Percolation of aligned and overlapping shape-anisotropic objects on lattices

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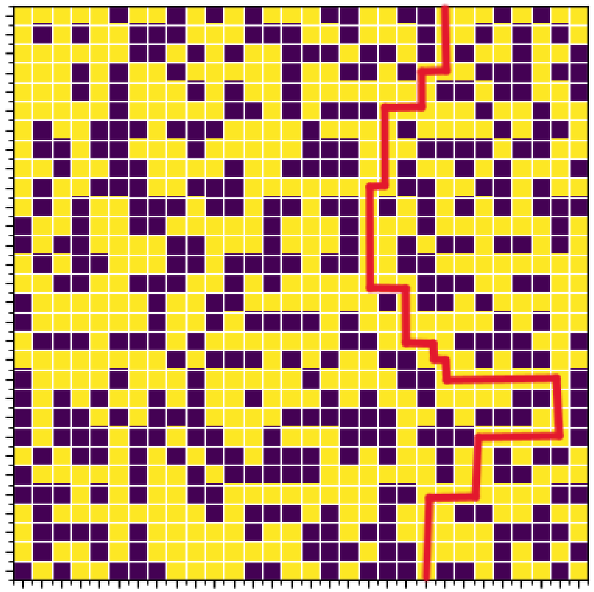
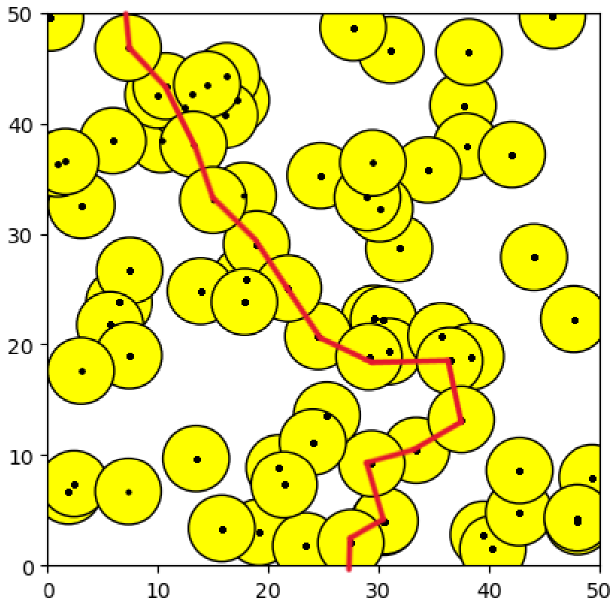
Outline of the talk

- Introduction to percolation
- Percolation of aligned overlapping anisotropic shapes on lattices
- Semi continuum models
- Conclusions

Percolation

- Model to study random and disordered media.
- Percolation phase transition : Emergence of a spanning cluster.
- Classification : **Lattice percolation** and **Continuum percolation**





Control parameters:

Occupation probability(Lattice)

Number density(Continuum)

Order parameter:
Probability of a spanning cluster

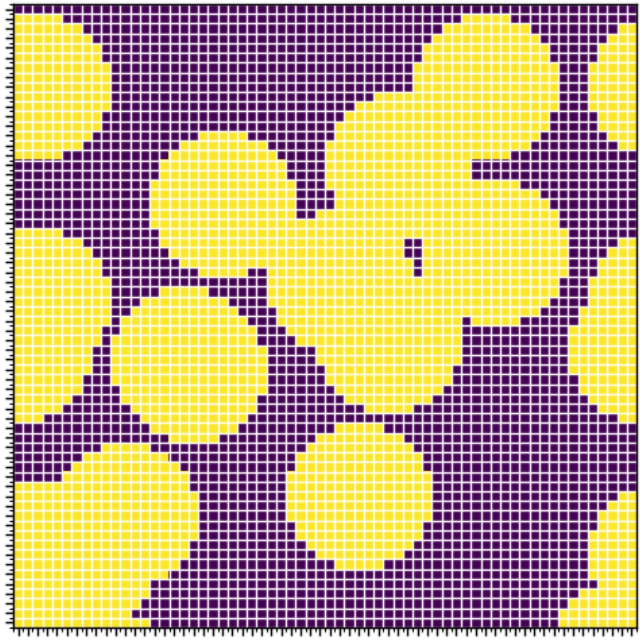
Transition point : Percolation threshold

