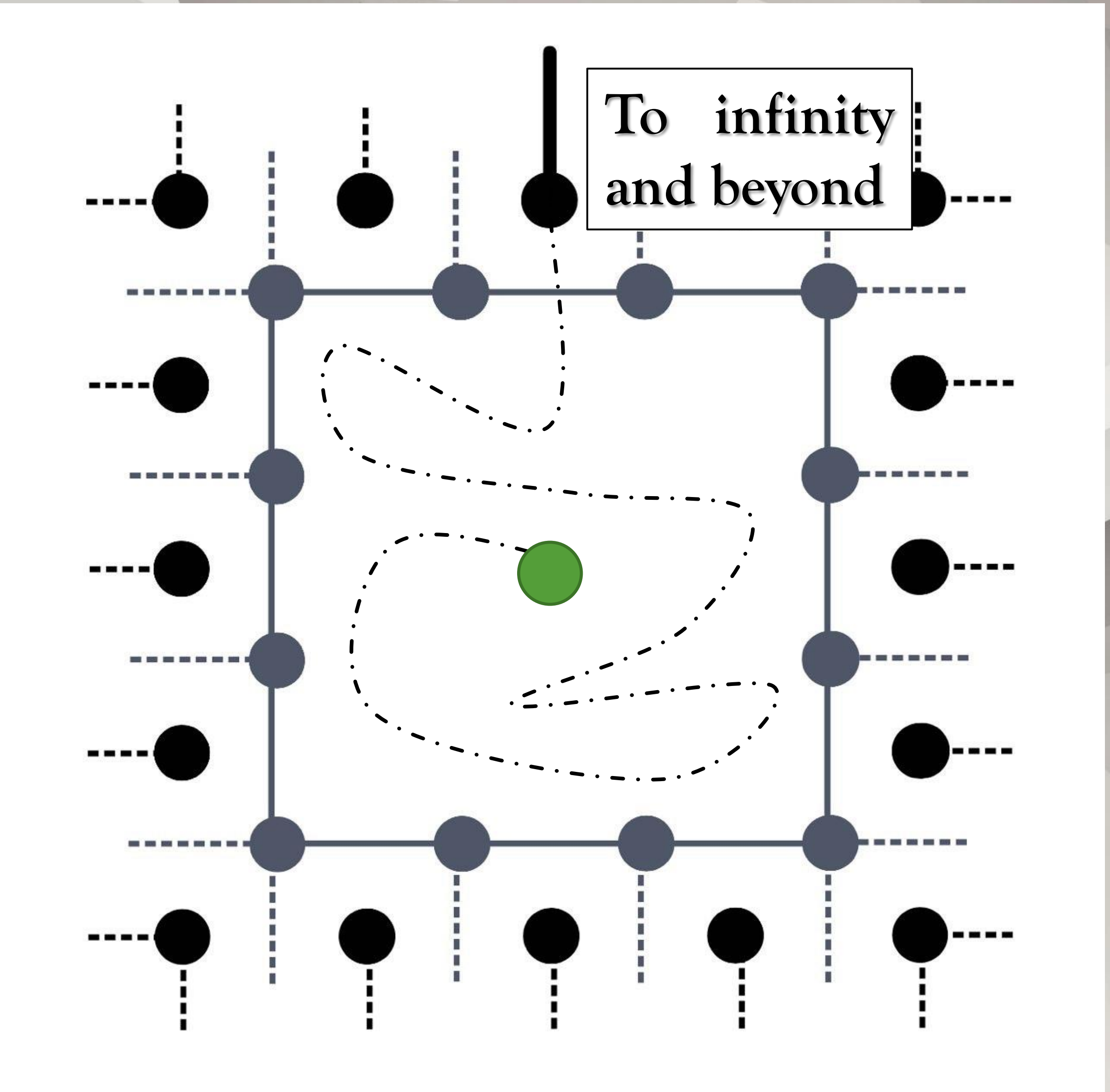

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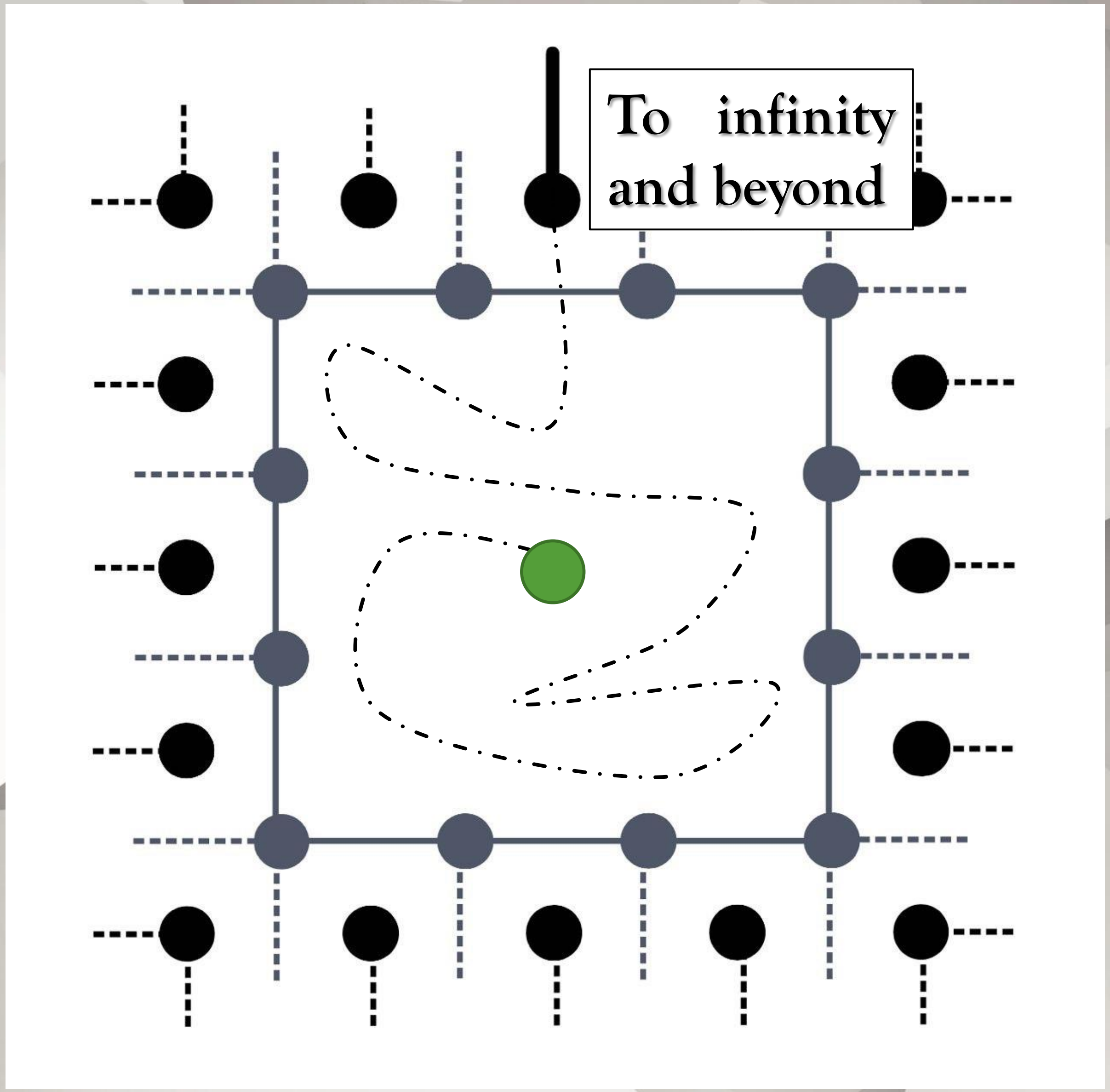

