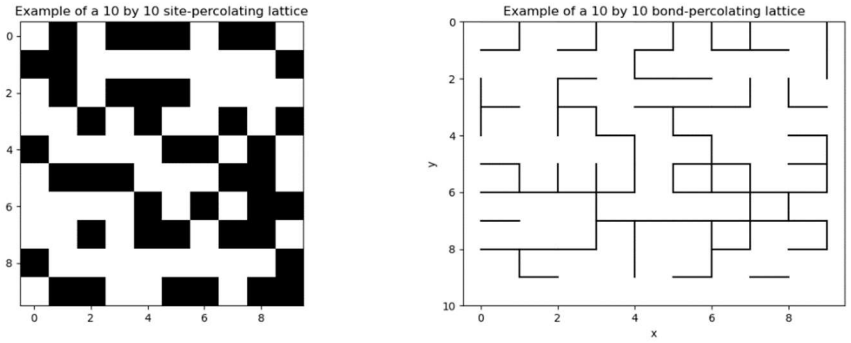
Simulating Percolation through Monte Carlo Methods

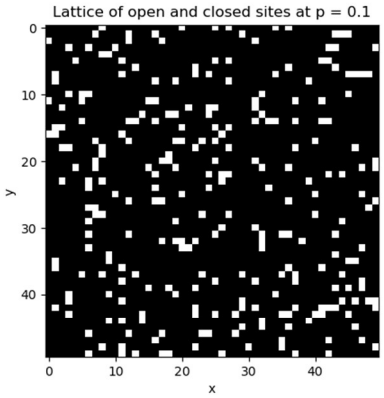
Percolations theories study porous materials and how different particles or liquids behave under this medium. Although there are many different types of percolation models, this report will investigate site percolation and bond percolation, focusing on site percolation problems. Site percolation can be imagined with a lattice of multiple sites [1] (Figure 1). Each site on the lattice has a probability (p) of being "open" and probability (1-p) of being "closed". An open site allows particles to go through and reside in its space, while a closed site is a solid barrier. Bond percolations are similar in theory, except paths are categorized instead of sites (Figure 1). Each site has potential paths to its neighboring site, and these paths are "open" with probability p and "closed" with probability (1-p).

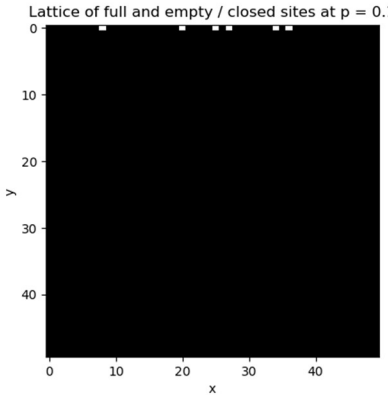


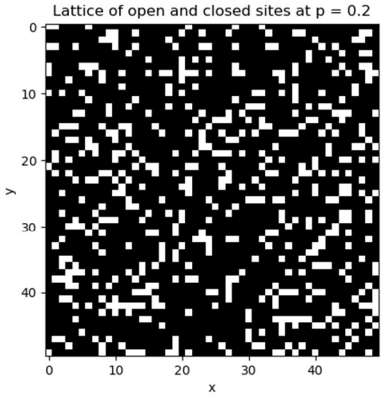
(Figure 1. Left figure shows an example of site percolation. Each black square is a closed site, and each white square is an open site. Right figure shows an example of bond percolation. Each dark line shows an open bond, and the absence of lines indicate a closed bond.)

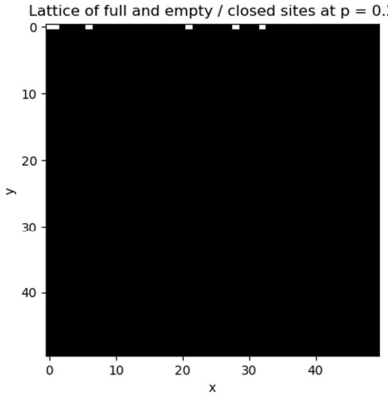
Site-percolation is ideal for modelling sinking water. For instance, given a few parameters, one can determine the likelihood of water permeating the soil to reach the crops' roots or the phase transition of superconductors [2]. The water-sinking phenomenon is computationally simulated below. The question raised is rather simple: with a material that has an occupation probability of p, what is the probability that water from the top layer can flow to the bottom?

