Percolation by a class of ballistic deposition and their universality classes

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I would like to dedicate this thesis to my loving parents ...

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 65,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 150 figures.

Muhammad Shahnoor Rahman
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Acknowledgements

And I would like to acknowledge ...

Abstract

This is where you write your abstract ...

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Chapter 1

Introduction

Percolation is one of the most studied problems in statistical physics. Its idea was first conceived by Paul Flory in the early 1940s in the context of gelation in polymers. Later, in 1957 it acquires the mathematical formulation due to the work of engineer Simon Broadbent and mathematician John Hammersley. Ever since then percolation theory has been studied extensively by scientists in general and physicits in particular.

1.1 Motivation and Objective

1.2 Method of Study

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Chapter 2

Scaling, Scale-Invariance and Self-Similarity

In physics we observe a natural phenomena and try to understand it using the existing knowledge. To do this we need to assign numbers to the observable quantities. If we can express it in numbers only then we can say we have acquired some knowledge about that quantity. And if we cannot do this then our knowledge is not complete about that quantity. This reveals the fact that physics is all about observation and measurement of physical quantities with the desire to acquire some knowledge about it and then use that knowledge to predict something that is yet to observe. For example, Albert Einstein predicted the existence of gravitational waves in 1916 in his general theory of relativity and the first direct observation of gravitational waves was made on 14 September 2015 and was announced by the LIGO and Virgo collaborations on 11 February 2016. Now, in order to understand the observation of a natural or artificial phenomena we need some tools. Since here we are trying to understand phase transition, finite size scaling (FSS) hypothesis is a great tool for the investigation. In this chapter we will try to understand the fundamentals which is based on Buckingham π theorem, self similarity and homogeneous functions.

2.1 Dimensions of Physical Quantity

In order to express physical quantities in terms of numbers we need a unit of measurement, since a number times unit tells us how much the quantity is larger or smaller with respect to the unit. The units of measurement are described as fundamental and derivative ones. The fundamental units of measurement are defined arbitrarily in the form of certain standards, while the derivative ones are obtained from the fundamental units of measurement by virtue

of the definition of physical quantities, which are always indications of conceptual method of measuring them. An example involving fundamental and derivative unit of measurement is velocity. Since velocity is measured by how much distance an object travels per unit time, the unit of velocity is the ratio of distance or length over time. It is expressed as $[v] = LT^{-1}$, where L is the unit of length and T is the unit of time. The unit of length and time are fundamental here and the unit of velocity is the derivative of these two. A system of units of measurement is a set of fundamental units of measurement sufficient to measure the properties of the class of phenomena under consideration. For example the *CGS* system where length is measurement in terms of centimeter, mass is measured in terms of gram and the *SI* system where the mass is measured in terms of kilogram, length is measured in terms of meter and in both system time is measured in terms of second.

Dimension of physical quantity determines by what amount the numerical value must be changed if we want to go to another system of units of measurement. For instance, if the unit of length is decreased by a factor L and the unit of time is decreased by a factor T, the unit of velocity is smaller by the factor of LT^{-1} than the original unit, so the numerical value of velocity would scaled up by a factor of LT^{-1} owing to the definition of equivalence.
The changes in the numerical values of physical quantities upon passage from one systems of units of measurement to another within the same class are determined by their dimensions. The functions that determines the factor by which the numerical value of a physical quantity changes upon transition from systems of unit of measurement to another system within a given class is called the dimension function or, the dimension of that physical quantity.We emphasize that the dimension of a given physical quantity is different in different classes of systems of units. For example, the dimension of density I in the MLT class is $[\rho] = ML^{-3}$ whereas in the FLT class it is $[\rho] = FL^{-4}T^{-2}$ [3, 86].

2.2 Buckingham π Theorem

A part of physics is about modeling physical phenomenon. And while doing it, the first thing is to identify the relevant variables, and then relate them using known physical laws. For simple phenomenon this task is not hard since it involves deriving some quantitative relationship among the physical variables from the first principles. But when dealing with complex systems we need a systematic way of dealing with the problem of reducing number of parameters. In these situations constructing a model in a systematic manners with minimum input parameters that can help analyzing experimental results has been a useful method. One of the simplest way is based on dimensional analysis. Its function is to reduce a

large number of parameters into a manageable set of parameters. Buckingham π theorem is one of the most suitable and studied mathematical process to deal with this kind of problems.

Buckingham π theorem describes dimensionless variables obtained from the power products of governing parameters denoted by $\Pi_1, \Pi_2, \ldots$ etc. When investigating a certain dimensional physical quantity (governed) that depend on other n dimensional variables then this theorem provide us a systematic way to reduce the degrees of freedom of a function. Using this theorem we reduce a function of n variables problems into a function of k dimensionless variable problem if each of the k dimensional variable of original n variables can be expressed in terms of the $n-k$ dimensionally independent variable [25].

The relationship found in physical theories or experiments can always be represented in the form

$$a = f(a_1, a_2, \ldots, a_n) \tag{2.1}$$

where the quantities $a_1, a_2, \ldots, a_n$ are called the governing parameters. It is always possible to classify the governing parameters a_i's into two groups using the definition of the dependent and independent variables. Let the arguments $a_{k+1}, \ldots, a_n$ have the independent dimensions and the dimensions of the arguments $a_1, a_2, \ldots, a_k$ can be expressed in terms of the dimensions of the governing independent parameters $a_{k+1}, \ldots, a_n$ in the following way

$$\begin{aligned}
[a_1] &= [a_{k+1}]^{\alpha_1} \ldots [a_n]^{\gamma_1} \\
[a_2] &= [a_{k+1}]^{\alpha_2} \ldots [a_n]^{\gamma_2} && (2.2) \\
&\vdots && (2.3) \\
[a_k] &= [a_{k+1}]^{\alpha_k} \ldots [a_n]^{\gamma_k}
\end{aligned}$$

The dimension of the governed parameter a must also be expressible in terms of the dimensionally independent governing parameters $a_1, \ldots, a_k$ since a does not have independent dimension and hence we can write

$$[a] = [a_{k+1}]^{\alpha} \ldots [a_n]^{\gamma} \tag{2.4}$$

Thus, there exist number α, γ such that 2.4 holds. We have set of governing parameters.

$$\Pi_1 = \frac{a_1}{[a_{k+1}]^{\alpha_1} \dots [a_n]^{\gamma_1}} \tag{2.5}$$

$$\Pi_2 = \frac{a_2}{[a_{k+1}]^{\alpha_2} \dots [a_n]^{\gamma_2}} \tag{2.6}$$

$$\vdots \tag{2.7}$$

$$\Pi_k = \frac{a_k}{[a_{k+1}]^{\alpha_k} \dots [a_n]^{\gamma_k}} \tag{2.8}$$

and a dimensionless governed parameter

$$\begin{aligned} \Pi &= \frac{a}{[a_{k+1}]^{\alpha} \dots [a_n]^{\gamma}} \\ &= \frac{f(\Pi_1, \dots \Pi_k, a_{k+1}, \dots, a_n)}{[a_{k+1}]^{\alpha} \dots [a_n]^{\gamma}} \end{aligned} \tag{2.9}$$

The right hand side of equation 2.9 clearly reveals that the dimensionless quantity Π is a function of $a_{k+1}, \dots, a_n, \Pi_1, \dots, \Pi_k$, i.e.,

$$\Pi \equiv F(a_{k+1}, \dots, a_n, \Pi_1, \dots, \Pi_k) \tag{2.10}$$

The quantities $\Pi, \Pi_1, \dots, \Pi_k$ are obviously dimensionless, and hence upon transition from one system of unit to another inside a given class their numerical values must remain unchanged. At the same time, according to the above, one can pass to a system of units of measurement such that any of the parameters of $a_{k+1}, \dots, a_n$, say for example, a_{k+1}, is changed by an arbitrary factor, and the remaining ones are unchanged. Upon such transition the first argument of F is unchanged arbitrarily, and all other arguments of the function remain unchanged as well as its value Π. Hence, it follows $\frac{\delta F}{\delta_{a_{k+1}}} = 0$ and entirely analogously $\frac{\delta F}{\delta_{a_{k+2}}} = 0, \dots, \frac{\delta F}{\delta_{a_n}} = 0$. Therefore, the relation 2.10 is in fact represented by a function of k arguments and proves it is independent of $a_{k+1}, \dots, a_n$, that is,

$$\Pi = \Phi(\Pi_1, \dots, \Pi_k) \tag{2.11}$$

and the function f can be written in the following special form (by combining **??**)

$$f(a_1, \dots, a_k, \dots, a_n) = a_{k+1}^{\alpha} \dots a_n^{\gamma} \Phi(\Pi_1, \dots, \Pi_k) \tag{2.12}$$

equation 2.12 is known as the Buckingham Π theorem. It constitutes one of the central statements in dimensional analysis and has great bearings on scaling theory.