Upper Bound for p_c

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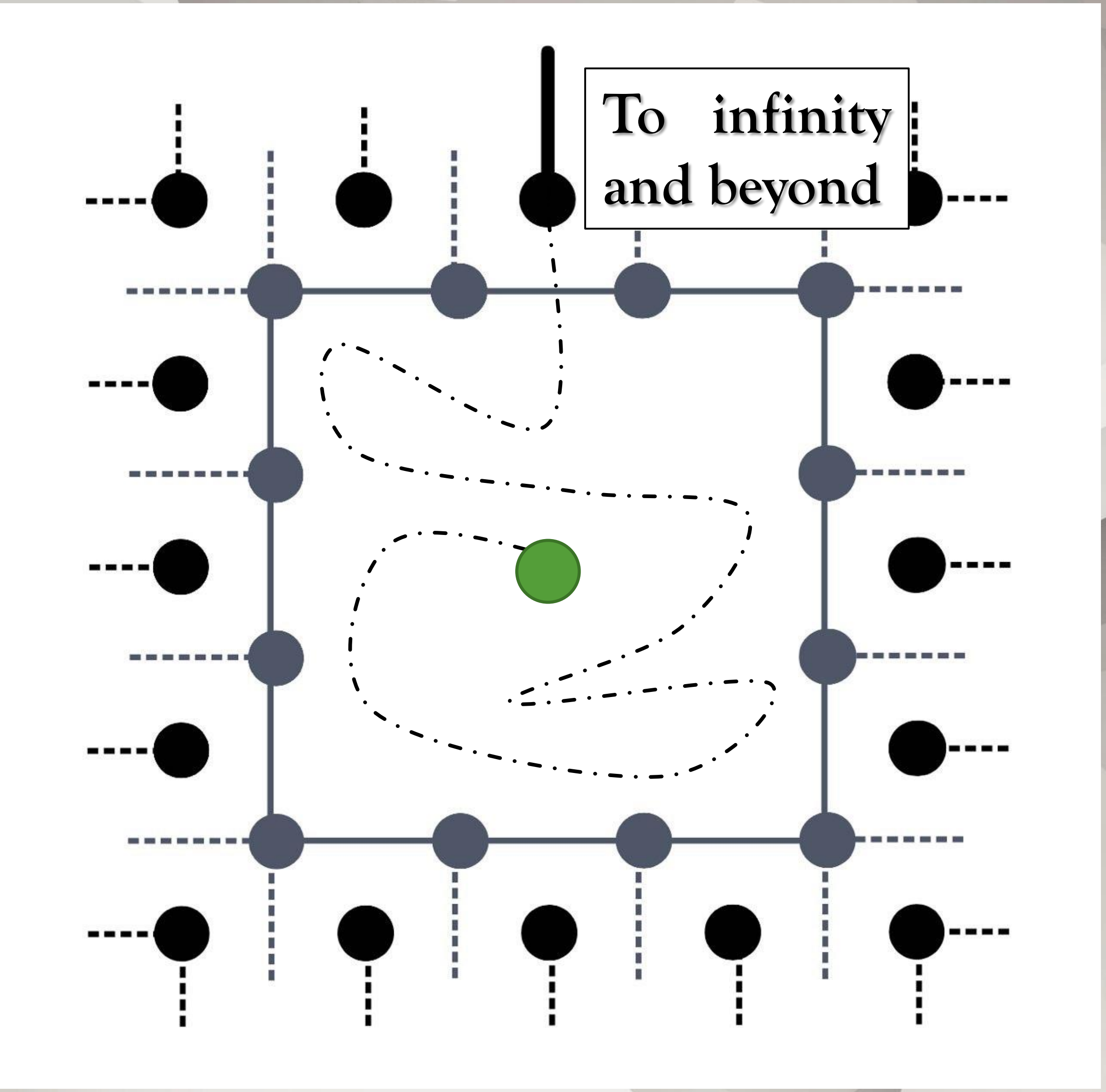
Dual Graph

Upper Bound

Finite Length Path

$$p_c \leq \frac{2}{3}$$



Recap

There exists a critical probability p_c that divides the two phases and is such that

$$\frac{1}{d-1} \leq p_c \leq \frac{2}{3}$$

for any number of dimensions $d \geq 2$.