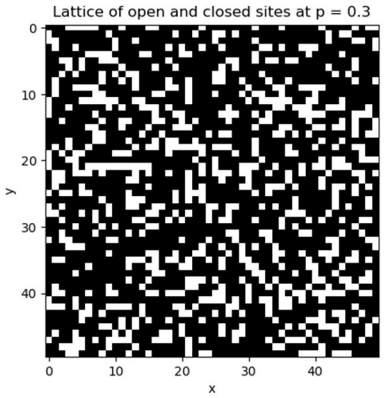
The program conducts Monte Carlo simulations using recursive programming. As a result, the simulation can "follow" the water flow by recursively checking its neighboring sites for openness. The downside to this method is that Python 3.8 has a small recursion depth limit, hence the program is unable to simulate site clusters that are too large. However, the depth limit is a minor issue for the purposes of this report, as it is capable of simulating sufficiently large lattices at 150 by 150. The program simulates percolation and plots the lattices (Figure 2).

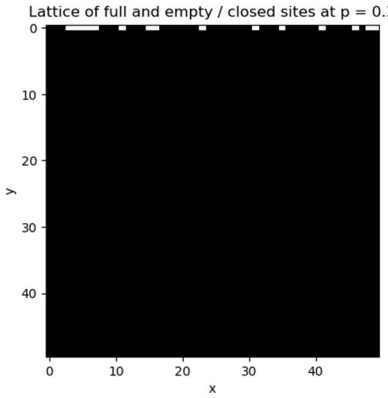

Lattice of open and closed sites at p = 0.1
0
10
20
30
40
y
0
10
20
30
40
x

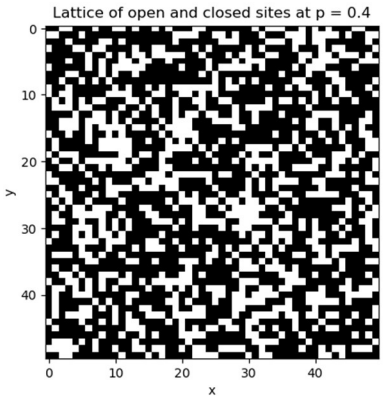

Lattice of full and empty / closed sites at p = 0.1
0
10
20
30
40
y
0
10
20
30
40
x

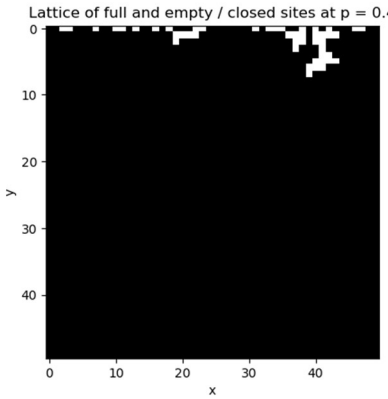

Lattice of open and closed sites at p = 0.2
0
10
20
30
40
y
0
10
20
30
40
x

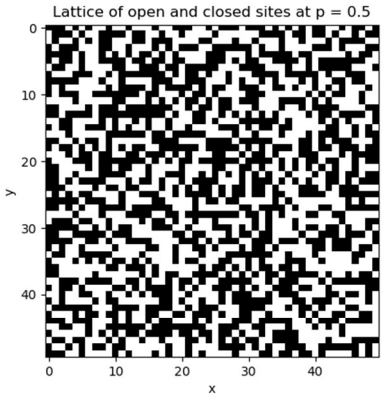

Lattice of full and empty / closed sites at p = 0.2
0
10
20
30
40
y
0
10
20
30
40
x