2.2.1 An Example

An explicit example using this theorem is needed for better understanding it's application. The simplest example that can describe basic features of Buckingham Π theorem is the area of a right triangle and Pythagorean theorem.
Consider a right triangle where three sides are of size a, b and c and for definiteness, the smaller of its acute angles θ. Assume that we are to measure the area S of the triangle. The area S can be written in the following form

$$S = S(a,b,c) \tag{2.13}$$

However, the definition of two governing parameters a and b can be expressed in terms of c alone since we have

$$[a] \sim [c] \text{ and } [b] \sim [c] \tag{2.14}$$

and so is true for the governed parameter S as we can write the dimensional relation $[S] \sim \left[c^2\right]$. We therefore can define two dimensionless parameters

$$\Pi_1 = \sin\theta = a/c \tag{2.15}$$

$$\Pi_2 = \cos\theta = b/c \tag{2.16}$$

and the dimensionless governed paremeter

$$\Pi = \frac{S}{c^2} = c^{-2} S(c\Pi_1, c\Pi_2, c) \equiv F(c, \Pi_1, \Pi_2) \tag{2.17}$$

Now it is possible to pass from one unit of measurement to another system of unit of measurement within the same class and upon such transition the arguments Π_1, Π_2 of the function F and the function itself remain unchanged. It implies that the function F is independent of c and hence we can write

$$\Pi = \phi(\Pi_1, \Pi_2) \tag{2.18}$$

However, Π_1 and Π_2 both depends on the dimensionless quantity θ and hence we can write

$$S = c^2 \phi(\theta) \tag{2.19}$$

where the scaling function $\phi(\theta)$ is universal in character. In order to further capture the significance of equation 2.19 we rewrite it as

$$\frac{S}{c^2} \sim \phi(\theta) \tag{2.20}$$

This result has far reaching consequences. For instance, consider that we have a right triangle of any arbitrary sides $a' \neq a$, $b' \neq b$ and $c' \neq c$ but have the same acute angle θ as before. This can be ensured by choosing an arbitrary point on the hypotenuse of the previous triangle and drop a perpendicular on the base b. Consider that the area of the new triangle is S' yet we will have

$$\frac{S}{c^2} = \frac{S'}{(c')^2} \tag{2.21}$$

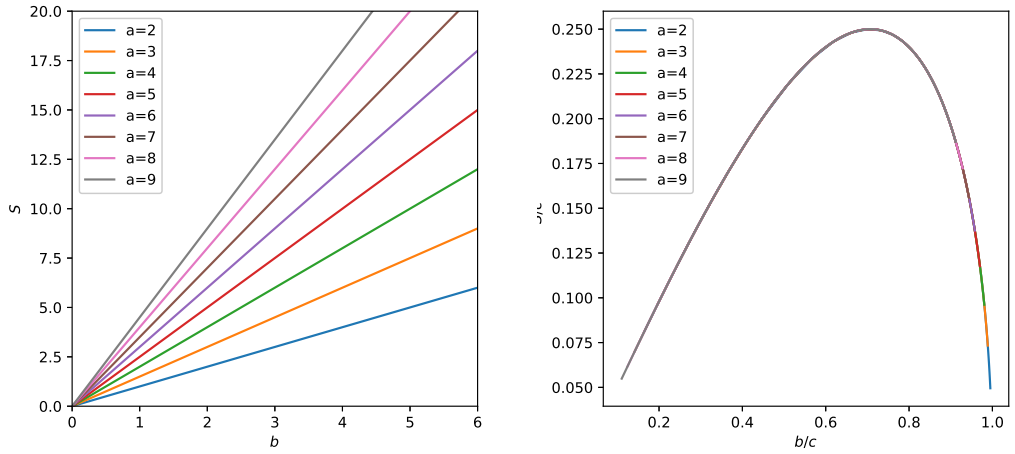
since the numerical value of the ratio of the area over the square of the hypotenuse depends on the angle θ. It implies that if we plot the ratio of the area over the square of the hypotenuse as a function θ all the data points should collapse onto a single curve regardless of the size of the hypotenuse and the respective areas of the right triangle. In fact, the details calculation reveals that

$$\phi(b/c) = \frac{1}{2}\sin\theta \tag{2.22}$$

This data collapse implies that if two or more right triangles which have one of the acute angle identical then such triangles are similar. We shall see later that whenever we will find data collapse between two different systems of the same phenomenon then it would mean that the corresponding systems or their underlying mechanisms are similar. Similarly, if we find that data collected from the whole system collapsed with similarly collected data from a suitably chosen part of the whole system then we can conclude that part is similar to the whole, implying self-similarity. On the other hand, if we have a set of data collected at many different times for a kinetic system and find they all collapse onto a single curve then we can say that the same system at different times are similar. However, similarity in this case is found of the same system at different times and hence we may coin it as temporal self-similarity.

2.3 Similarity and Self-Similarity

The concept of physical similarity is a natural generalization of the concept of similarity in geometry. For instance, two triangles are similar if they differ only in the numerical values of the dimensional parameters, i.e. the lengths of the sides, while the dimensionless parameters, the angles at the vertices are identical for the two triangles. Analogously,



(a) S vs b graph. b is the base of the triangle which is varied for a single θ.

(b) S/c^2 vs b/c graph. This each graph contains information about all triangle with a certain acute angle, meaning the entire graph contains information about every right triangle.

Fig. 2.1 Application of Buckingham Π theorem in a right triangle

physical phenomena are called similar if they differ only in their numerical values of the dimensional governing parameters; the values of the corresponding dimensionless parameters $\Pi_1, \ldots, \Pi_k$ are being identical. In connection with this definition of similar phenomena, the dimensionless quantities are called similarity parameters. The term *self-similarity* is, as the term itself suggests, a structure or process and a part of it appear to be similar to the whole when compared. This also means that a self-similar structure is infinite in theory. Therefore the fundamental principle of a self-similar structure is the repetition of a unit pattern on different scales.

2.3.1 An example

At this point a real world example will be helpful. Suppose we need to build an airplane. Obviously it's a billion dollar project. If we try to build the airplane directly without first building a prototype then we will wasting time, money and man power. Because we can not build an actual working airplane without following certain steps. First we need to build a small-scale model of the airplane. Then we need to test the model for performance. If it is satisfying then we can start building a prototype using the knowledge obtained from the

experimentation on the model. Here the model and the prototype are similar to each other. That's why this method works. Since only the dimensional parameters are scaled.

2.3.2 Diving Into Similarity

Let us consider two similar phenomena, one of which will be called the prototype and the other the model. For both phenomena there is some relation of the form

$$\alpha = f(a_1, a_2, a_3, b_1, b_2) \tag{2.23}$$

where the function f is the same for both cases by the definition of similar phenomena, but the numerical values of the governing parameters a_1, a_2, a_3, b_1, b_2 are different. Thus for prototype we have

$$\alpha_p = f(a_1^{(p)}, a_2^{(p)}, a_3^{(p)}, b_1^{(p)}, b_2^{(p)}) \tag{2.24}$$

and for model we have

$$\alpha_m = f(a_1^{(m)}, a_2^{(m)}, a_3^{(m)}, b_1^{(m)}, b_2^{(m)}) \tag{2.25}$$

where the index p denotes quantities related to the prototype and the index m denotes quantities related to the model. Consider that b_1 and b_2 are dependent variable and thus they are expressed in terms of a_1, a_2, a_3 in both model and prototype systems. Using dimensional analysis we find for both phenomena

$$\Pi^{(p)} = \Phi(\Pi_1^{(p)}, \Pi_2^{(p)}) \tag{2.26}$$

and

$$\Pi^{(m)} = \Phi(\Pi_1^{(m)}, \Pi_2^{(m)}) \tag{2.27}$$

where the function Φ must be the same for the model and the prototype. By the definition of similar phenomena the dimensional quantities must be identical in both the cases such as in the prototype and in the model, i.e.,

$$\Pi_1^{(m)} = \Pi_1^{(p)} \tag{2.28}$$

$$\Pi_2^{(m)} = \Pi_2^{(p)} \tag{2.29}$$

It also follows that the governed dimensionless parameter satisfies

$$\Pi^{(m)} = \Pi^{(p)} \tag{2.30}$$

Returning to dimensional variables, we get from the above equation

$$a_p = a_m \left(\frac{a_1^{(p)}}{a_1^{(m)}}\right)^{q_1} \left(\frac{a_2^{(p)}}{a_2^{(m)}}\right)^{q_2} \left(\frac{a_3^{(p)}}{a_3^{(m)}}\right)^{q_3} \tag{2.31}$$

which is a simple rule for recalculating the results of measurements on the similar model for the prototype, for which direct measurement may be difficult to carry out for one reason or another.

The conditions for similarity of the model to the prototype-equality of the similarity parameters Π_1, Π_2 for both phenomena show that it is necessary to choose the governing parameters $b_1^{(m)}, b_2^{(m)}$ of the model as to guarantee the similarity of the model to the prototype

$$b_1^{(m)} = b_1^{(p)} \left(\frac{a_1^{(m)}}{a_1^{(p)}}\right)^{\alpha_1} \left(\frac{a_2^{(m)}}{a_2^{(p)}}\right)^{\beta_1} \left(\frac{a_3^{(m)}}{a_3^{(p)}}\right)^{\gamma_1} \tag{2.32}$$

and

$$b_2^{(m)} = b_2^{(p)} \left(\frac{a_1^{(m)}}{a_1^{(p)}}\right)^{\alpha_2} \left(\frac{a_2^{(m)}}{a_2^{(p)}}\right)^{\beta_2} \left(\frac{a_3^{(m)}}{a_3^{(p)}}\right)^{\gamma_2} \tag{2.33}$$

whereas the model parameters $a_1^{(m)}, a_2^{(m)}, a_3^{(m)}$ can be chosen arbitrarily. The simple definitions and statements presented above describe the entire content of the theory of similarity.

2.3.3 Self-Similarity

A system is called self-similar When a small part of the system is similar to the whole system. A self similar structure is created by repetition of a unit pattern or a simple rule over different size scales [72]. Although the term "self-similarity" itself is explanatory, some example gives better insight.