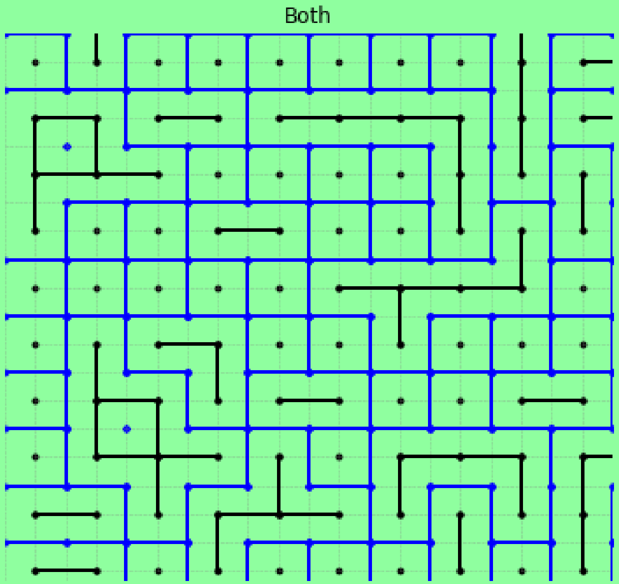
Actual value for p_c

Actual value for p_c

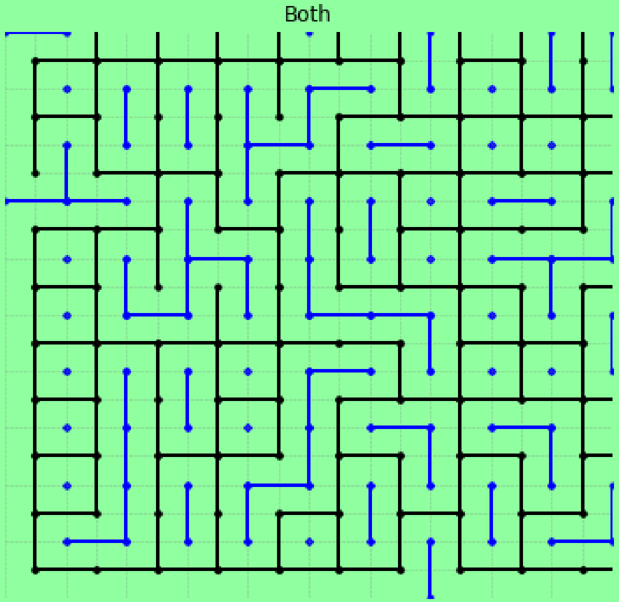
Theoretical considerations

Actual value for p_c

Theoretical considerations



$$p_{primal} = 0.30$$
$$p_{dual} = 0.70$$



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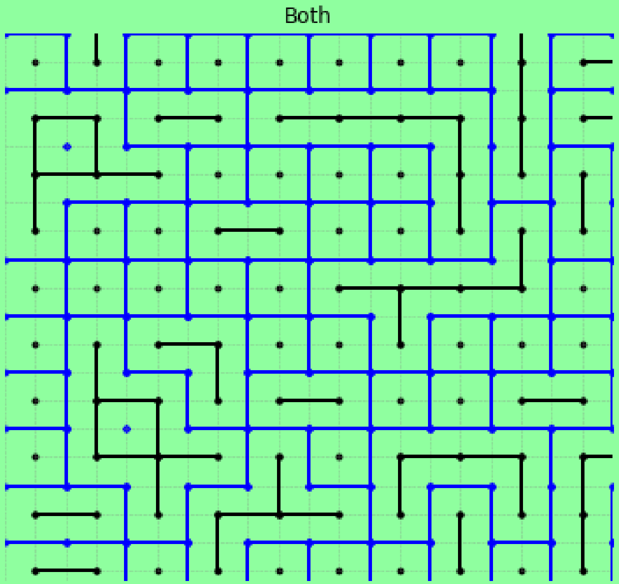

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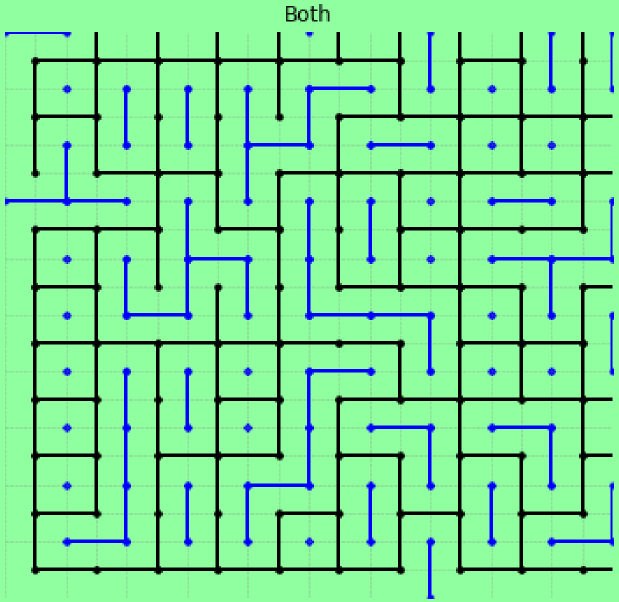

$$p_{primal} = 0.70$$
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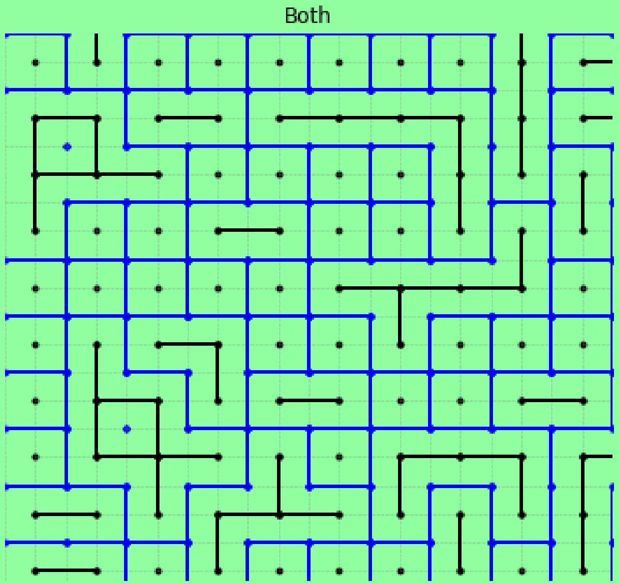
Actual value for p_c

Theoretical considerations

$$p_{dual} = 1 - p_{primal}$$



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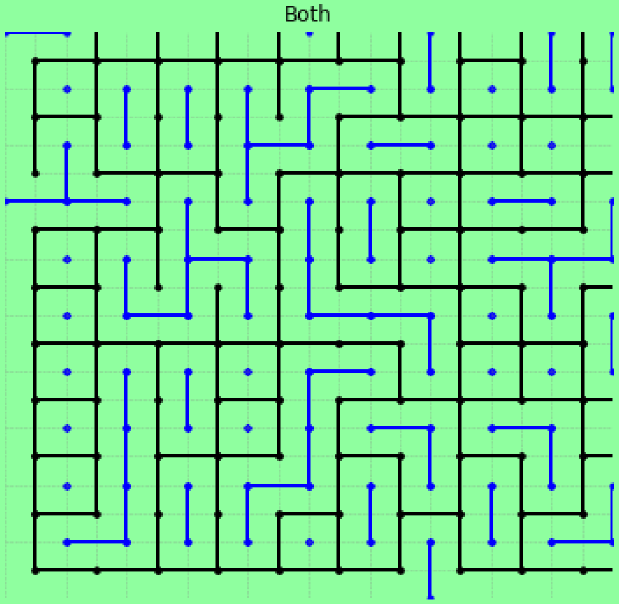

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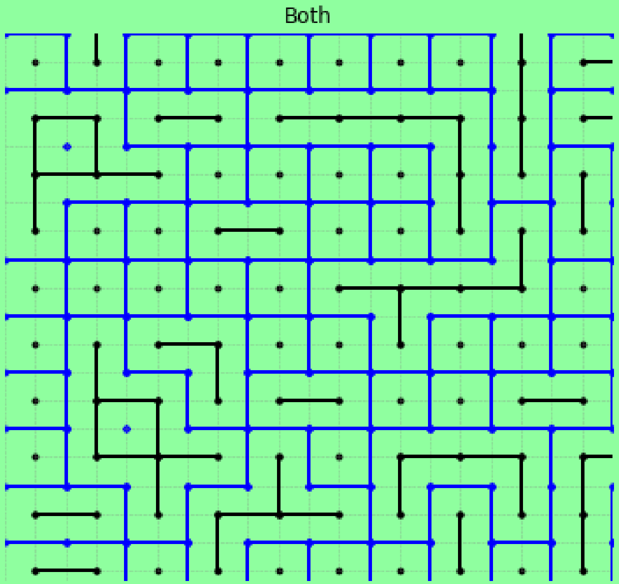
Actual value for p_c

Theoretical considerations

$$p_{dual} = 1 - p_{primal}$$

$$p_c^{dual} = 1 - p_c^{primal}$$



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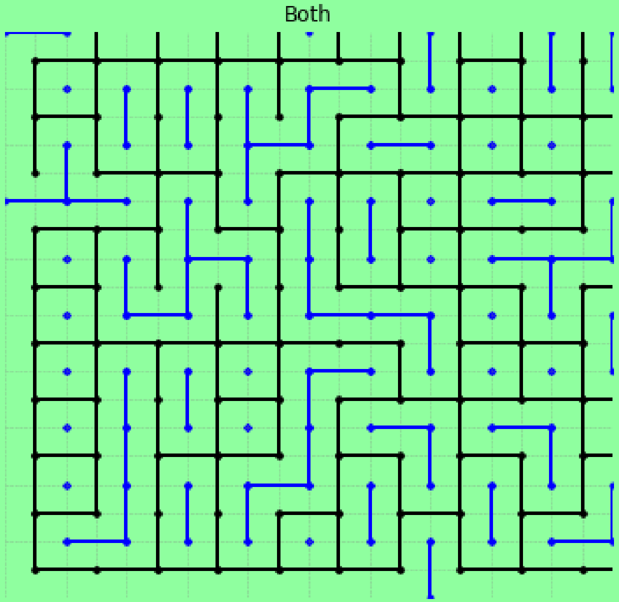