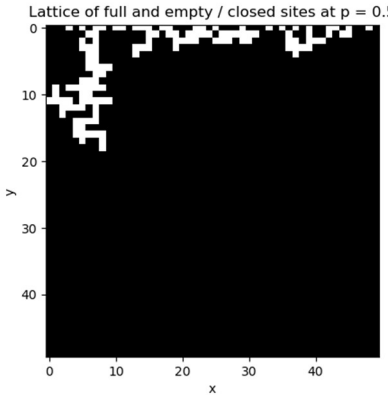

Lattice of open and closed sites at p = 0.3
0
10
20
30
40
y
0
10
20
30
40
x

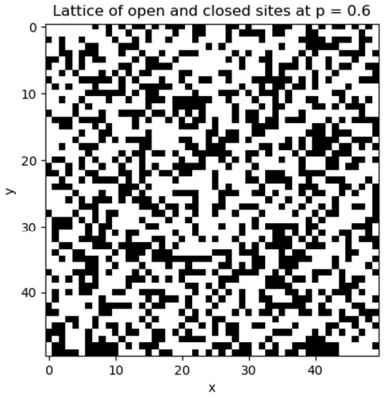

Lattice of full and empty / closed sites at p = 0.3
0
10
20
30
40
y
0
10
20
30
40
x

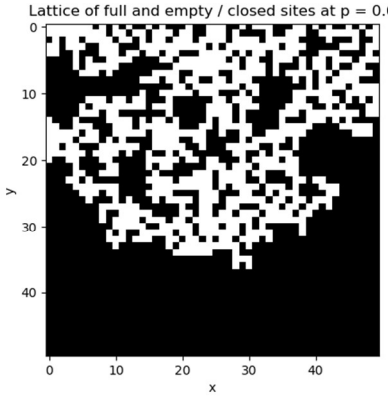

Lattice of open and closed sites at p = 0.4
0
10
20
30
40
y
0
10
20
30
40
x

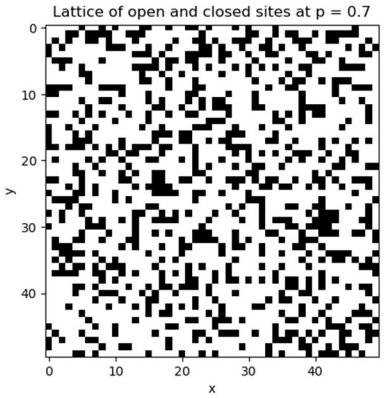

Lattice of full and empty / closed sites at p = 0.4
0
10
20
30
40
y
0
10
20
30
40
x