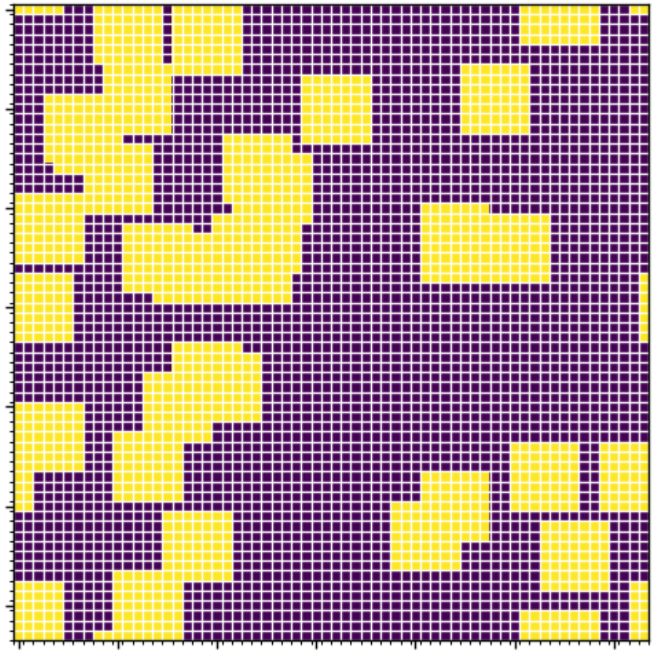
Percolation of extended overlapping shapes on lattices

- Extended shapes on lattices : Discs, squares, rectangles, sticks, diamonds etc.(Koza et.al 2014, Brzeski et.al 2022).

- Interpolates between lattice and continuum

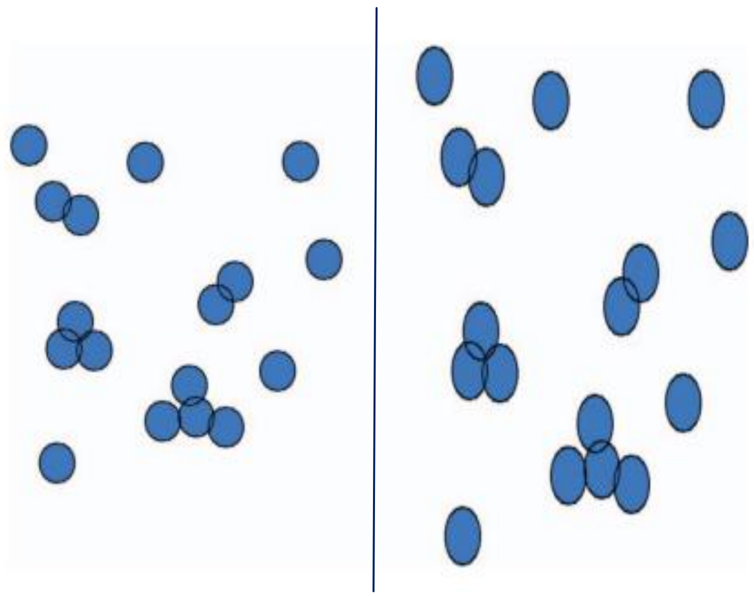
- Features : Multisite occupancy and multiple occupancy.

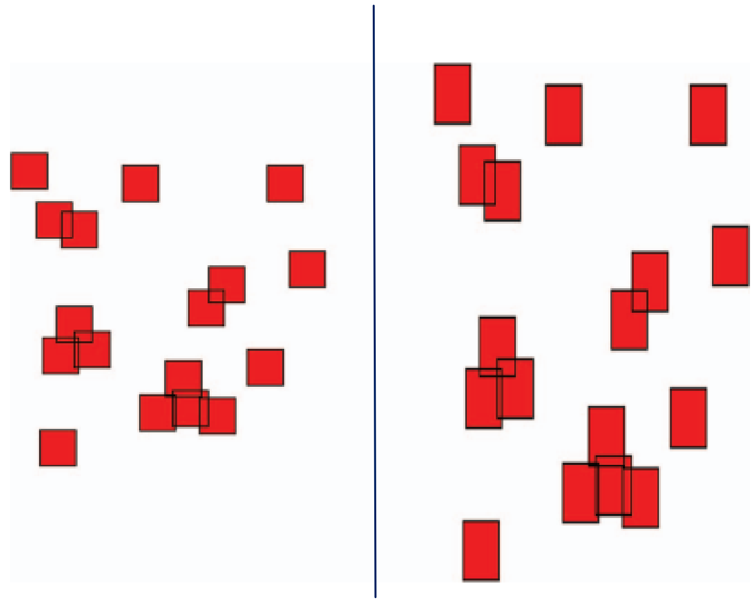




Motivation

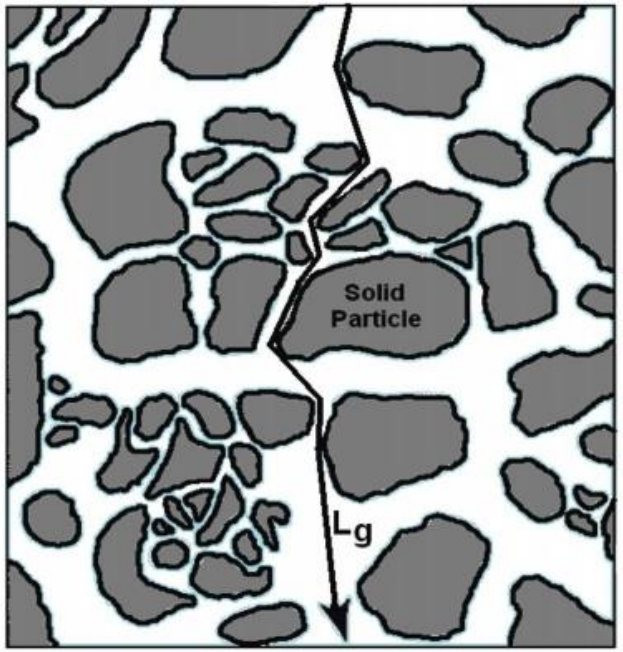
- How does anisotropic shapes show discrete to continuum transition?
- 2D continuum model of aligned rectangles : Percolation threshold independent of aspect ratio. (Klatt et.al, 2017).
- Affine symmetry is present in continuum cases(Torquato, 2012) .