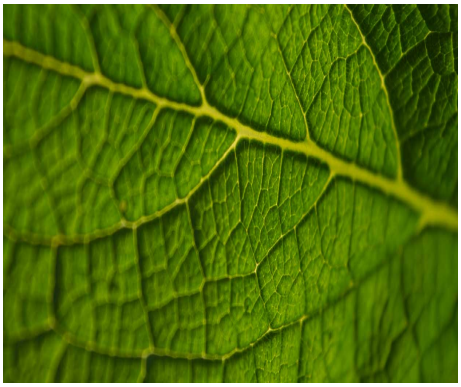
The cauliflower head contains branches or parts, which when removed and compared with the whole found to be very much the same except it is scaled down. These isolated branches can again be decomposed into smaller parts, which again look very similar to the whole as well as of the branches. Such self-similarity can easily be carried through for about three to four stages. After that the structures are too small to go for further dissection. Of course, from the mathematical point of view the property of self-similarity may be continued through an infinite stages though in real world such property sustain only a few stages 2.2.

There are plenty of other examples of self similarity in nature. Snowflakes exhibit self-similar branching patterns 2.3. The growth in aggregating colloidal particles are statistically self-similar. A leafless tree branches 2.3 in a self-similar fashion, each length splitting into

(a) A cauliflower

(b) Disection of cauliflower

Fig. 2.2 Self-Similarity in Cauliflower



(a) Leaf

(b) Snowflake

(c) Blood vessel

(d) Leafless Tree

Fig. 2.3 Self-Similarity examples

two or more branches. This branch pattern is repeated on smaller and smaller length scales till the tree top is reached. The veins of the leaves also branch in a self similar manner 2.3. The decimal number system is a construct that uses the idea of self-similarity. If we look a meter stick, we shall see that a decimeter range with its marks looks like a meter range with its marks, only smaller by a factor of 10. This pattern of meter stick makes it very easy to note readings. The human brain is also a complex network of neurons which organize in self-similar patterns. From quantum particle paths, lightning bolts, blood vessels 2.3, aggregation of bacteria all are example of self-similarity.

One thing must be mentioned although it is understandable from the above discussion is that a system is to be called self-similar in the statistical sense even if it is not visible to the eye [71].

2.4 Scaling Hypothesis

2.4.1 Dynamic Scaling

Dynamic scaling (sometimes known as Family-Vicsek scaling [41, 96]) is the litmus test of showing that an evolving system exhibits self-similarity. A function $f(x,t)$ is said to obey dynamic scaling if one of the variable t strictly denotes time and if it satisfies

$$f(x,t) \sim t^{\theta}\phi(x/t^{z}) \tag{2.34}$$

where t is independent variable and θ and z are fixed by the dimensional relation $\left[t^{\theta}\right] = [f]$ and $[t^{z}] = [x]$ respectively, while $\phi(\xi)$ is known as the scaling function. Sometimes it is also written in the following form

$$f(x,t) \sim x^{\omega}\phi(x/t^{z}) \tag{2.35}$$

where x is consider independent variable.

Buckingham π-theorem can provide a systematic processing procedure to obtain the dynamic scaling form and at the same time appreciate the fact that the second form is not mathematically sound. An interesting aspect of the structure of the dynamic scaling form given by equation 2.34 is that the distribution function $f(x,t)$ at various moments of time can be obtained from one another by a similarity transformation

$$x \to \lambda^{z}x \tag{2.36}$$

$$t \to \lambda t \tag{2.37}$$

$$f \to \lambda^{\theta} \tag{2.38}$$

revealing the self-similar nature of the function $f(x,t)$.

To derive it one has to know first that one of the two governing parameters can be assumed to be independent. Let us assume that t is chosen to be an independent parameter and hence x can be expressed in terms of t

$$x \sim t^z \tag{2.39}$$

It implies that we can choose t^z as unit of measurement or yard-stick and quantify x in terms of dimensionless quantity $\xi = x/t^z$. Here, the quantity ξ is a number that tells how many t^z we need to measure x. If t is independent quantity then we can also express f in units of t^θ to obtain yet another dimensionless quantity $\phi = f(x,t)/t^\theta$ where the exponent θ is fixed by the dimensional requirement $[f] = \left[t^\theta\right]$. Since ϕ is a dimensionless quantity its numerical value can only depend on dimensionless quantity ξ not on a dimensional quantity t. We can then immediately obtain the scaling form given by Eq. 2.34. On the other hand, had we choose x to be independent parameter instead of t then following the same argument we would have the following scaling 2.35.

2.4.2 Finite Size Scaling

Finite-size scaling, as formulated by Fisher and Barber [43] concerns itself with the manner in which this rounding or crossover occurs. In a finite-size system, there are in principle three length scales involved: ξ, L and the microscopic length a which governs the range of the interactions. Thermodynamic quantities thus may in principle depend on the dimensionless ratios ξ/a and L/a. The finite-size scaling hypothesis assumes that, close to the critical point, the microscopic length drops out. Thus, if we consider a quantity such as the ferromagnetic susceptibility χ, which behaves like near the critical point in the infinite system, then in the finite geometry characterized by a size L,

$$\chi = \chi^{\gamma/\nu}\phi(\xi/L) \tag{2.40}$$

Equation of this sorts is used in any phase transition model.

The finite-size scaling (FSS) [6] has been extensively used as a very powerful tool for estimating finite size effects specially in the second order phase transition near the critical temperature T. The various response functions, typically the second derivative of the free energy F, in second order phase transition diverges. Such transitions are clasified by a set of critical exponents which characterize the critical point. The best known example of second

order phase transition is the paramagnetic to ferromagnetic transition where

$$M \sim (T - T_c)^{\beta} \tag{2.41}$$

$$\chi_M \sim (T - T_c)^{-\gamma} \tag{2.42}$$

$$C_V \sim (T - T_c)^{-\alpha} \tag{2.43}$$

$$\xi \sim (T - T_c)^{-\nu} \tag{2.44}$$

where, M, χ_M, C_V, ξ are Magnetization, Susceptibility, Heat capacity, Correlation length respectively. These relations are only true in the thermodynamic limit in the sense that the system size is infinite. However, we can work in simulation and experiment with finite size L^d where correlation length $\xi \sim L$. Finite size scaling thus provides a means of extrapolating various results for infinite systems.

According to finite size scaling (FSS) hypothesis, a function $f(\varepsilon, L)$ with $\varepsilon = T - T_c$ is said to obey finite size scaling if it can be expressed as

$$f(\varepsilon, L) \sim L^{-\omega/nu} \phi(\varepsilon L^{1/\nu}) \tag{2.45}$$

However, using the Buckingham π-theorem we not only obtain the correct scaling form but we also gain a deeper insight into the problem as it provides a systematic processing procedure. For instance, as we know that the correlation length ξ in the limit $L \to \infty$ diverges like $\xi \sim \varepsilon^{\nu}$ near the critical point and it bear the dimension of length. We therefore can either choose L as an independent parameter and measure ξ,i.e., $T - T_c$, in unit of L. Consequently we can measure L in unit of $T - T_c$ assuming it as an independent parameter. Choosing the later case we can define a dimensionless quantity

$$\pi = \frac{L}{\xi} = L(T - T_c)^{\nu} \tag{2.46}$$

and the corresponding dimensionless governing parameter is

$$\Pi = \frac{f(\varepsilon, L)}{\xi^{\omega}} = \phi(\pi) \tag{2.47}$$

Following the argument of the π-theorem we can immediately write that

$$f(\varepsilon, L) \sim (T - T_c)^{-\nu\omega} \phi(L(T - T_c)^{\nu}) \tag{2.48}$$

On the other hand had we chosen L as an independent parameter then the similar treatment would yield

$$f(\varepsilon, L) \sim L^{\theta}\phi(\{L(T-T_c)^{\nu}\}^{-1}) \tag{2.49}$$

Till to date neither of the two scaling forms obtained following π theorem are in use in their strict form. Instead, what is done traditionally are as follows. The important point is that if $\pi = L/\xi$ is dimensionless then so is

$$\pi^{1/\nu} = (L/\xi^{1/\nu}) = (T-T_c)L^{1/\nu} \tag{2.50}$$

It also means that we can choose L as independent parameter and express $(T-T_c)$ in unit of $L^{-1/\nu}$ to make the dimensionless quantity coincide with $\pi^{1/\nu}$. Then f too can be expressed in unit of L^{θ} which according to the prescription of π-theorem we have the following FSS scaling form

$$f(\varepsilon, L) \sim L^{\theta}\phi((T-T_c)L^{1/\nu}) \tag{2.51}$$

which is the same as the traditional scaling form given by 2.45 if we find θ negative and it is related to the exponent ν via $\theta = -\omega/\nu$.

A quantitative way of interpreting how the experimental data exhibits finite-size scaling is done by invoking the idea of data-collapse method - an idea that goes back to the original observation of Rushbrooke. That is, the values of $f(\varepsilon, L)$ for different system size L can be made to collapse on a single curve if $fL^{\omega/\nu}$ is plotted against $\varepsilon L^{1/\nu}$. It implies that systems of different sizes are all similar that also include system where $L \to \infty$. The method of data-collapse therefore comes as a powerful means of establishing scaling. It is extensively used to analyze and extract exponents especially from numerical simulations. We shall elucidate it further in the upcoming chapters.

2.5 Homogeneous Functions and Scale-Invariance

In mathematics, a homogeneous function is one with multiplicative scaling behaviour: if all its arguments are multiplied by a factor, then its value is multiplied by some power of this factor.