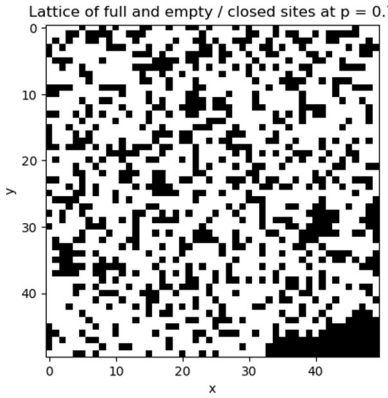

Lattice of open and closed sites at p = 0.5
y
x

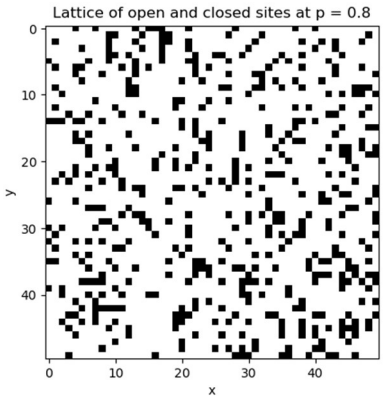

Lattice of full and empty / closed sites at p = 0.5
y
x

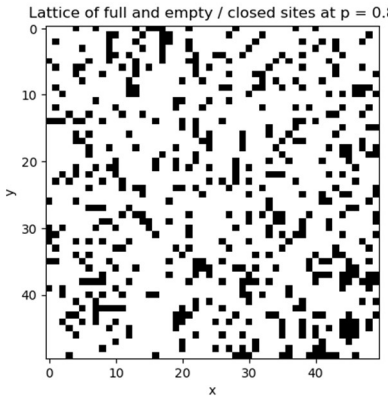

Lattice of open and closed sites at p = 0.6
y
x


Lattice of full and empty / closed sites at p = 0.6
y
x


Lattice of open and closed sites at p = 0.7
y
x

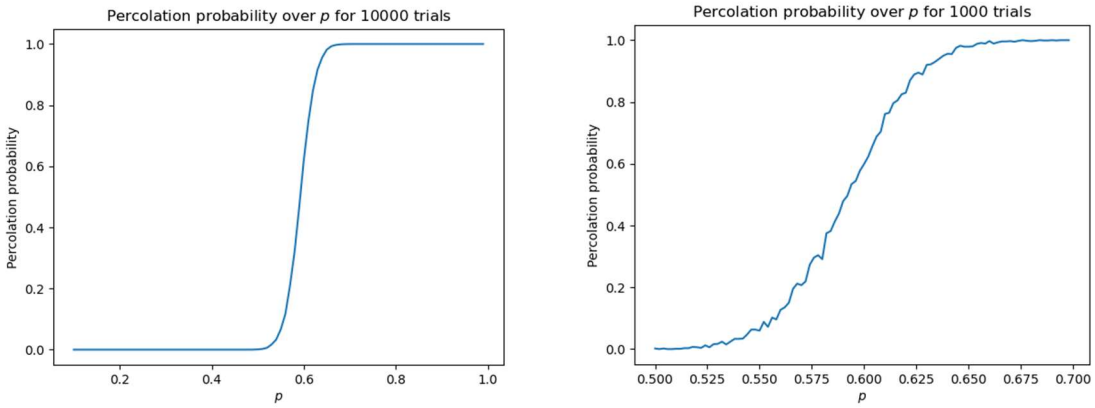

Lattice of full and empty / closed sites at p = 0.7
y
x


Lattice of open and closed sites at p = 0.8
y
x


Lattice of full and empty / closed sites at p = 0.8
y
x

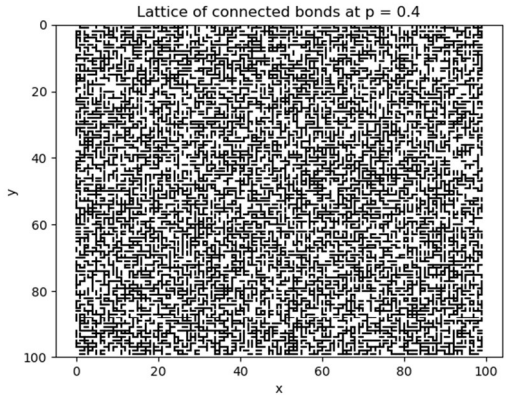
(Figure 2. The above figure shows simulation of site percolation with a variety of occupational probability p. The left diagrams show randomly generated lattices, where white squares are open and black squares are closed. The right diagrams show behaviour of water that enters from open sites on the top edge. White squares are open and filled sites, and black squares are closed or empty sites.)

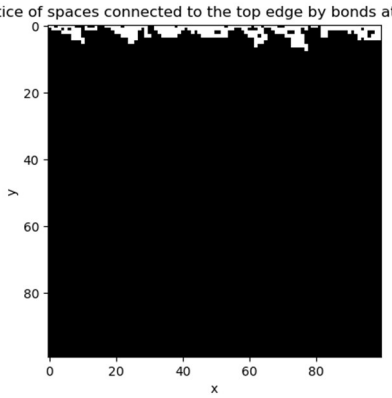
Intuitively, the material is more permeable when the probability of an open site is larger, making the medium more "porous". As a result, water is more likely to reach the bottom of the lattice. Furthermore, the system seemingly transitions from non-percolating to percolating between p=0.5 and p=0.7. Theoretically, the phase transition should be at approximately p=0.5925 [4]. This number can be numerically estimated below using the program. Initially all simulations result in no percolation, while, eventually, every simulation percolates. Hence, the phase transition can be estimated at around p=5.9, which corresponds to the literature (Figure 3).

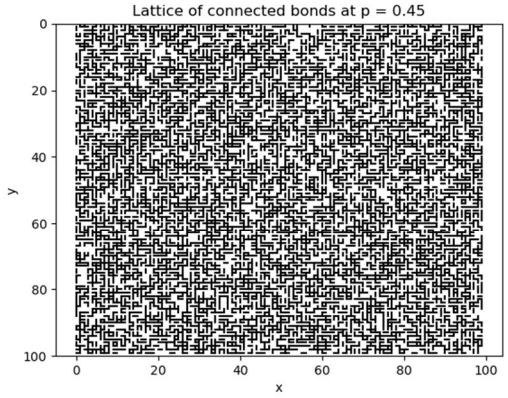


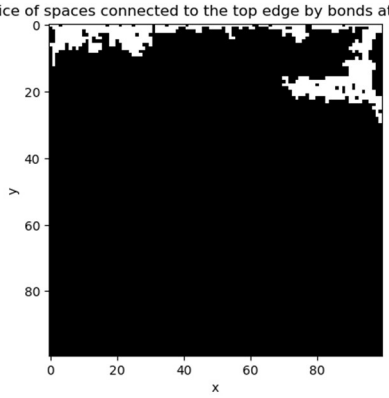
(Figure 3. The probability of water percolating over 10000 and 1000 trials is plotted in this figure.)