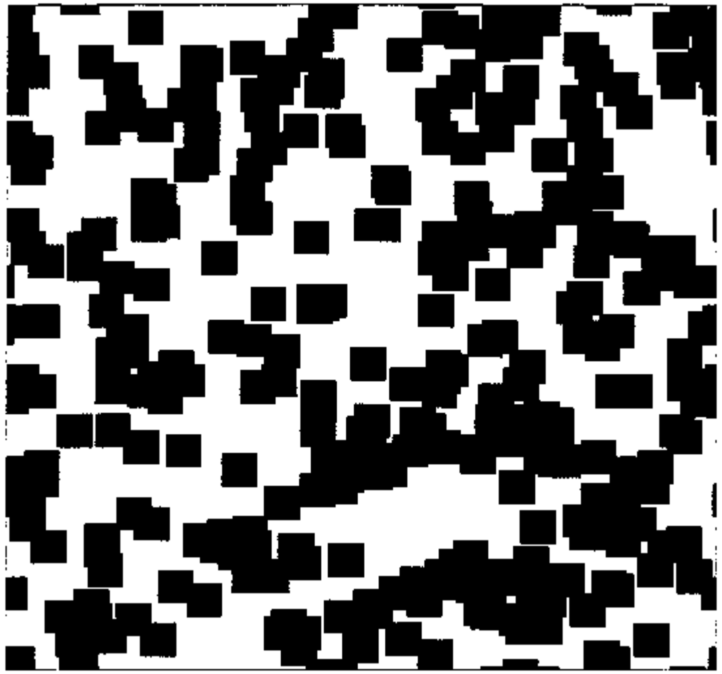


Lattices do not have such a symmetry under scaling

- Aligned overlapping rectangle model useful in study of transport properties in porous media. (Koponen et.al 1997)