For example, a homogeneous function of two variables x and y is a real-valued function that satisfies the condition

$$f(\lambda x, \lambda y) = \lambda^{k} f(x, y) \tag{2.52}$$

for some constant k and all real numbers λ . The constant k is called the degree of homogeneity [7].

2.5.1 One variable function

A function is called scale-invariant or scale-free if it retains its form keeping all its characteristic features intact even if we change the measurement unit or scale. Mathematically, a function $f(r)$ is called scale-invariant or scale-free if it satisfies

$$f(\lambda x) = g(\lambda) f(x) \; \forall \lambda \tag{2.53}$$

where $g(\lambda)$ is yet unspecified function. That is, one is interested in the shape of $f(\lambda x)$ for some scale factor λ which can be taken to be a length or size rescaling. For instance dimensional functions of physical quantity are always scale-free since they obey power monomial law. It can be rigorously proved that the function that satisfies 2.53 should always have power law of the form $f(x) \sim x^{-\alpha}$.
Let us first set $r = 1$ to obtain $f(\lambda) = g(\lambda) f(1)$. Thus $g(\lambda) = f(\lambda)/f(1)$ and equation 2.53 can be written as

$$f(\lambda x) = \frac{f(\lambda) f(x)}{f(1)} \tag{2.54}$$

The above equation is supposed to be true for any λ, we can therefore differentiate both sides with respect to λ to yield

$$x f'(\lambda x) = \frac{f'(\lambda) f(x)}{f(1)} \tag{2.55}$$

where f' indicates the derivative of f with respect to its argument. Now we set $\lambda = 1$ and get

$$x f'(x) = \frac{f'(1) f(x)}{f(1)} \tag{2.56}$$

This is a first order differential equation which has a solution

$$f(x) = f(1) x^{-\alpha} \tag{2.57}$$

where $\alpha = -f(1)/f'(1)$. There it is proven that the power law is the only solution that can satisfy 2.53. We can also prove that $g(\lambda)$ has a power law form as well.
Power law distribution of the form $f(x) \sim x^{-\alpha}$ are said to be scale free since the ratio $\frac{f(\lambda r)}{f(x)}$ depends on λ alone. Thus the distribution does not need a characteristic scale. If we change the unit of measurement of x by a factor of λ, the numerical value of $f(x)$ will change by a factor of $g(\lambda)$, without affecting the shape of the function f.

2.5.2 Generalized Homogeneous Function

A function $f(x,y)$ of two independent variables x and y is said to be a generalized homogeneous function if for all values of the parameter λ the function $f(x,y)$ satisfies,

$$f(\lambda^a x, \lambda^b y) = \lambda f(x,y) \tag{2.58}$$

where a,b are arbitrary numbers. In contrast to the homogeneous functions defined in the previous section **??** generalized homogeneous functions can not be written as $f(\lambda x, \lambda y) = \lambda^p f(x,y)$, because 2.58 can not be generalized any further to the following form,

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x,y) \tag{2.59}$$

choosing $p = 1$ in the above equation yields

$$f(\lambda^{a/p} x, \lambda^{b/p} y) = \lambda f(x,y) \tag{2.60}$$

Similarly an statement converse is also valid and the equation above is no more general than the form in the equation 2.58. Another equivalent form of 2.58 is as follows,

$$f(\lambda x, \lambda^b y) = \lambda^p f(x,y) \tag{2.61}$$

Similarly

$$f(\lambda^a x, \lambda y) = \lambda^p f(x,y) \tag{2.62}$$

Note that there are at least two undetermined parameters a and b for a generalized homogeneous function. Now let use see what happens if we choose $\lambda^a = 1/x$ to set in equation 2.58,

$$f(1, \frac{y}{x^{b/a}}) = x^{-\frac{p}{a}} \tag{2.63}$$

$$f(x,y) = x^{p/a} f(y/x^{b/a}) \tag{2.64}$$

This combining and hence the simplification of two variables x and y into a single term has far reaching consequence in Windom scaling **??**in the theory of phase transition and critical phenomena.

Chapter 3

Phase Transition

The term phase transition is generally use to describe the transition between solid, liquid or gaseous states and in some cases the plasma state. It is one of the most studied problem in physics. Phase transition is a process where below a critical point the system behaves in one way whereas above that point the system behaves in a completely different way. There is a control parameter in phase transition. It can be temperature T or magnetic field H. For example in ferromagnet to paramagnet transition temperature is the control parameter and for normal to superconductor transition both temperature and magnetic field are the control parameter.

3.1 Classification

3.1.1 Ehrenfest classification

Paul Ehrenfest classified phase transitions based on the behavior of the thermodynamic free energy as a function of other thermodynamic variables [60]. Under this scheme, phase transitions were labeled by the lowest derivative of the free energy that is discontinuous at the transition.

First-order phase transitions exhibit a discontinuity in the first derivative of the free energy with respect to some thermodynamic variable [19]. The various solid/liquid/gas transitions are classified as first-order transitions because they involve a discontinuous change in density, which is the (inverse of the) first derivative of the free energy with respect to pressure.

Second-order phase transitions are continuous in the first derivative (the order parameter, which is the first derivative of the free energy with respect to the external field, is continuous across the transition) but exhibit discontinuity in a second derivative of the free energy [19]. These include the ferromagnetic phase transition in materials such as iron, where the

magnetization, which is the first derivative of the free energy with respect to the applied magnetic field strength, increases continuously from zero as the temperature is lowered below the Curie temperature. The magnetic susceptibility, the second derivative of the free energy with the field, changes discontinuously. Under the Ehrenfest classification scheme, there could in principle be third, fourth, and higher-order phase transitions.

Though useful, Ehrenfest's classification has been found to be an incomplete method of classifying phase transitions, for it does not take into account the case where a derivative of free energy diverges (which is only possible in the thermodynamic limit). For instance, in the ferromagnetic transition, the heat capacity diverges to infinity. The same phenomenon is also seen in superconducting phase transition.

3.1.2 Modern classifications

In the modern classification scheme, phase transitions are divided into two broad categories, named similarly to the Ehrenfest classes:[60]

First-order phase transitions are those that involve a latent heat. During such a transition, a system either absorbs or releases a fixed (and typically large) amount of energy per volume. During this process, the temperature of the system will stay constant as heat is added: the system is in a "mixed-phase regime" in which some parts of the system have completed the transition and others have not. Familiar examples are the melting of ice or the boiling of water (the water does not instantly turn into vapor, but forms a turbulent mixture of liquid water and vapor bubbles).

Second-order phase transitions are also called continuous phase transitions. They are characterized by a divergent susceptibility, an infinite correlation length, and a power-law decay of correlations near criticality. Examples of second-order phase transitions are the ferromagnetic transition, superconducting transition (for a Type-I superconductor the phase transition is second-order at zero external field and for a Type-II superconductor the phase transition is second-order for both normal-state—mixed-state and mixed-state—superconducting-state transitions) and the superfluid transition. In contrast to viscosity, thermal expansion and heat capacity of amorphous materials show a relatively sudden change at the glass transition temperature [80] which enables accurate detection using differential scanning calorimetry measurements

3.1.3 Basic Properties of the classes

Some basic properties of the two classes of phase transition is listed below.

First Order

1. Latent heat of nucleation in growth
2. Symmetry may or may not be broken
3. Discontinuous change in entropy

Second Order

1. No Latent heat or meta-stable state
2. Sysmmetry is always broken
3. Continuous change in entropy

At the event of critical point of phase transition there might exists a meta-stable state, where both phases exists simultaneously. At the meta-stable state the control parameter or temperature (in case of thermal phase transition, e.g., ice to water or water to vapor) does not change but there is a change (usually large) in heat which give rise to discontinuity of the first derivative of free energy, i.e., entropy 3.2.1 4.5.3. And if the entropy is continuous then the latent heat is zero which is the signature of second order transition.

3.2 Thermodynamic Quantities

The first explicit statement of the first law of thermodynamics, by *Rudolf Clausius* in 1850, referred to cyclic thermodynamic processes.

In all cases in which work is produced by the agency of heat, a quantity of heat is consumed which is proportional to the work done; and conversely, by the expenditure of an equal quantity of work an equal quantity of heat is produced.

$$\Delta E = Q + W \tag{3.1}$$

where, Q is the net quantity of heat supplied to the system by its surroundings and W is the net work done by the system. The IUPAC convention for the sign is as follows: All net energy transferred to the system is positive and net energy transferred from the system is negative. Clausius also stated the law in another form, referring to the existence of a function of state of the system, the internal energy, and expressed it in terms of a differential equation for the increments of a thermodynamic process.

In a thermodynamic process involving a closed system, the increment in the internal energy is equal to the difference between the heat accumulated by the system and the work done by it.

For quasi-static process

$$dU = \delta Q - \delta W \tag{3.2}$$
$$= dQ - PdV \tag{3.3}$$

U is the internal energy. here $W = -PdV$ since work done by the system on the environment if the product PdV whereas the work done on the system is $-PdV$ for pressure P and volume change dV.
The term heat for Q means "that amount of energy added or removed by conduction of heat or by thermal radiation", rather than referring to a form of energy within the system. The internal energy is a mathematical abstraction that keeps account of the exchanges of energy that befall the system.