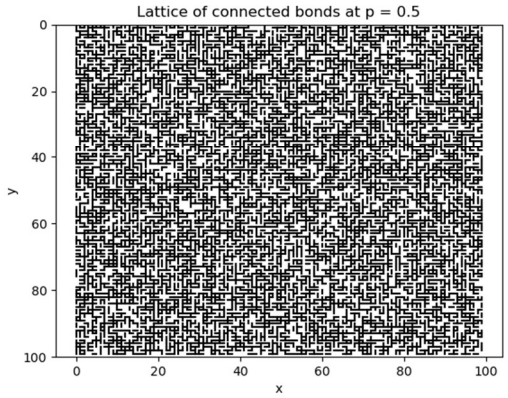
Although bond percolation is similar in theory, its computational method is drastically different, which is reflected through its program. The program requires one to store information of the bonds instead of the sites. However, the phenomenon observed in this scenario replicates that of site percolation (Figure 4). Percolation is more likely with lower p, and the material becomes more porous.

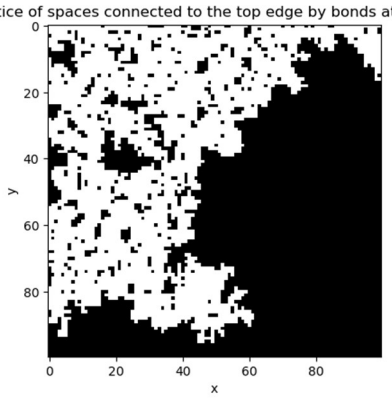

Lattice of connected bonds at p = 0.4
y
x

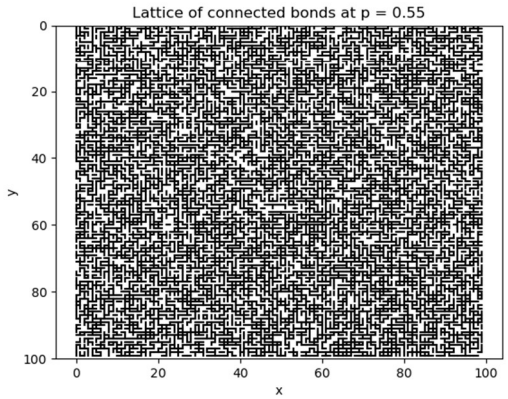

Lattice of spaces connected to the top edge by bonds at p = 0.4
y
x

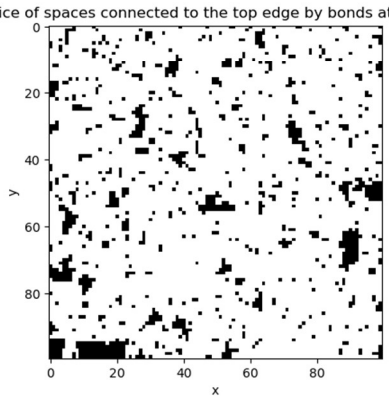

Lattice of connected bonds at p = 0.45
y
x


Lattice of spaces connected to the top edge by bonds at p = 0.45
y
x


Lattice of connected bonds at p = 0.5
y
x

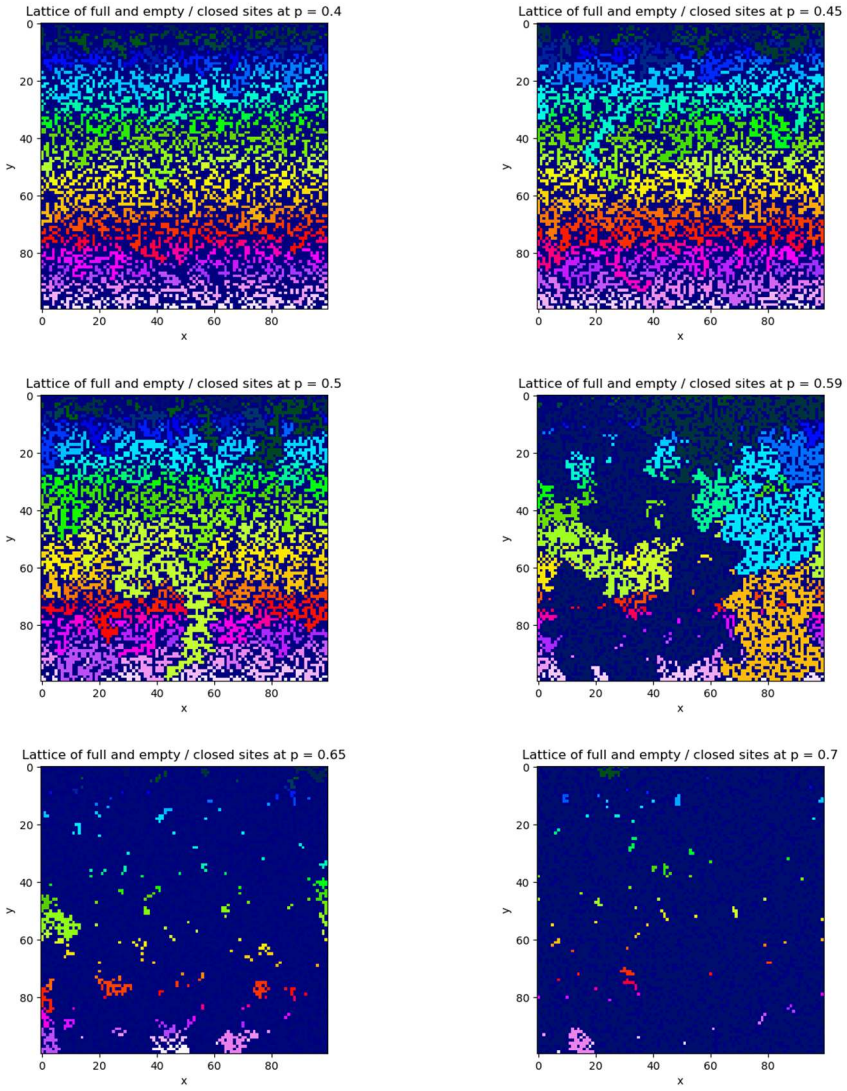

Lattice of spaces connected to the top edge by bonds at p = 0.5
y
x


Lattice of connected bonds at p = 0.55
y