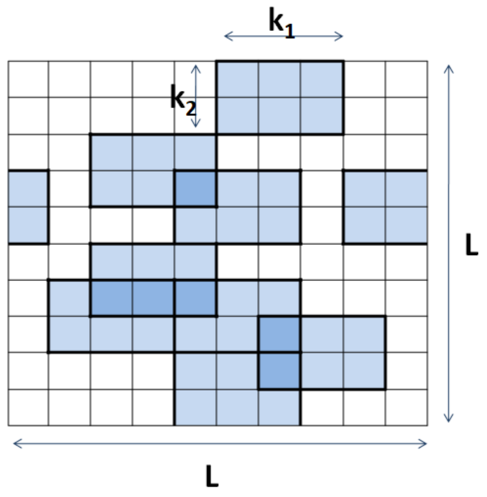
Ghanbarian et.al 2013

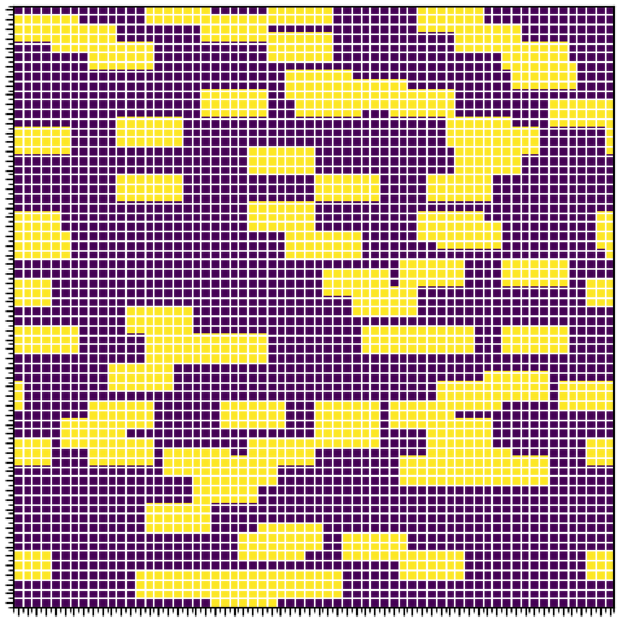


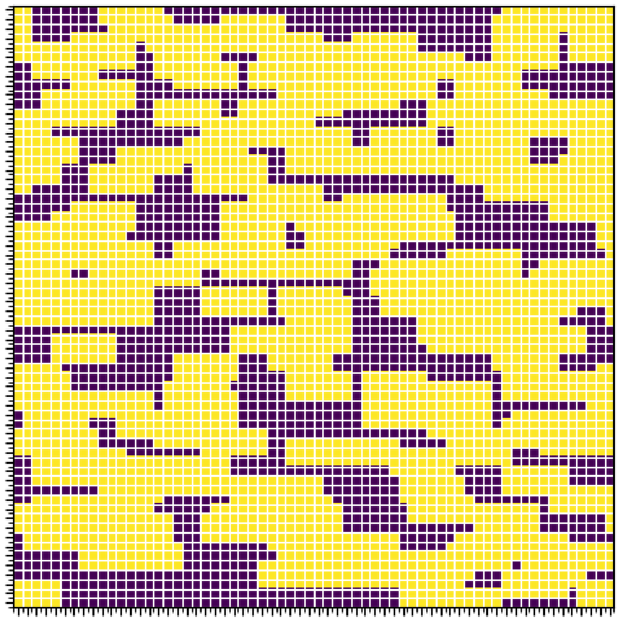
Koponen et.al 1997

Percolation of aligned and overlapping rectangle model

- Typical example of anisotropic shapes on lattices.
- Connected path of rectangles in vertical direction : Spanning cluster
- $\phi = 1 - \exp(-\eta)$, ϕ – Density of occupied sites, η – Areal density.







k_1 x k_2 rectangles in L x L system
2D square lattice

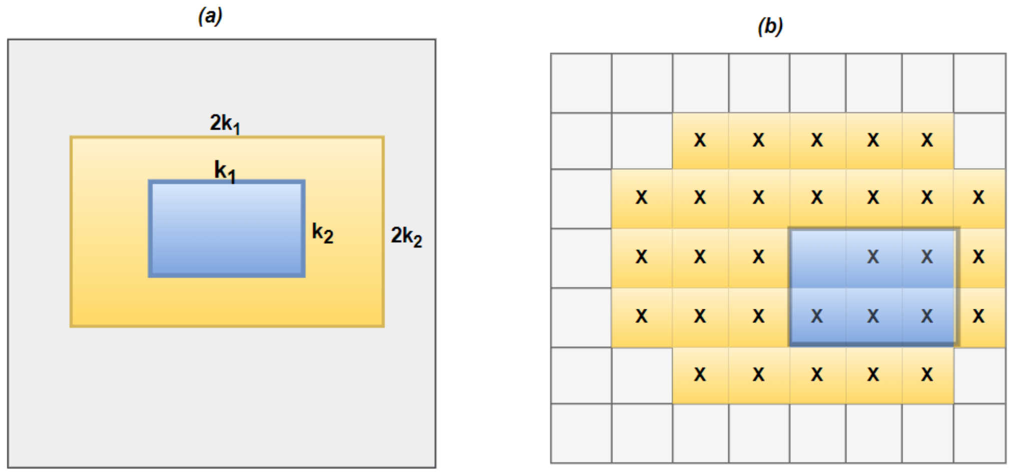
Excluded volume theory

- Analytic approximation technique to obtain percolation threshold $\boldsymbol{\phi_c}$ **(Critical density of occupied sites).**

- **Excluded volume theory :** Product of number density of basic percolating units and average excluded volume is an invariant quantity for similar systems at criticality (Balberg et.al 1984, Balberg 1987).

$$n_c V_{ex} = B_c$$

- **n=η/V** gives : $\phi_c = 1 - \exp(-B_c \frac{V}{Vex})$



Excluded area/volume is a connectedness factor in lattice systems

V_{ex}(Continuum)=$\mathbf{4k_1k_2}$

V_{ex}(Lattice)= $\mathbf{(2k_1+1)(2k_2+1)-5}$

Lattice version of excluded volume theory predictions

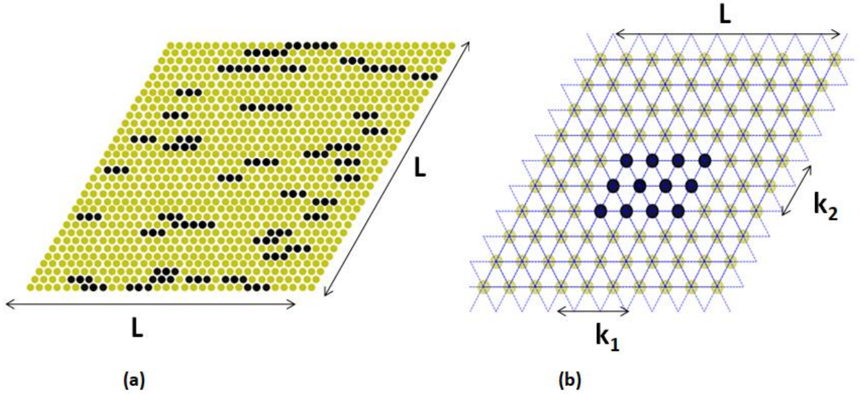
- For aligned rectangles :

$$\phi_c^{k_1,k_2} \approx 1 - exp(-B_c \frac{k_1 k_2}{(2k_1+1)(2k_2+1)-5})$$

- Theory predicts :
  - For width k_2=1 , threshold is monotonically decreasing with k_1.
  - For width k_2=2, threshold is a constant.
  - For width k_2=3, threshold is monotonically increasing with k_1.