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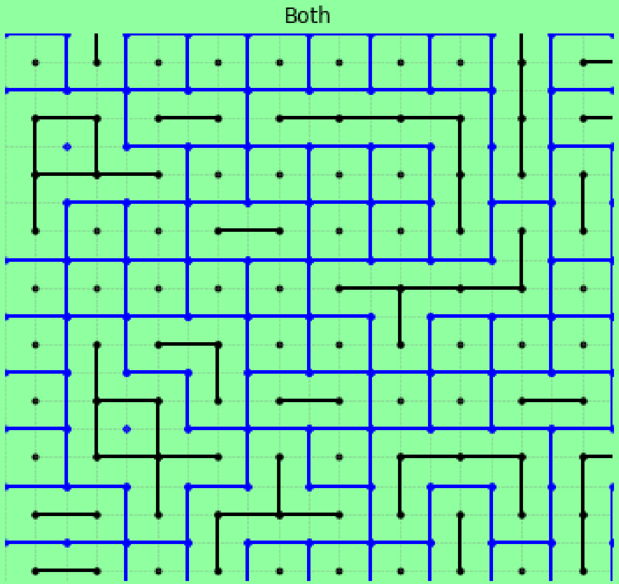

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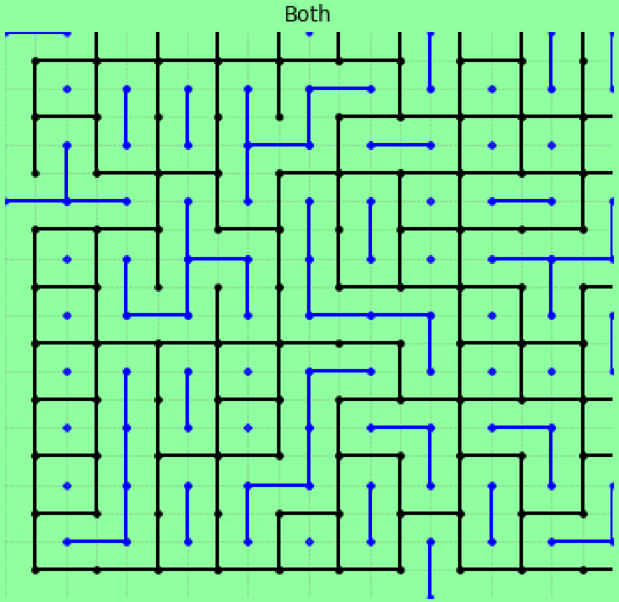

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Actual value for p_c

Theoretical considerations

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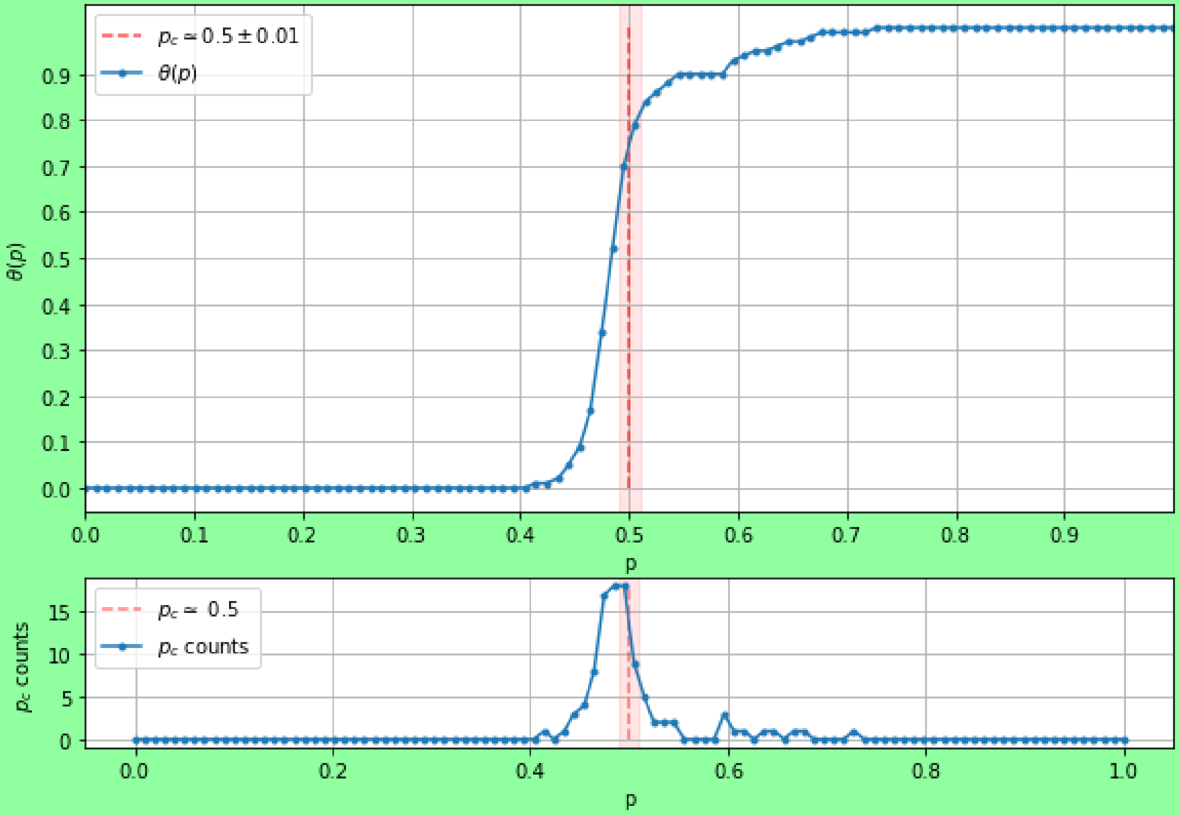
$$p_c^{dual} = 1 - p_c^{primal}$$

$$p_c^{dual} = p_c^{primal}$$

$$p_c^{dual} = p_c^{primal} = \frac{1}{2}$$



Actual value for p_c

Theoretical considerations

Monte Carlo Simulations

$\exists$ of Infinite Cluster

Kolmogorov's Zero-One Law

∃ of Infinite Cluster

Kolmogorov's Zero-One Law

If $\boldsymbol{p > p_c}$ it exists

$$0 < P(\{\text{cluster of the origin is infinite}\}) \le P(\{\exists \text{ infinite cluster on any point}\})$$