For quasi-static state we can write

$$dQ = TdS \tag{3.4}$$

where S is the entropy of the system and T is the temperature. Thus we can write for canonical ensemble

$$dU = TdS - PdV \tag{3.5}$$

such that $E = E(S,V)$ and for grand canonical ensemble

$$dU = TdS - pdV + \mu dN \tag{3.6}$$

where $U = U(S,V,N)$. But a problem arises, since there is no device we currently posses that can measure entropy. So we use Legendre transformation to change variable dependency

$$\begin{aligned} dU &= TdS - pdV \\ &= TdS + SdT - SdT - PdV \\ d(U - TS) &= -SdT - PdV \\ dA &= -SdT - PdV \end{aligned} \tag{3.7}$$

where $A = A(T,V)$ is the Helmholtz free energy. We can perform another Legendre transformation in 3.7 as follows

$$\begin{aligned} dA &= -SdT - PdV - VdP + VdP \\ d(A+PV) &= -SdT + VdP \\ dG &= -SdT + VdP \end{aligned} \tag{3.8}$$

where $G = G(T,P)$ is the Gibbs free energy.

3.2.1 Entropy

One of the most important concept in Statistical Mechanics is entropy. The notion of entropy was first introduced in physics by a German scientist Rudolf Clausius who laid the foundation for the second law of thermodynamics in 1850 by examining the relation between heat transfer and work. The second law of thermodynamics states that the total entropy of an isolated system can never decrease over time. Therefore the direction toward which entropy increases monotonically is the direction of time. Monotonically means that it can increase or keep constant but never decrease. The term entropy is used in many other branches of science, sometimes distant from physics or mathematics (such as sociology), where it no longer maintains its rigorous quantitative character. Usually, it roughly means disorder, chaos, decay of diversity or tendency toward uniform distribution of kinds [38].

Entropy is considered as a quantity about the disorderness of a system. This kind of disorder is the number of states a system can take on. So what are the states of a system? Imagine a cube of volume $1cm^3$, filled with one particular gas. At a particular time if we can label all the molecules of the gas uniquely then at next moment most of the molecule will change their positions due to their random motion. Then we will not be able to identify each molecule with their previous label. This process of identifying the labels of the molecules are easier if it's a liquid and even more easier in it's solid form. Since temperature increases the random motion of the molecules, as the temprature rises it is more difficult to identify those molecules. Thus at high temperature a system has higher entropy. Another thing to mention about it's volume. If a larger volume is selected then obviously the number of possible states will increase therefore entropy will increase.

Example If we were ot compare the entropy of the moon and the sun, the above discussion tells us that the sun has higher entropy than the moon. The reason is that the sun is much much larger than the moon and has much higher temperature than the moon. Therefor the number of possible states will be larger for the sun than the moon.

In Classical Physics, entropy is seen as a magnitude which in every time is proportional to the quantity of energy that at that time cannot be transformed into mechanical work. Using the above interpretation, entropy plays a central role in the formulation of the second law of thermodynamics which states that in an isolated physical system, any transformation leads to an increase of its entropy.

In Probability Theory, the entropy of a random variable measures the uncertainty over the values which can be reached by the variable.

In Information Theory, the entropy of the compression of a message (for example, of a file from a computer), quantifies the content of the information of the message to have the minimum lost of information in the compression process previous to its transmission.

In Abstract Theory of Dynamical Systems, the entropy measures the exponential complexity of the system or the average flow of information per unit of time [14].

So it is already explicit that the concept of entropy is not easy to grasp and frequently entropy is seen as very mysterious quantity and that's why it received a very large number of interpretations, explications, applications. In order to understand how the complex concept of entropy emerged, in this chapter we will give a brief history and will review the works of Clausius, Boltzmann, Shannon and Rényi.

Clausius Entropy

As mentioned Earlier in this section The concept and name of entropy originated in the early 1850s in the work of Rudolf Julius Emmanuel Clausius $(1822-1888)$ and that work was at first primarily concerned with the question of which cycle is best suited for the conversion of heat into work and which substance is best used for the conversion [31].

Clausius based his argument on the plausible axiom that heat cannot pass by itself from a cold to a hot body. In order to exploit that axiom Clausius considered two competing Carnot cycles (see figure 3.1) working in the same temperature range, one as a heat engine and one as a refrigerator; the refrigerator consumes the work the engine provides. By comparing the amounts of heat Q passed from top to bottom and vice versa, he came to the conclusion that among all efficiencies the efficiency of a Carnot cycle is maximum and universal. 'Maximum' means that no cycle in the same range of temperature has a bigger efficiency than a Carnot cycle, and 'universal' means that all working substances provide the same efficiency in a Carnot cycle [28]. It is easy to calculate the efficiency of the Carnot engine of an ideal gas:

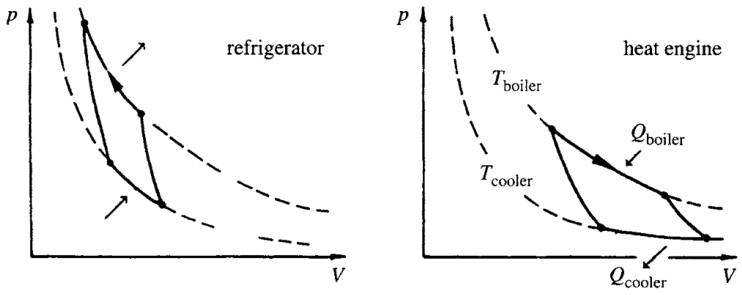


Fig. 3.1 Two competing Carnot engines, pressure (P) versus volume (V) - diagrams [12]

$$\begin{aligned}\eta &= \frac{W}{Q_{boiler}} \\ &= \frac{Q_{boiler} - Q_{cooler}}{Q_{boiler}} \\ &= 1 - \frac{Q_{cooler}}{Q_{boiler}} \qquad (3.9) \\ &= 1 - \frac{T_{cooler}}{T_{boiler}} \qquad (3.10)\end{aligned}$$

where T is the Kelvin temperature. And, since by Clausius's result this efficiency is universal, it holds not only for ideal gases but for all substances, be they water, mercury, sulphur, or steel. Nicolas Léonard Sadi Carnot anticipated Clausius by 30 years, but no one could understand Carnot's reasoning. Carnot believed in the caloric theory of heat, by which the heat passing through the cycle from boiler to cooler is unchanged in amount. This is quite wrong and it is a kind of miracle that Carnot, despite his erroneous concepts, obtained a correct result. Carnot's trouble was that he did not know the balance of energy, or the first law of thermodynamics, which states that

$$\begin{aligned}dU &= dQ - dW \qquad (3.11) \\ &= dQ - PdV \qquad (3.12)\end{aligned}$$

since

$$dW = PdV \qquad (3.13)$$

This equation holds, if the work is expended reversibly for the volume change. With that superior knowledge Clausius showed that it is not the heat that passes through the cycle from boiler to cooler unchanged in amount. He proved that from equation 3.10

$$\frac{Q}{T}\Big|_{\text{boiler}} = \frac{Q}{T}\Big|_{\text{heater}} \qquad (3.14)$$

nd decided to define the entropy change to be the ratio of heat flow to temperature: [94]

$$\Delta S_{\text{thermo}} = \frac{Q}{T} \tag{3.15}$$

He also showed that in an arbitrary process, the change of entropy, satisfies the inequality

$$dS \geq \frac{dQ}{T} \tag{3.16}$$

This important relation is known as the second law of thermodynamics. We will now discuss the significance of this law. First, we stick to reversible process, where the equality holds in equation 3.16. We may then eliminate dQ between the first and second laws, we obtain the Gibbs equation

$$dS = \frac{1}{T}(dU + PdV) \tag{3.17}$$

In an adiabatic irreversible process, $dQ = 0$ and equation 3.16 one has the fundamental relation between entropy and irresponsibility. In words

In a closed system (adiabatic), the entropy cannot decrease, it remains constant or increase [17]

But the irreversible increase of entropy is not a property of the microscopic laws of nature. Because the microscopic laws of nature are time-reversal invariant. For example the Maxwell's equations are time reversible or the laws governing the motion of electrons of atoms are also time reversible. Thus the direction of time cannot be determined from microscopic laws of nature. But since entropy always increase monotonically, the direction in which entropy increases (or remains constant) is the direction of time [94].

Also by differentiating equation 3.8 with respect to T keeping P constant we can get an expression for entropy in terms of the Gibbs free energy.

$$S = -\frac{dG}{dT} \tag{3.18}$$

similar expression is obtained from 3.7. Thus entropy is indeed the first derivative of free energy with respect to the control parameter T.

Boltzmann Entropy

Another intuitive interpretation of entropy is as a measure of the disorder in a system. Liquids have higher entropy than crystals intuitively because their atomic positions are less orderly [94]. Ludwig Boltzmann interpreted the entropy function as statistical entropy using probability theory. Around 1900 there was a fierce debate going on between scientists

whether atoms really existed or not. Boltzmann was convinced that they existed and realized that models that relied on atoms and molecules and their energy distribution and their speed and momentum, could be of great help to understand physical phenomena. Because atoms where supposed to be very small, even in relatively small systems, one faces already a tremendous number of atoms. For example: one mole of water contains about 6.023×10^{23} molecules! Clearly it is impossible to track the energy and velocity of each individual atom. Therefore, Boltzmann introduced a mathematical treatment using statistical mechanical methods to describe the properties of a given physical system (for example the relationship between temperature, pressure and volume of one liter of air).