For aligned rectangles of width 2, threshold is independent of its length!

- Theory predicts similar results for triangular lattice as well :
  - For width k_2=1, threshold is a constant.
  - For width k_2=2, threshold is monotonically increasing



Excluded volume theory results for various shapes

Shape	Lattice	CCVF ϕ_c from discrete excluded volume theory	Limiting Values of ϕ_c
Rectangles of size $k_1 \times k_2$	2D Square	$1-\exp\left(-B_c\frac{k_1k_2}{(2k_1+1)(2k_2+1)-5}\right)$	$1-\exp\left(-B_c\frac{k_2}{4k_2+2}\right)$ $(k_1\to\infty$, finite $k_2)$
Squares $(k_1 = k_2 = k)$	2D Square	$1-\exp\left(-B_c\frac{k^2}{(2k+1)^2-5}\right)$	0.6667 $(k\to\infty)$, $B_c = 4.3953711(5)$
Diamonds of linear size k	$2D$ Square	$1-\exp\left(-B_c\frac{k^2+1}{4k(k+1)}\right)$	$1-\exp\left(-B_c/4\right)$ $(k\to\infty)$
Cubes $(k_1 = k_2 = k_3 = k)$	3D Cubic	$1-\exp\left(-B_c\frac{k^3}{(2k-1)^3+6(2k-1)^2-1}\right)$	0.2773 $(k\to\infty)$, $B_c = 2.5978(5)$
Sticks of length k_1	3D Cubic	$1-\exp\left(-B_c\frac{k_1}{5(2k_1-1)+1}\right)$	0.22877 $(k_1\to\infty)$, $B_c = 2.5978(5)$
Parallelograms of size $k_1 \times k_2$	2D Triangular	$1-\exp\left(-B_c\frac{k_1k_2}{(2k_1+1)(2k_2+1)-3}\right)$	$1-\exp\left(-B_c\frac{k_2}{4k_2+2}\right)$ $(k_1\to\infty$, finite $k_2)$

Limiting values are finite

Some interesting predictions of excluded volume theory

- Length independence of threshold (k_2=2) can be extended to higher dimensions.(Hyper cuboids in d-dimensions, for e.g. in 3-dim k_2=2 and k_3=4)

- Define a parameter $s = \frac{|n_v - n_h|}{|n_v + n_h|}$ for fraction of rectangles having mixed orientation.(Tarasevich et.al 2012)

- s=1(fully aligned), s=0(isotropic).

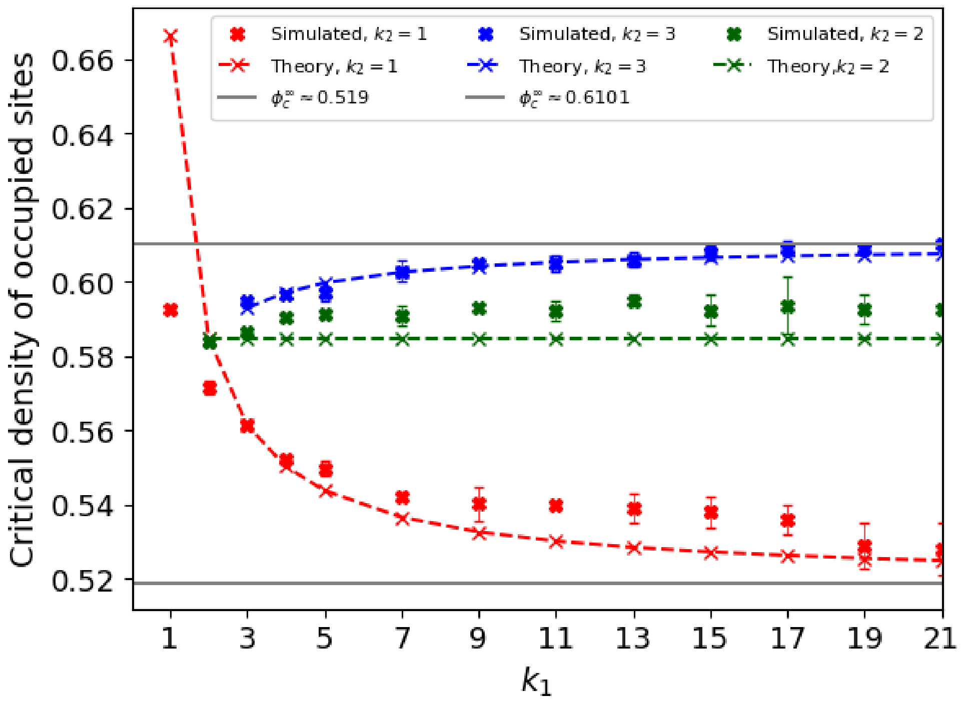
- s-dependent expression for excluded volume:

$$V_{ex} = \left(\frac{1+s}{2}\right)^2((2k_1+1)(2k_2+1)-5) + \left(\frac{1-s}{2}\right)^2((2k_1+1)(2k_2+1)-5) + \frac{1-s^2}{4}((k_1+k_2+1)^2-4) + \frac{1-s^2}{4}((k_1+k_2+1)^2-4)$$