∃ of Infinite Cluster

Kolmogorov's Zero-One Law

If $p > p_c$ it exists

If $p < p_c$ it does NOT exists

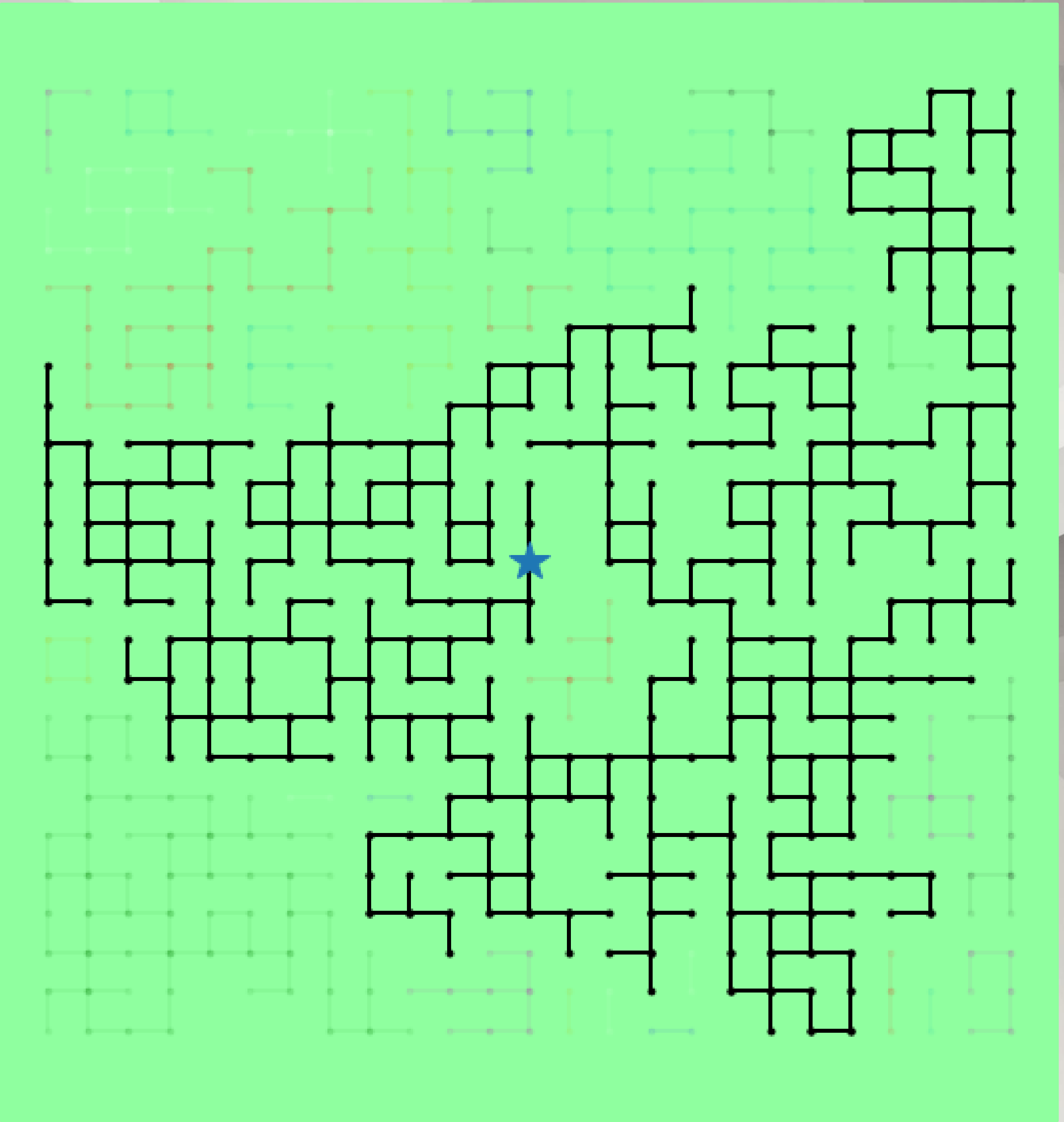
∃ of Infinite Cluster

Kolmogorov’s Zero-One Law

If $p > p_c$ it exists

If $p < p_c$ it does NOT exists

How many infinite clusters?



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Kolmogorov's Zero-One Law

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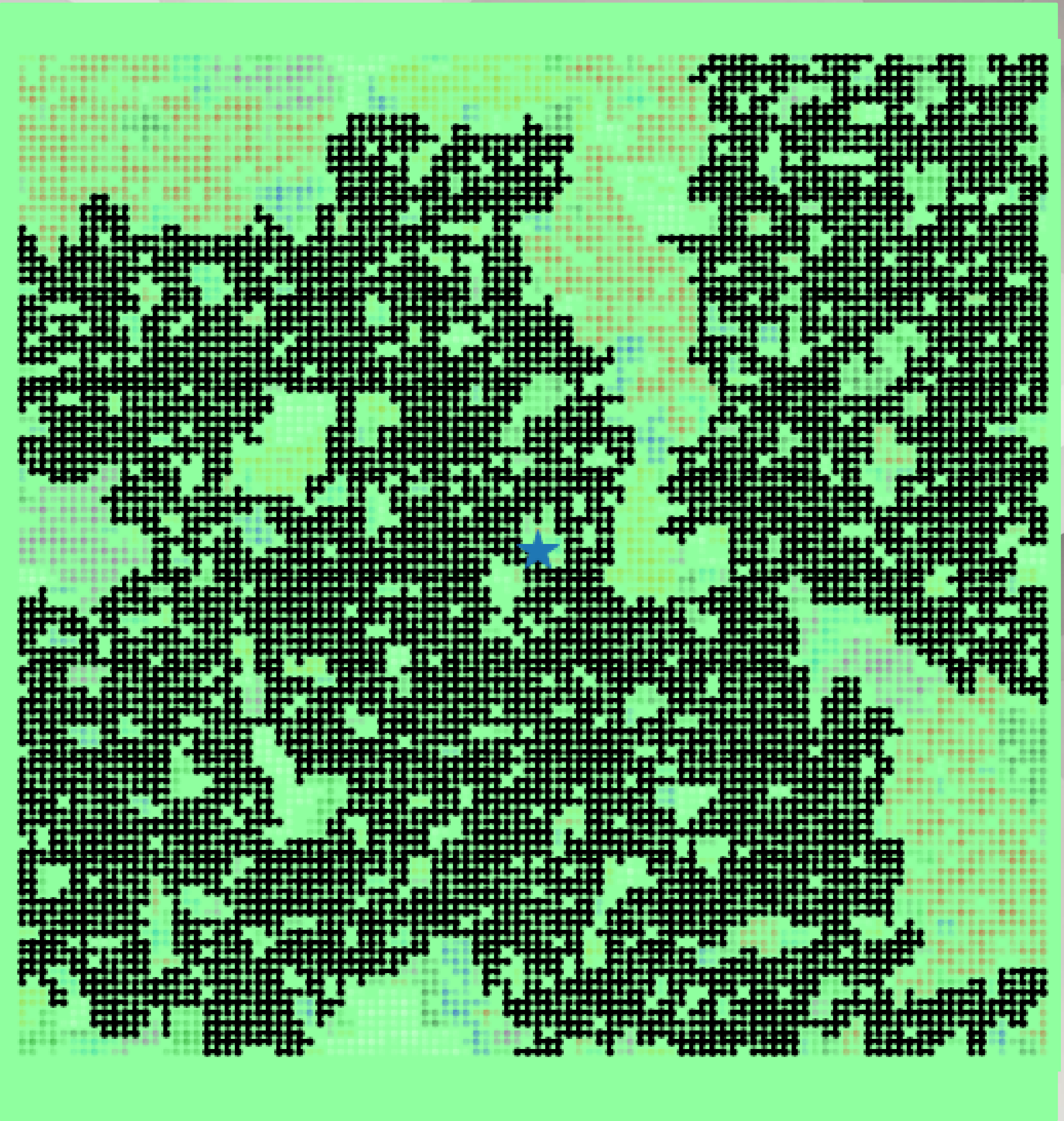