x


Lattice of spaces connected to the top edge by bonds at p = 0.55
y
x

(Figure 4. The above figure shows simulation of bond percolation with a variety of occupational probability p. The left diagrams show randomly generated lattices, where dark lines are open and connected bonds. The right diagrams show behaviour of water that is only allowed to cross connected bonds when it enters from the top edge. White squares sites where water resides.)

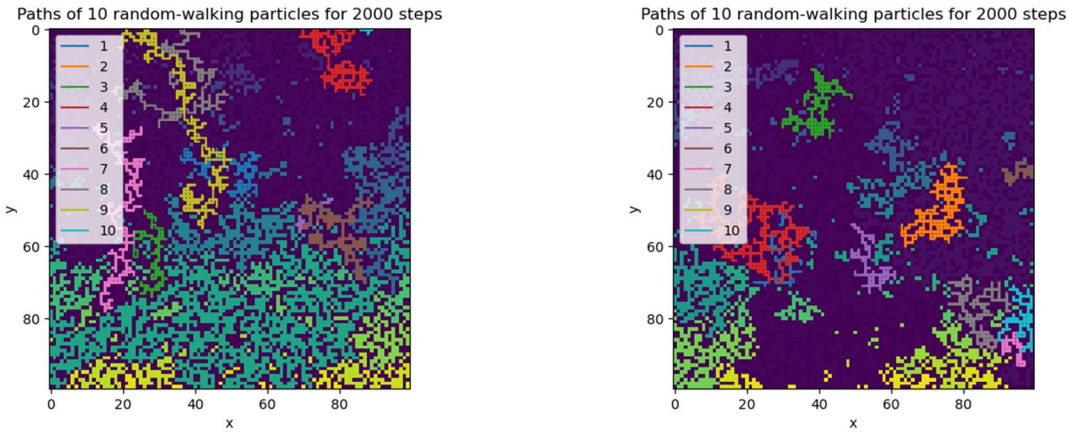
Cluster shapes and sizes are also topics of interest for percolation theories. Each cluster is a group of connected sites. As one might expect, the number of clusters and their sizes are subject to variations under different occupational probabilities. These concepts are able to model the physical world, where glasses shatter in varying sizes depending on the strength of its molecular bonds; therefore, humans can applicably create safety glasses that shatter in tiny pieces when p is small [2].