- For all s<1 and for large k_1 , ϕ_c always monotonically decreases. S=1 trends are unique

Simulation studies

- Percolation probability vs density of occupied sites is obtained for various system sizes.
- Threshold calculated for increasing values of k_1 for particular width k_2.
- Width dependent trends in threshold



Scaling relation for threshold determination:

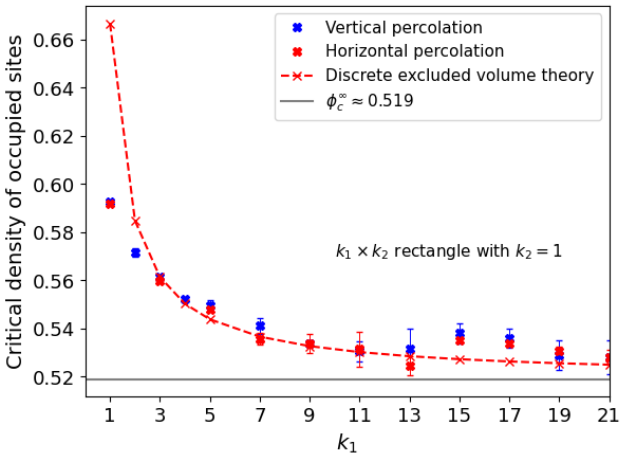
$$\phi_c(L)=B*\Delta(L)+\phi_c(\infty).$$

K_2=1, ϕ_c monotonically decreases.

K_2=2, ϕ_c is nearly a constant.

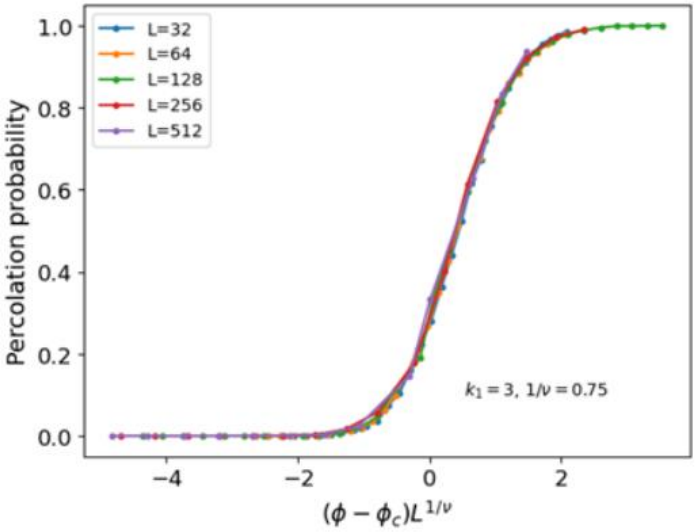
K_2=3, ϕ_c monotonically increases.

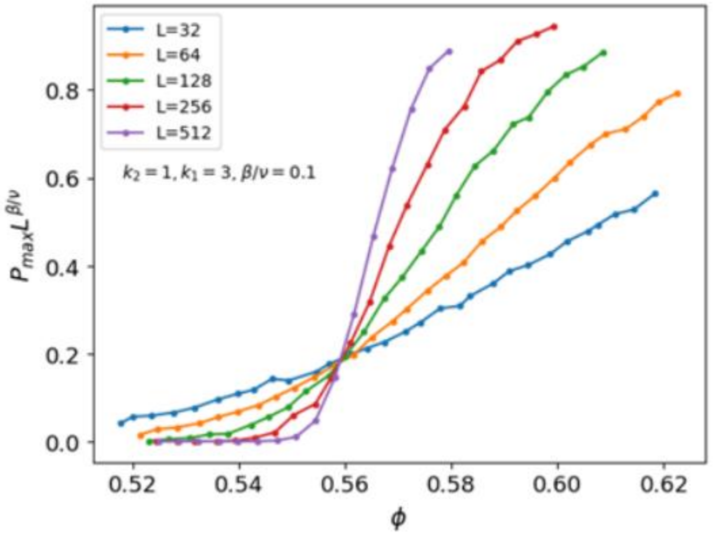
Some related findings…



- Model of aligned rectangles show isotropy in threshold.
- Model belongs to standard percolation universality class.
- Increase of rectangle alignment(s-parameter) leads to increase of threshold.

$P(\varphi) = f((\varphi - \varphi_c)L^{1/\nu})$ $\quad P_{max}(\varphi) = L^{-\beta/\nu}F((\varphi - \varphi_c)L^{1/\nu})$





Exponents:

β≈0.133
ν≈1.33
σ≈0.3948
γ≈2.36
τ≈2.05

Continuum limit of lattice models

- Limiting value **ϕ_c ($k \to \infty$)** from discrete excluded volume theory.

- Previous studies for symmetric shapes suggests : **Continuum percolation of aligned objects can be regarded as a limit of corresponding discrete model.** (Koza et.al 2016)

- Special limiting case ($k_1 \to \infty, k_2$=const) is finite and different from continuum threshold of rectangles.