Boltzmann's idea behind statistical mechanics was to describe the properties of matter from the mechanical properties of atoms or molecules. In doing so, he was finally able to derive the Second Law of Thermodynamics around 1890 and showed the relationship between the atomic properties and the value of the entropy for a given system. It was Max Planck who formulated the expression of entropy of the ideal gas system based on Boltzmann's results [89]. The Boltzmann entropy formula or Boltzmann-Planck entropy formula is

$$S = k_B \log \Omega \tag{3.19}$$

S is called the Planck entropy or Boltzmann entropy. Here k_B is the Boltzmann constant (ideal gas constant R divided by Avogadro's number N) which equals to $1.4 \times 10^{-23}\ J/K$), and Ω, comes from the German *Wahrscheinlichkeit*, meaning probability, which is often referred to as disorder. In another way we can define it as the number of microstates (often modeled as quantum states) with the given macrostate. Macrostate is any particular arrangement of atoms where we look only on average quantities. Any individual arrangement defining the properties (e.g. positions and velocities) of all the atoms for a given macrostate is a microstate. For a microstate it matters what individual particles do, for the macrostate it does not.

The logarithm is used because it simplifies the computations and reproduced the property of additivity of entropy, in the sense that the entropy of two systems sums instead of multiplies. In equation 3.19, the entropy S increases when Ω increases. More microstates give raise to more disorder hence higher entropy. Besides for only one possible microstate, entropy is zero. The notion of disorder is an intuitive notion depending of the system to be considered. In the case of a gas, it is considered it in a ordered state if its molecules have a distribution of energies or positions very different of those random which means the Boltzmann distribution. The most disordered states are the most probable and as consequence have the most entropy. Another consequence is that in the universe the disorder tends to increase [14].

From there, it is a short conceptual jump to the second Law (total entropy tends to increase, and all spontaneous processes increase entropy). In summary, the thermodynamic definition of entropy provides the experimental definition of entropy, while the probabilistic definition of entropy extends the concept, providing an explanation and a deeper understanding of its nature [11].

These definitions of entropy is of no use in our model. However we can use the Boltzmann entropy with a few modification to get Shannon entropy [95]. This process of getting Shannon entropy from Boltzmann entropy and how does it help us is described in section 4.5.3.

3.2.2 Specific Heat

Heat capacity is a physical quantity which is the ratio of the heat added to an object to the resulting temperature change [52]. Note that removing heat is just like adding negative heat. The unit of heat capacity if joule per kelvin j/K. And it's dimensional form is $L^2MT^{-2}\Theta^-1$. The specific heat is the amount of heat per unit mass ($1kg$) required to raise the temperature by one kelvin($1K$).

Heat capacity is an *extensive* property of matter (it is proportional to the size of the system). When expressing the same phenomenon as an *intensive* property, the heat capacity is divided by the amount of substance, mass, or volume, thus the quantity is independent of the size or extent of the sample. The molar heat capacity is the heat capacity per unit amount (SI unit: mole) of a pure substance, and the specific heat capacity, often called simply specific heat, is the heat capacity per unit mass of a material. In some engineering contexts, the volumetric heat capacity is used.

Temperature represents the average randomized kinetic energy of constituent particles of matter relative to the centre of mass of the system, while heat is the transfer of energy across a system boundary into the body other than by work or matter transfer. Translation, rotation, and vibration of atoms represent the degrees of freedom of motion which classically contribute to the heat capacity of gases, while only vibrations are needed to describe the heat capacities of most solids, as shown by the Dulong–Petit law [63].

The internal energy of a closed system changes by adding heat to the system or by the system performing work.

$$\Delta E_{system} = E_{in} - E_{out} \tag{3.20}$$

which is same expression as 3.2. If the heat is added at constant volume, then the second term of this relation vanishes to give

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \left(\frac{\partial Q}{\partial T}\right)_V \tag{3.21}$$

Another useful quantity is the heat capacity at constant pressure, C_P. This quantity refers to the change in the enthalpy of the system given by

$$H = U + PV \tag{3.22}$$

Thus the change in enthalpy is

$$\begin{aligned} dH &= dU + d(PV) \\ &= dQ + dW + PdV + VdP \\ &= dQ + VdP \end{aligned} \tag{3.23}$$

Therefore at constant pressure we have

$$C_P = \left(\frac{\partial H}{\partial T}\right)_P = \left(\frac{\partial Q}{\partial T}\right)_P \tag{3.24}$$

In general we can write the relationship between heat and temperature change as

$$C = \frac{Q}{dT} \tag{3.25}$$

where C is the specific heat. and we know

$$Q = TdS \tag{3.26}$$

we immediately get

$$C = T\frac{dS}{dT} \tag{3.27}$$

3.2.3 Order Parameter

An order parameter is a measure of the degree of order across the boundaries in a phase transition system. It's numerical usually ranges between $[0,1]$. At the critical point, the order parameter susceptibility will usually diverge.

An example of an order parameter is the net magnetization in a ferromagnetic system undergoing a phase transition. For liquid-gas transitions, the order parameter is the difference of the densities.

Order parameter does have a theoretical perspective. It arise from symmetry breaking. When this happens, one needs to introduce one or more extra variables to describe the state of the system. For example, in the ferromagnetic phase, one must provide the net magnetization,

whose direction was spontaneously chosen when the system cooled below the Curie point. Order parameter can be a function of more than one variable. In other words it can have more than one degree of freedom. It can also be defined for non-symmetry-breaking transitions.

3.2.4 Susceptibility

The first law of thermodynamics for a non magnetic system is obtainable from 3.5 using a conversion. For a magnetic system $P \to h$ and $V \to -m$, where h is the magnetic field and m is the magnetization. The negative sign for the magnetization is because of the fact that the magnetization increases with the increase of the magnetic field whereas the volume decreases as the pressure increases. Since we relate pressure to the magnetic field, to relate volume to magnetization we need to put a minus sign with it. Thus we get

$$dU = TdS + hdm \tag{3.28}$$
$$= TdS + SdT - SdT + hdm \tag{3.29}$$
$$d(U - TS) = -SdT + hdm \tag{3.30}$$
$$dA = -SdT + hdm \tag{3.31}$$
$$dA = -SdT + hdm + mdh - mdh \tag{3.32}$$
$$d(A - mh) = -SdT - mdh \tag{3.33}$$
$$dG = -SdT - mdh \tag{3.34}$$

where $A = A(T,m)$ is the Helmholtz free energy and $G = G(T,h)$ is the Gibbs free energy for the magnetic system. From the definition of free energy for a magnetic system 3.34 3.31 we can find the expression for entropy and magnetization in terms of free energy.

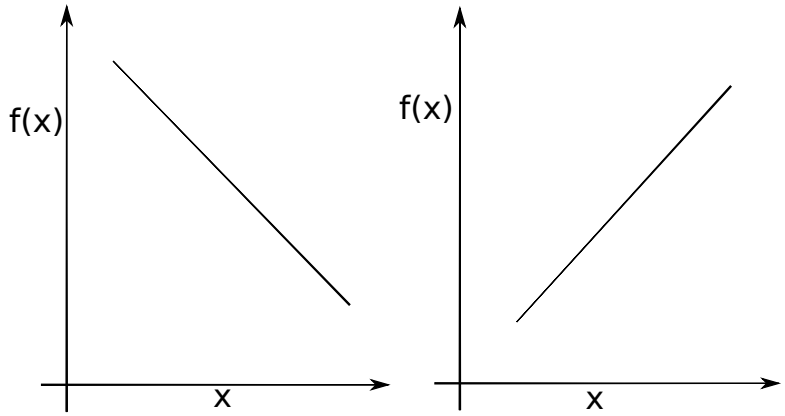
$$S = -\left(\frac{\partial G}{\partial T}\right)_h = -\left(\frac{\partial A}{\partial T}\right)_m \tag{3.35}$$

$$m = -\left(\frac{\partial G}{\partial h}\right)_T \tag{3.36}$$

$$h = \left(\frac{\partial A}{\partial m}\right)_T \tag{3.37}$$

And since the susceptibility is defined as the derivative of the magnetization with respect to the magnetic field, we get

$$\chi = \left(\frac{\partial m}{\partial h}\right)_h = -\left(\frac{\partial^2 G}{\partial h^2}\right)_T \tag{3.38}$$



(a) negative slope (b) positive slope

Fig. 3.2 shape of $f(x)$ from $f'(x)$

again we can write χ as

$$\begin{aligned} \chi &= \frac{1}{\frac{\partial h}{\partial m}} \\ &= \frac{1}{\frac{\partial^2 A}{\partial m^2}} \end{aligned} \tag{3.39}$$

3.3 Shapes of the Thermodynamic Quantities

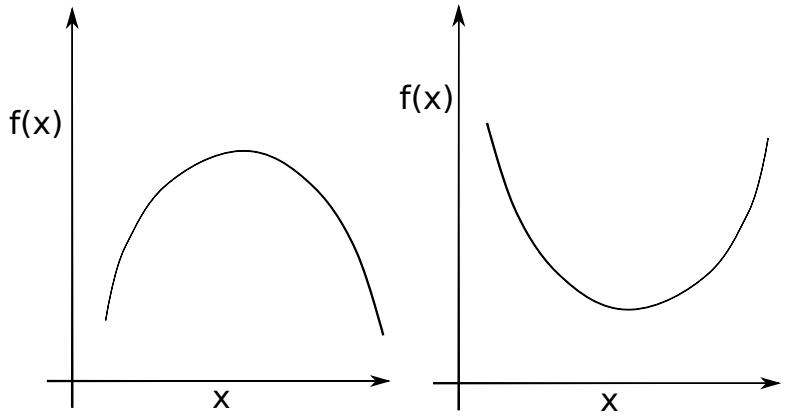
3.3.1 Calculus to determine the shapes

From the law of Calculus we can estimate the approximate shape of a function by it's first and second derivative. Say we have a function $f(x)$ and we want to estimate it's shape. If the first derivative of this function is negative (positive) the function is said to have decreasing (increasing) slope 3.2.