$\exists$ of Infinite Cluster

Kolmogorov's Zero-One Law

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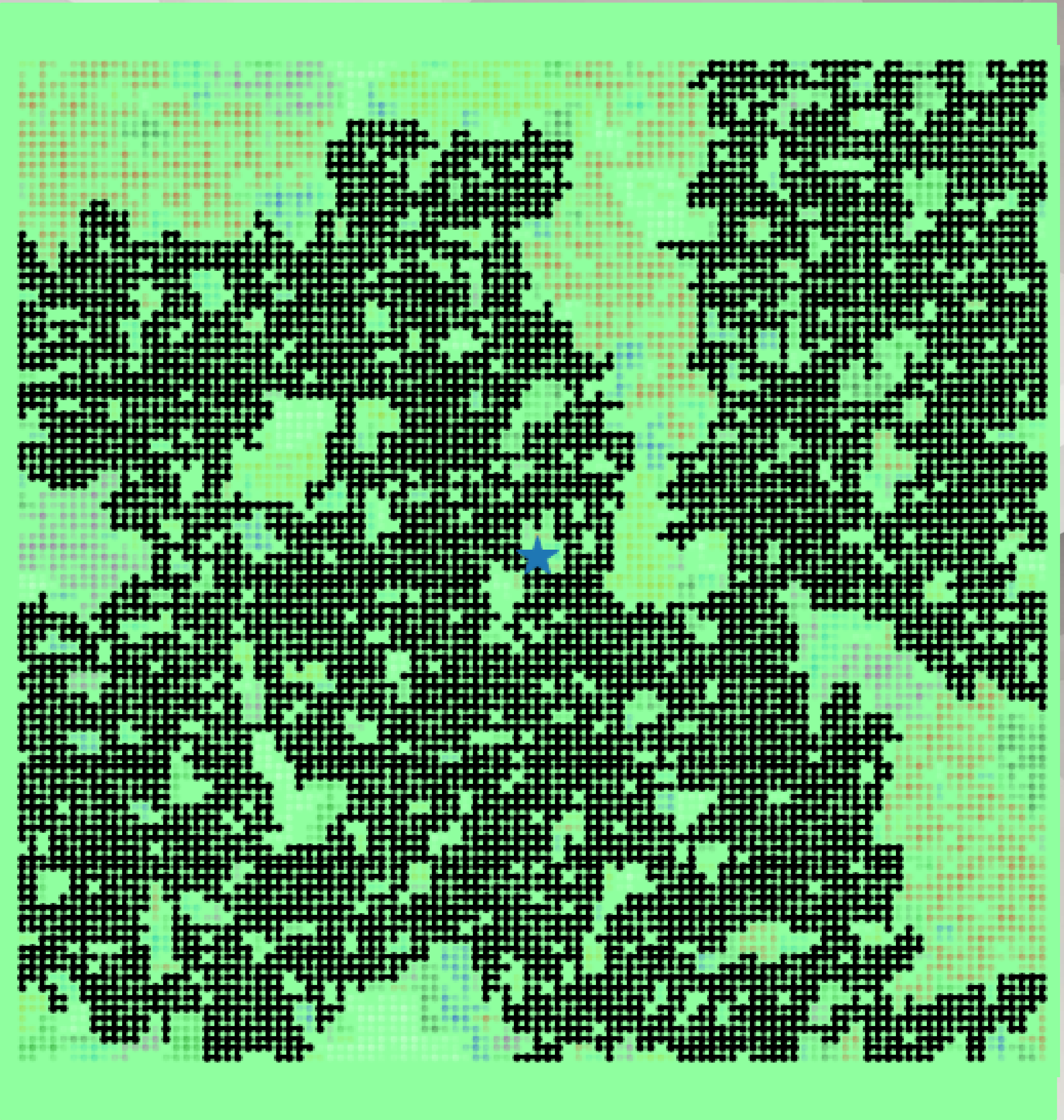
How many infinite clusters?



∃ of Infinite Cluster

Kolmogorov’s Zero-One Law

If $p > p_c$ it exists

If $p < p_c$ it does NOT exists

How many infinite clusters?

1

The Two Phases

Subcritical Phase

$$\exists \alpha(p) > 0 : P_p(|C| = n) \sim e^{-n\alpha(p)}$$

$$\textbf{as } n \to \infty$$

Supercritical Phase

$$e^{-\beta_1(p)} \leq e^{n^{(d-1)/d}} \, P_p(|C| = n) \leq e^{-\beta_2(p)}$$

$$\delta(p) = \lim_{n\to\infty} \left\{ -n^{-(d-1)/d} \log\left(P_p(|C| = n)\right) \right\}$$

Critical Exponents

At the critical point

$$P_{p_c}(|C| > n) \sim n^{-1/\delta}$$

as $n \to \infty$

Near the Critical Point

$$\gamma = \quad -\lim_{p \to p_c^-} \frac{\log \chi(p)}{log|p - p_c|}$$

$$\beta = \quad \lim_{p \to p_c^+} \frac{\log \theta(p)}{log(p - p_c)}$$

$$\delta^{-1} = \quad -\lim_{n \to \infty} \frac{\log P_{p_c}(|C| \geq n)}{log(n)}$$

The Two Phases

Subcritical Phase

$$\exists \alpha(p) > 0 : P_p(|C| = n) \sim e^{-n\alpha(p)}$$

as $n \to \infty$

Supercritical Phase

$$e^{-\beta_1(p)} \leq e^{n^{(d-1)/d}} P_p(|C| = n) \leq e^{-\beta_2(p)}$$

$$\delta(p) = \lim_{n \to \infty} \left\{ -n^{-(d-1)/d} \log\left(P_p(|C| = n)\right) \right\}$$

Virus Capsids Collapse

- Capsid of Hepatitis B (HBV)
- 120 dimer with T=4 icosahedral symmetry
- Experimental studies show no fragmented capsid with less than 90 dimers