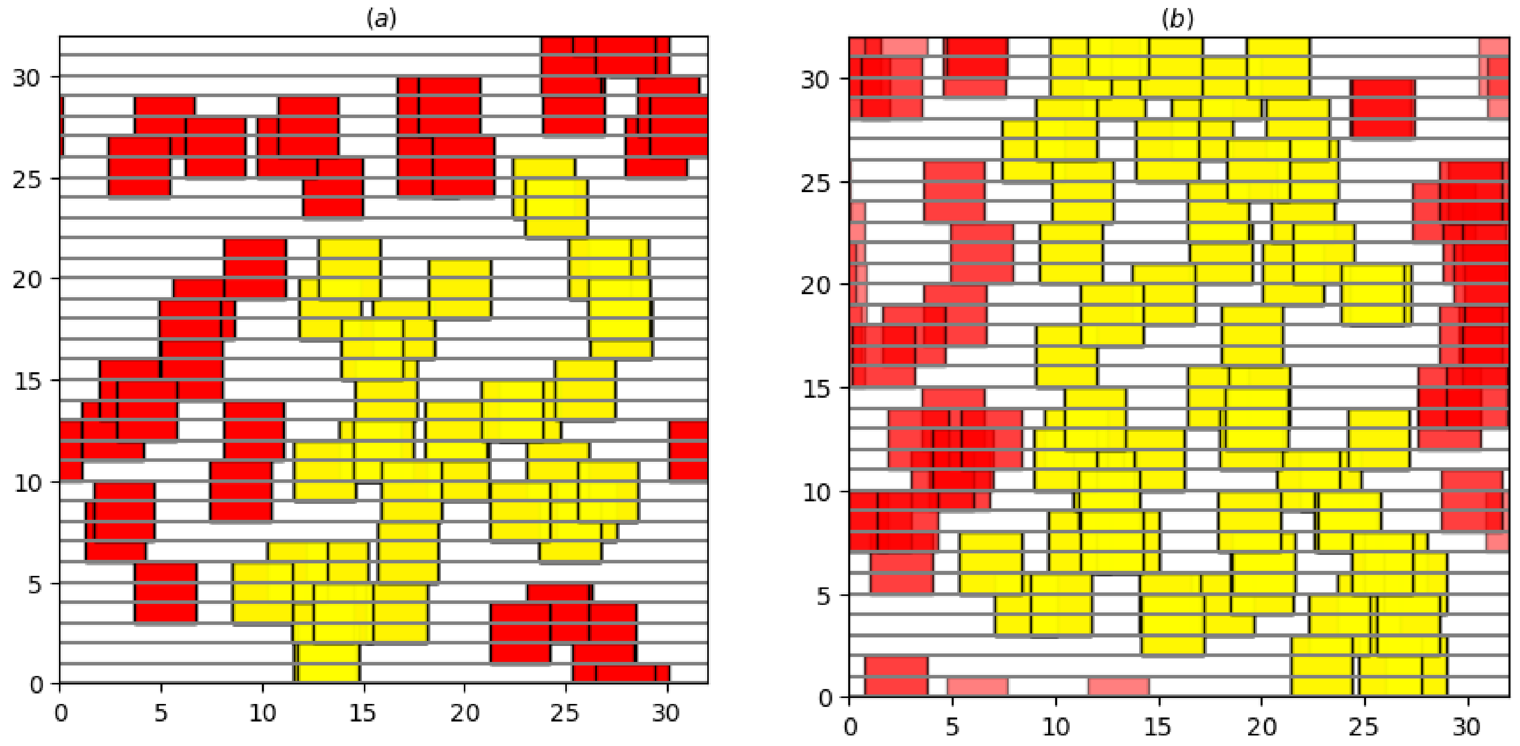
$$\phi_c^{k_1 \to \infty, k_2} \approx 1 - exp\left(-B_c \frac{k_2}{2(2k_2+1)}\right)$$

- Lattice spacing tending to zero in only one direction.

- A **semi continuum model** can be introduced as the continuum analogue of special limiting case.

Overlapping objects in lanes / Semi continuum models

- ❑ Objects in lanes have continuous x-coordinates, discrete y-coordinates.
- ❑ Object width as integer multiple of lane width.