If the second derivative of this function is negative (positive) the function is said to have concave (convex) shape 3.3. Thus if we know the sign of the first and second derivative we can approximate a shape of the function.

3.3.2 Free Energy

Now since we obtain from 3.8 that the entropy is the first derivative of the free energy 3.40 and from 3.45 specific heat is the second derivative of the free energy 3.41. Since the entropy is a positive quantity and specific heat is also a positive quantity we get that the first and second derivative of the free energy is negative which implies from the laws of calculus that



(a) concave (b) convex

Fig. 3.3 shape of $f(x)$ from $f''(x)$

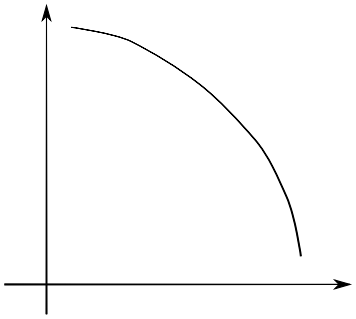


Fig. 3.4 Shape of the free energy

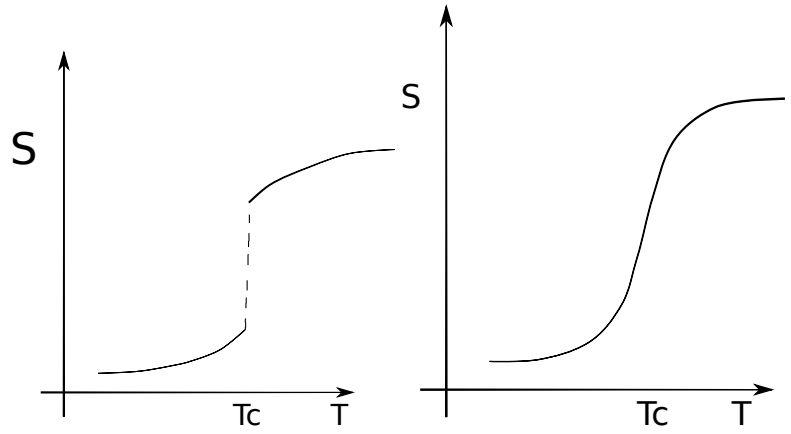
the shape of the free energy should be a decreasing concave curve 3.4 in other words concave shaped with negative slope.

$$S = -\frac{\partial G}{\partial T} \tag{3.40}$$

$$C = -\frac{\partial^2 G}{\partial T^2} \tag{3.41}$$

3.3.3 Entropy and Specific Heat

Now that we know the shapes of the free energy, the very next thing to do is to find the shape of the entropy. Since we can get entropy from differentiating the free energy with respect to temperature T we get the following shape 3.5. From the definition of the transition order we know that the first order transition is discontinuous and the second order transition continuous. Since the first order transition requires latent heat at the critical point the discontinuity is



(a) Entropy in first order transition (b) Entropy in 2nd order transition

Fig. 3.5 Shape of entropy

inevitable. Note that, since entropy measures disorderedness of a system it should increase with increasing temperature. Because the temperature is nothing but the average kinetic energy of the particles in the system. As the kinetic energy of the system increases with temperature, the particles tend to vibrate more and get higher average velocity. Thus making the system disordered. Therefore in a physical system entropy always increases with the increasing of temperature. If we find something different, as if, the entropy is decreasing with the increasing of temperature, there must be a problem somewhere. Just after knowing the shape of entropy one can anticipate the shape of specific heat, which is the derivative of the entropy with respect to temperature and is defined in 3.43. Using this and the shape of entropy we can get the shape of the specific heat immediately as follows

3.3.4 Order Parameter and Susceptibility

Since diamagnetic substances have negative susceptibilities ($\chi < 0$); paramagnetic, and ferromagnetic substances have positive susceptibilities ($\chi > 0$), and we are working for a phase transition model similar to paramagnet and ferromagnet transition, taking susceptibility to be positive is appropriate for our model. Now if susceptibility is positive then from 3.38 we get $\left(\frac{\partial^2 G}{\partial h^2}\right) < 0$ which means that the shape of the free energy for this case is concave from the knowledge of 3.3.1. And from 3.36 and the fact that the magnetic field h can be positive or negative, as it can change direction, the Gibbs free energy is negative, since it is the lowest binding energy.
Also from 3.39 we can say $\frac{\partial^2 A}{\partial m^2}$ is positive giving convex shape of the Helmholtz free energy.

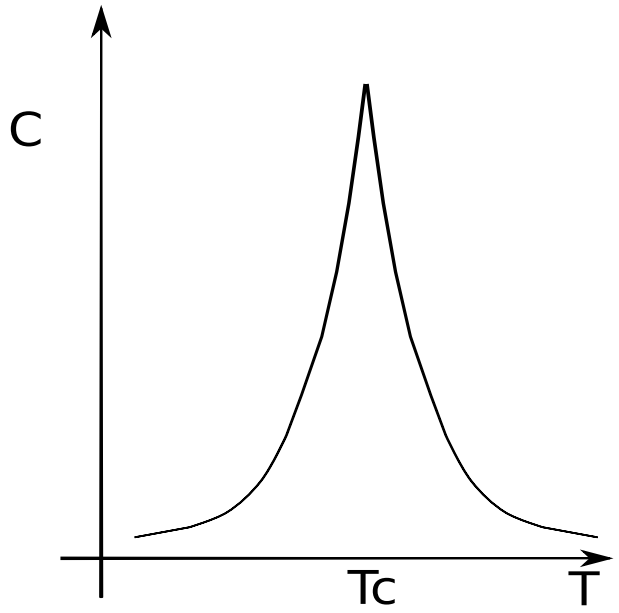


Fig. 3.6 Shape of Specific Heat and Susceptibility

And 3.37 tells us that since h can ve positive or negative, the Helmholtz free energy can have increasing or decreasing slope respectively.

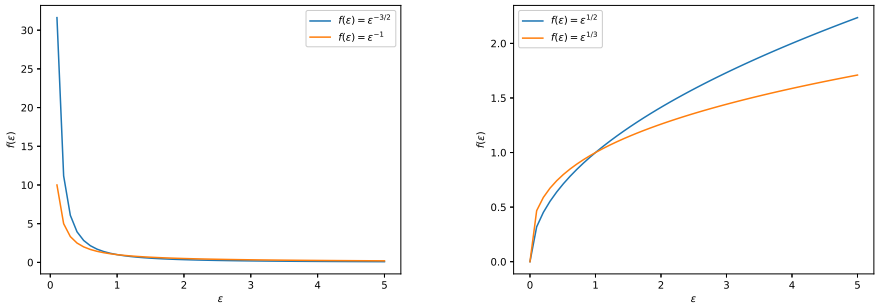
3.4 Response Functions

The Specific heat and Susceptibility are called the response function in thermodynamics and the definitions are as follows. The specific heat C_p or C_v is the derivative of the enthalpy with respect to the temperature at constant pressure or volume respectively.

$$C_x = \left(\frac{dQ}{dT}\right)_x \tag{3.42}$$

here x can be P for pressure or V for volume. And from 3.4 we can write

$$C_x = T\left(\frac{dS}{dT}\right) \tag{3.43}$$



(a) $f(\varepsilon) \sim \varepsilon^{\lambda}$ where $\lambda = -1, -3/2$ (b) $f(\varepsilon) \sim \varepsilon^{\lambda}$ where $\lambda = 1/2, 1/3$

Fig. 3.7 Function showing power law

To give the following

$$C_v = -T \left(\frac{\partial^2 A}{\partial T^2} \right)_v \tag{3.44}$$

$$C_p = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_p \tag{3.45}$$

Thus we can see that the response functions are the second derivative of the free energy.

3.5 Critical Exponents

Near the critical point there is, in general, a function that describes the behavior of the system that is mostly interesting. For thermodynamical system the temperature is the control parameter , thus that function depends on the temperature. But since we want the information at the critical point, $(T - T_c)/T_c$, instead of T is a better parameter to address. In equation

$$\varepsilon = \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1 \tag{3.46}$$

ε is considered a better parameter. Thus a function $f(\varepsilon)$ is used instead of $f(T)$. Using the fact that in the vicinity of T_c the function $f(\varepsilon)$ exhibits power law

$$f(\varepsilon) \sim \varepsilon^{\lambda} \tag{3.47}$$

The following figures shows some function that exhibit power law To see this more closely,

we can expand any function $f(\varepsilon)$ as a power series of ε

$$f(\varepsilon) = A\varepsilon^{\lambda}(1 + B\varepsilon^{a} + C\varepsilon^{b} + ...) \tag{3.48}$$

Near T_c only the first term is dominating. We had the Gibbs free energy (for a magnetic system)

$$G = G(T,h) \equiv G(\varepsilon,h) \tag{3.49}$$

since ε is a better parameter. Assuming that G is a generalized Homogeneous function. Therefore from the realization of section 2.5 we can write

$$G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) = \lambda G(\varepsilon,h) \tag{3.50}$$

differentiating equation 3.50 with respect to h

$$\begin{aligned}
\frac{\partial G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\partial h} &= \lambda \frac{\partial G(\varepsilon,h)}{\partial h} \\
\frac{\partial G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\partial \lambda^{a_h} h}\lambda^{a_h} &= \lambda \frac{\partial G(\varepsilon,h)}{\partial h} \\
\lambda^{a_h} G'(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda G'(\varepsilon,h) \\
-\lambda^{a_h} m(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= -\lambda m(\varepsilon,h) \\
m(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda^{1-a_h} m(\varepsilon,h) \qquad (3.51) \\
& \qquad (3.52)
\end{aligned}$$

Here m is the magnetization or order parameter. The figure 3.8 shows the general shape of the order parameter.