CrossMark

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PAPER

Molecular jenga: the percolation phase transition (collapse) in virus capsids

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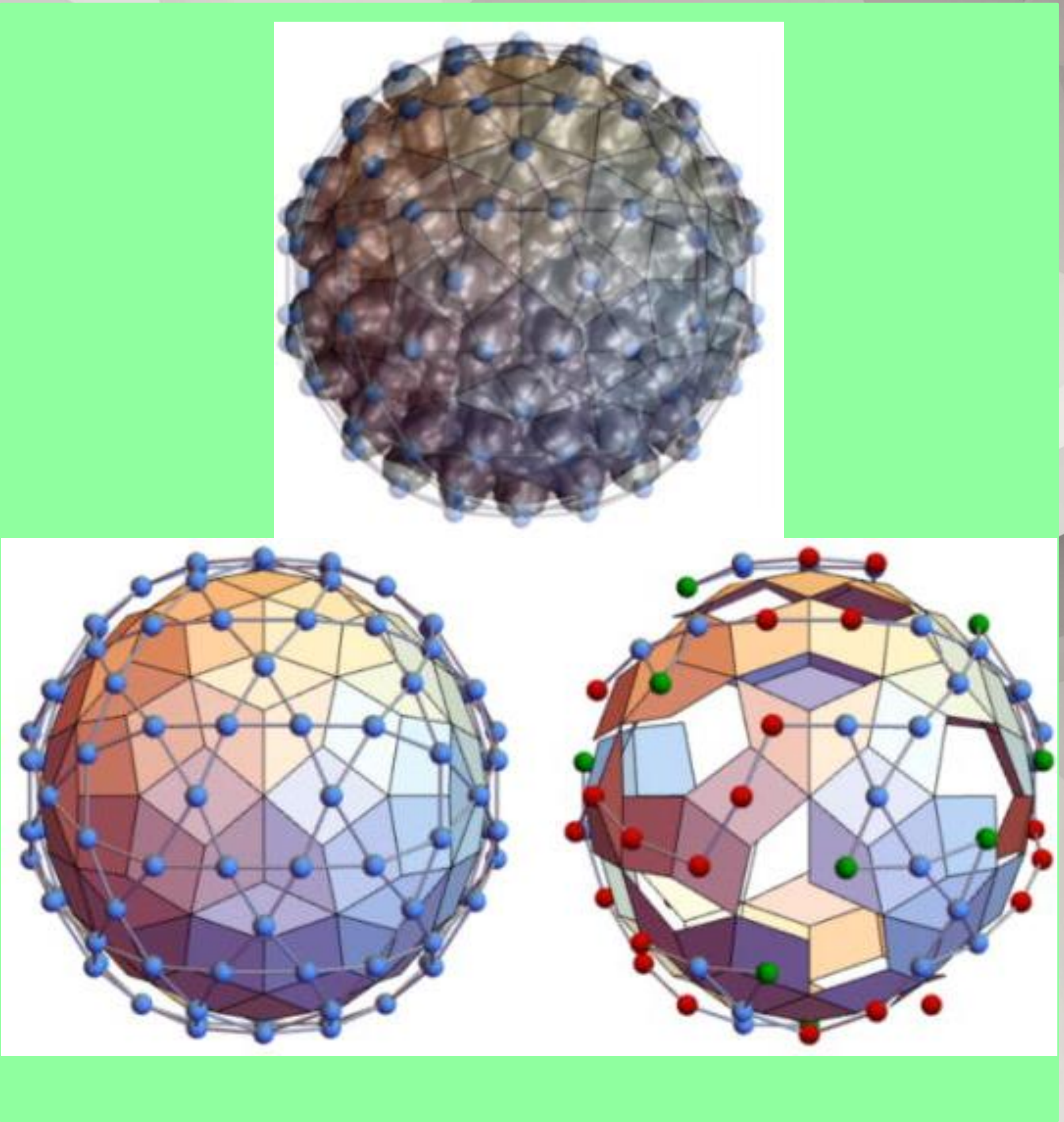
Keywords: capsid, hepatitis B virus, self-assembly, icosahedral symmetry

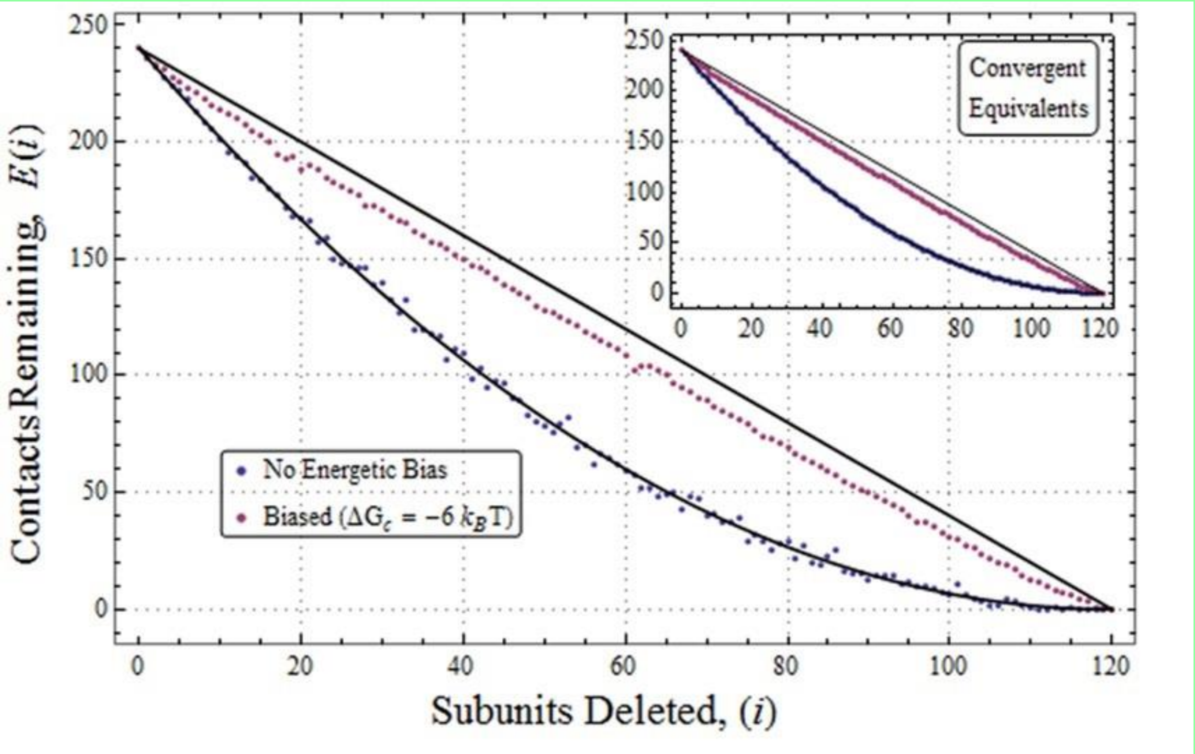
Abstract

Virus capsids are polymeric protein shells that protect the viral cargo. About half of known virus families have icosahedral capsids that self-assemble from tens to thousands of subunits. Capsid disassembly is critical to the lifecycles of many viruses yet is poorly understood. Here, we apply a graph and percolation theory to examine the effect of removing capsid subunits on capsid stability and fragmentation. Based on the structure of the icosahedral capsid of hepatitis B virus (HBV), we constructed a graph of rhombic subunits arranged with icosahedral symmetry. Though our approach neglects dependence on energetics, time, and molecular detail, it quantitatively predicts a percolation phase transition consistent with recent *in vitro* studies of HBV capsid dissociation. While the stability of the capsid graph followed a gradual quadratic decay, the rhombic tiling abruptly fragmented when we removed more than 25% of the 120 subunits, near the percolation threshold observed experimentally. This threshold may also affect results of capsid assembly, which also experimentally produces a preponderance of 90 mer intermediates, as the intermediate steps in these reactions are reversible and can thus resemble dissociation. Application of percolation theory to understanding capsid association and dissociation may prove a general approach to relating virus biology to the underlying biophysics of the virus particle.