Objects of width 3 in lanes

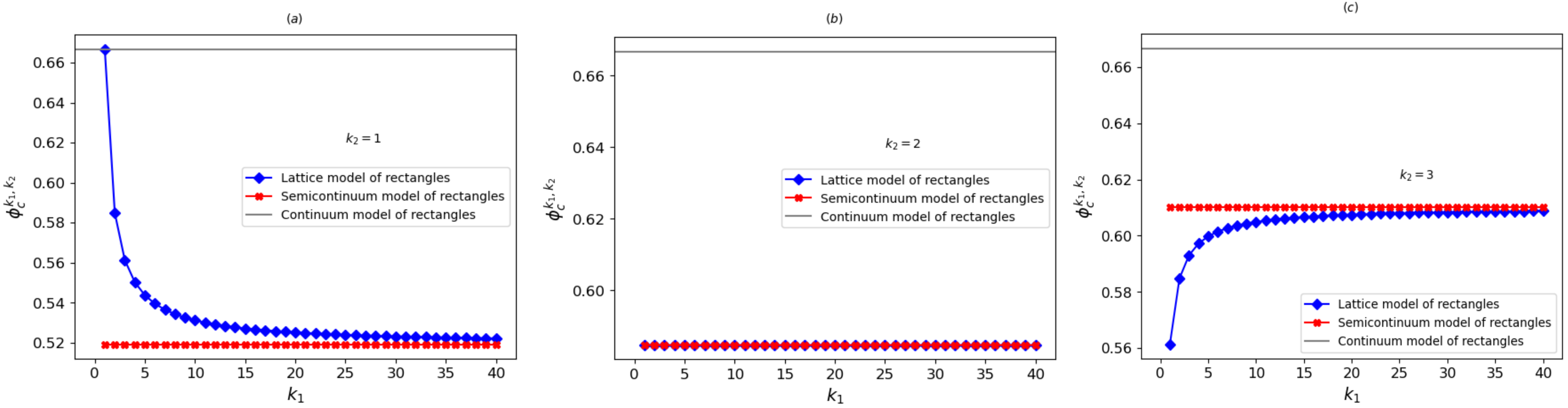
No restriction on overlapping in x-direction. Objects that overlap or share edges are connected.

Excluded volume V_{ex}:

$$2k_1(2k_2+1)$$

Theory predictions : A comparison

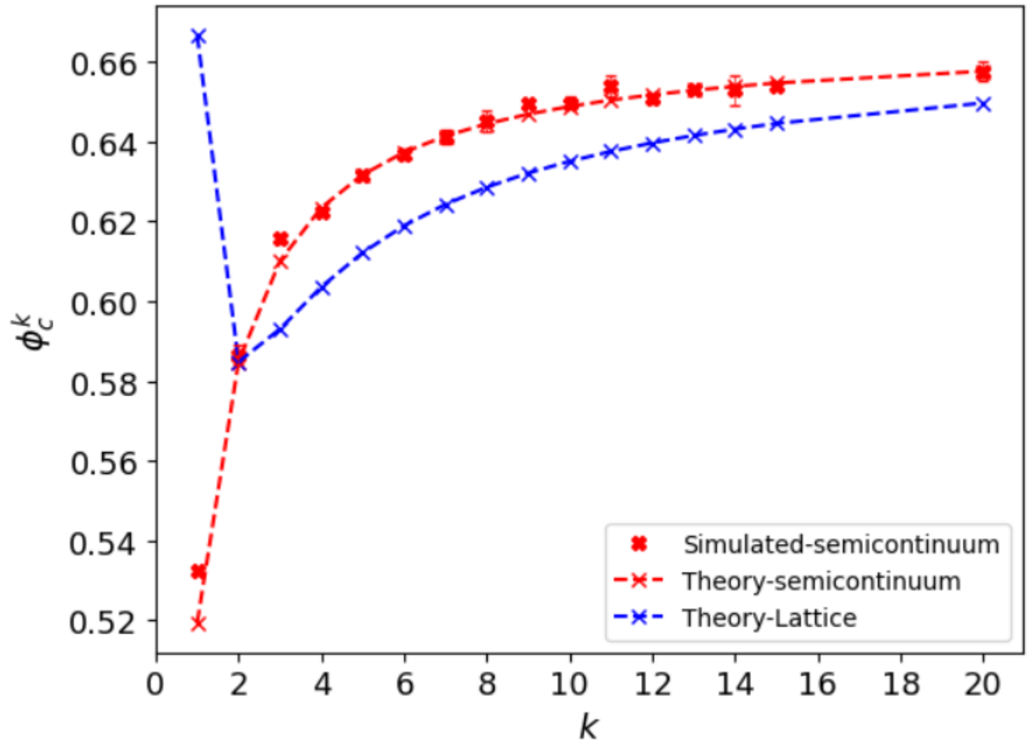
- Semi continuum model of rectangles : Width dependent phenomena is observed.



- Threshold is independent of length k_1 for a particular width k_2.

A comparison for overlapping squares in lanes

- Comparison between theory predictions for overlapping square model in lattice and semi continuum



Lattice model :
Non monotonic

Semi continuum model:
Monotonic increase

Conclusions

- Lattice version of excluded volume theory yield predictions of higher accuracy for aligned overlapping objects on lattices.
- Shape anisotropy leads to width dependent trends in percolation threshold of systems.
- Similar trends can be obtained for anisotropic shapes on other lattices and dimensions.
- Width dependent trends are unique for s=1(fully aligned) cases.
- For shape anisotropic objects, special limiting case ($k_1 \to \infty$, k_2= const) appears as semi continuum model.
- Semi continuum models show a width dependent phenomena.

Reference : Jasna C K, V. Sasidevan. Effect of shape asymmetry on percolation of aligned and overlapping objects on lattices. Preprint. arXiv : 2308.12932

Thank You…