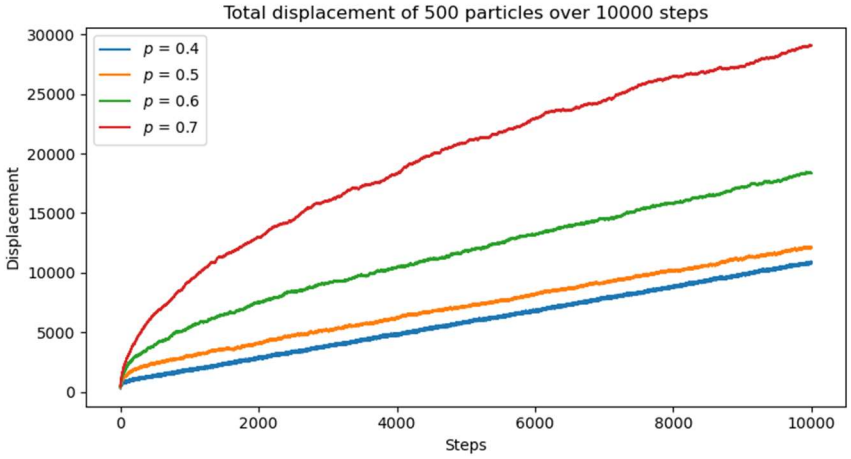
(Figure 5. Each lattice has different clusters that are represented by different colours. Occupational probability increases from the top left to the bottom right.)

Figure 5 categorizes clusters using colours. When p is small, there are many clusters in the lattice, and each of which has a small area. When p is large, there is one large spanning cluster, with other clusters. The rainbow effect in small p values indicate that the clusters are small because the colour corresponds to the cluster ID. Since the program reads the sites from top left to bottom right, the cluster ID increases regularly to go through the colour map, as these sites are often new clusters that require a new cluster ID.

Random-walk particle diffusion can be simulated in percolation clusters. When particles that are subject to Brownian motion reside in a porous medium, its diffusion around the environment is an important observation [5].



(Figure 6. Above are two simulations of 10 particles that navigate through random clusters in Brownian motion. Each line is the path of a random-walking particle)



(Figure 7. The figure shows total displacement of 500 random-walking particles under varying occupational probabilities)

Figure 6 shows the motion of random-walking particles when they are in porous materials. The closed sites act as barriers that obstruct diffusion. A simulation of many particles over a large number of steps show the distinctive features of movements under different

occupational probabilities (Figure 7). The total displacement of the particles over time is significantly higher with lower p, since cluster sizes are larger, providing each particle with a larger area to move within. Additionally, the difference in total displacement between p=0.4 and p=0.5 is significantly smaller than that between p=0.6 and p=0.7. This phenomenon is explained by the phase transition, where large clusters combine after the threshold of p=0.5925, resulting in a high probability that each random particle is dropped into a large cluster.

References

1. Stauffer, D., & Aharony, A. (2018). Introduction to percolation theory. CRC press.
2. Sahini, M., & Sahimi, M. (2003). Applications of percolation theory. CRC Press.
3. Mastering recursive programming. (n.d.). Retrieved from https://developer.ibm.com/technologies/linux/articles/l-recurs
4. Van den Berg, J. (1981). Percolation theory on pairs of matching lattices. Journal of Mathematical Physics, 22(1), 152-157.
5. Havlin, S., & Ben-Avraham, D. (1987). Diffusion in disordered media. Advances in physics, 36(6), 695-798.