Hypothesis

- Capsid can be modelled as a 2D graph
- Fragmentation is seen as percolation on finite graph
- Dimers are assumed completely identical



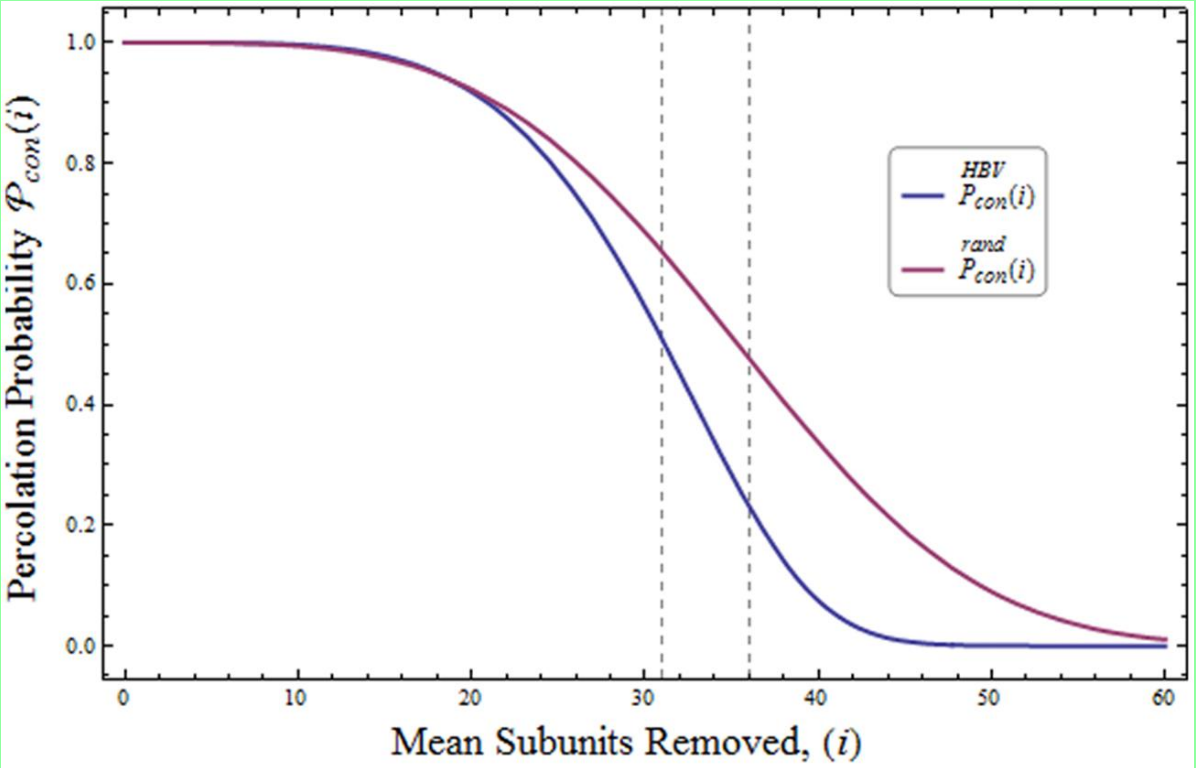
Dimer-Dimer interaction

No dimer-dimer interaction

$$\bar{E}(i) \simeq E_0 - \bar{k}_o i + \frac{\bar{k}_0}{2}\frac{i}{V_0} i$$

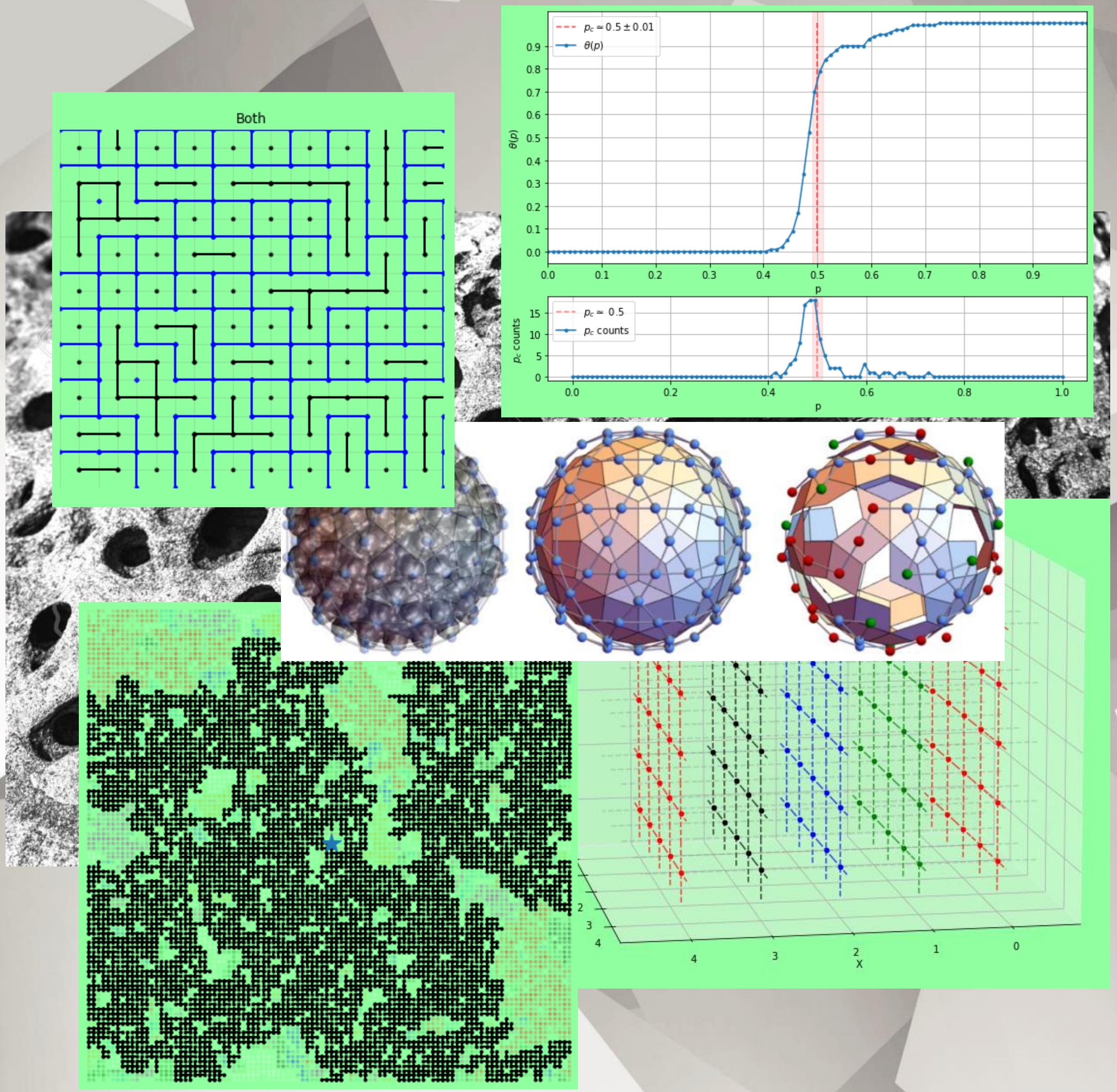
Dimer-dimer interaction

$$\bar{E}(i) \simeq E_0 - \frac{E_0}{V_0} i$$



Percolation Probability

- Fragmentation is defined as maximum change of percolation probability
- Fragmentation occurs at 25%
- Similar results are obtained with other graphs



Conclusions

About the model

The analogies with the Ising Model are due to **random cluster model.**

About applications

Quantitative predictions seems forced but qualitative behaviour is enlightening.

References

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