Setting $h = 0$ in equation 3.52

$$\begin{aligned}
m(\lambda^{a_\varepsilon}\varepsilon) &= \lambda^{1-a_h} m(\varepsilon) \\
m(1) &= \lambda^{1-a_h} m(\varepsilon) \\
m(1) &= \varepsilon^{-\frac{1-a_h}{a_\varepsilon}} m(\varepsilon) \\
m(\varepsilon) &= \varepsilon^{\beta} m(1) \qquad (3.53)
\end{aligned}$$

where

$$\beta = \frac{1-a_h}{a_\varepsilon} \tag{3.54}$$

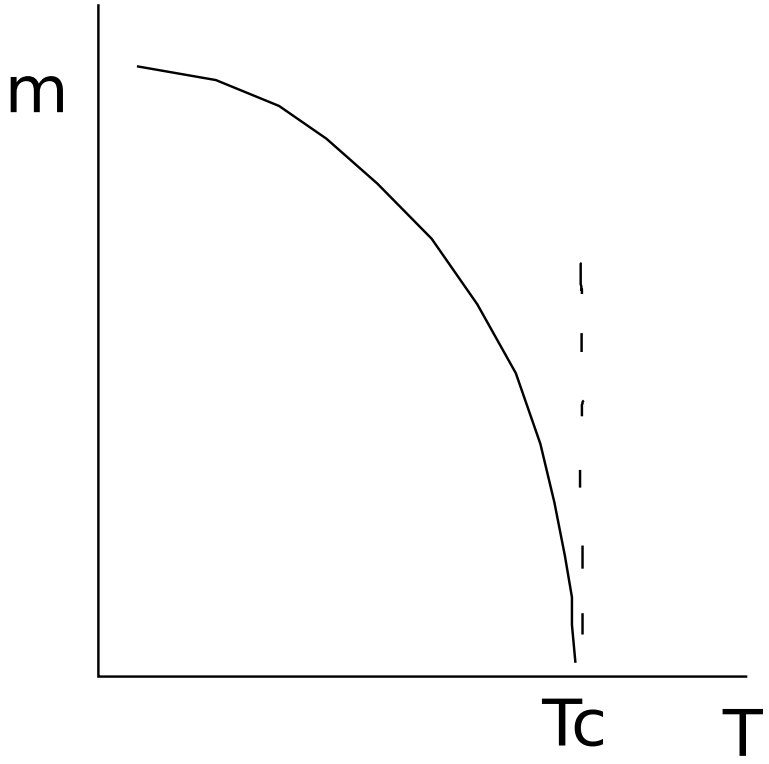


Fig. 3.8 General shape of Order Parameter

Note that, setting $\lambda^{a_\varepsilon}\varepsilon = 1$ gives $\lambda = \varepsilon^{-1/a_\varepsilon}$.
Setting $\varepsilon = 0$ in equation 3.52

$$\begin{aligned} m(\lambda^{a_h}h) &= \lambda^{1-a_h}m(h) \\ m(1) &= h^{-\frac{1-a_h}{a_h}}m(h) \\ m(h) &= m(1)h^{\delta} \end{aligned} \tag{3.55}$$

where

$$\delta = \frac{a_h}{1-a_h} \tag{3.56}$$

Again, note that, setting $\lambda^{a_h}h = 1$ gives $\lambda = h^{-1/a_h}$
Now, Since the response functions are the second derivative of the free energy 3.4, by

differentiating 3.50 twice with respect to ε we get the Specific Heat

$$\begin{aligned}
\lambda^{2a_\varepsilon} G''(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda G''(\varepsilon, h) \\
\lambda^{2a_\varepsilon} \frac{\partial G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\left(\frac{1}{T_c}\right)^2 \partial T^2} &= \lambda G''(\varepsilon, h) \\
\lambda^{2a_\varepsilon} C(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) &= \lambda C(\varepsilon, h)
\end{aligned} \tag{3.57}$$

We have used $\varepsilon = \frac{T}{T_c} - 1$ and $d\varepsilon = \frac{1}{T_c} dT$. Now setting $h = 0$ we get from 3.57

$$\begin{aligned}
\lambda^{2a_\varepsilon} C(\lambda^{a_\varepsilon}\varepsilon) &= \lambda C(\varepsilon) \\
C(1) &= \lambda^{1-2a_\varepsilon} C(\varepsilon) \\
&= \varepsilon^{-\frac{1-2a_\varepsilon}{a_\varepsilon}} C(\varepsilon) \\
C(\varepsilon) &= \varepsilon^{-\alpha} C(1)
\end{aligned} \tag{3.58}$$

We have used the value of λ when we set $\varepsilon\lambda^{a_\varepsilon} = 1$ and the exponent

$$\alpha = \frac{2a_\varepsilon - 1}{a_\varepsilon} \tag{3.59}$$

Again by differentiating 3.50 twice with respect to h we get the susceptibility. Then we set $h = 0$ to get only ε dependency.

$$\begin{aligned}
\lambda \frac{\partial^2 G(\varepsilon, h)}{\partial h^2} &= \lambda^{2a_h} \frac{\partial^2 G(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h)}{\partial h^2} \\
\lambda \chi(\varepsilon, h) &= \lambda^{2a_h} \chi(\lambda^{a_\varepsilon}\varepsilon, \lambda^{a_h}h) \\
\chi(\varepsilon) &= \lambda^{2a_h - 1} \chi(\lambda^{a_\varepsilon}\varepsilon) \\
\chi(\varepsilon) &= \varepsilon^{-\gamma} \chi(1)
\end{aligned} \tag{3.60}$$

Similar to previous case, We have used the value of λ when we set $\varepsilon\lambda^{a_\varepsilon} = 1$ and the exponent is

$$\gamma = \frac{2a_h - 1}{a_\varepsilon} \tag{3.61}$$

3.5.1 List of Thermodynamic Quantities that Follows Power Law

The exponent that scales Specific heat is called α

$$C \sim \varepsilon^{-\alpha} \tag{3.62}$$

The exponent that scales order-parameter is called β

$$m \sim \varepsilon^{\beta} \tag{3.63}$$

Another exponent that scales order-parameter is called δ, but it relates the order parameter with the magnetic field, h

$$m \sim h^{\delta} \tag{3.64}$$

The exponent that scales susceptibility is called γ

$$\chi \sim \varepsilon^{-\gamma} \tag{3.65}$$

Note that these quantities only follows power law near T_c.

3.5.2 Rushbrooke Inequality

$$\alpha + 2\beta + \gamma \geq 2 \tag{3.66}$$

but the equality is often obtain theoretically which is shown below in the present case

$$\begin{aligned} \alpha + 2\beta + \gamma &= \frac{2a_\varepsilon - 1}{a_\varepsilon} + \frac{2(1-a_h)}{a_\varepsilon} + \frac{2a_h - 1}{a_\varepsilon} \\ &= \frac{2a\varepsilon}{a\varepsilon} \\ &= 2 \end{aligned}$$

Thus the Rushbrooke inequality is satisfied.

3.5.3 Griffiths Inequality

$$\alpha + \beta(1+\delta) = 2 \tag{3.67}$$

Let's do a quick check to see if this is also satisfied.

$$\begin{aligned}\alpha+\beta(1+\delta) &= \frac{2a_\varepsilon-1}{a_\varepsilon}+\frac{1-a_h}{a_\varepsilon}\left(1+\frac{a_h}{1-a_h}\right)\\ &= \frac{2a_\varepsilon-1}{a_\varepsilon}+\frac{1}{a_\varepsilon}\\ &= \frac{2a_\varepsilon}{a_\varepsilon}\\ &= 2\end{aligned} \tag{3.68}$$

So the Griffiths Inequality is also satisfied.

3.6 Ising Model

For a very long time scientists have been trying to understand phase transition in different aspects. And for this purpose many different models have been provided for decades. The first model was provided by physicist Ernst Ising as a mathematical model of ferromagnetism in statistical mechanics. The Ising model was invented by the physicist Wilhelm Lenz (1920), who gave it as a problem to his student Ernst Ising. The one-dimensional Ising model has no phase transition and was solved by Ising (1925) himself in his 1924 thesis [59]. But he provided a model in 1 dimension and proved that in 1 dimension phase transition is not possible and concluded that it is not possible in higher dimension as well. But it was proved later that in dimension $d \geq 2$ phase transition is possible [100, 74] which proved Ising wrong about his conclusion but he certainly gave a good insight for phase transition and hence the naming.

Consider a set Λ of lattice sites, each with a set of adjacent sites forming a d-dimensional lattice. For each lattice site $k \in \Lambda$ there is a discrete variable σ_k such that $\sigma_k \in \{+1,-1\}$, representing the site's spin. A spin configuration $\sigma = (\sigma_k)_{k\in\Lambda}$ is an assignment of spin value to each lattice site.

For any two adjacent sites $i, j \in \Lambda$ there is an interaction J_{ij}. Also a site $j \in \Lambda$ has an external magnetic field h_j interacting with it. The energy of a configuration σ is given by the Hamiltonian

$$H(\sigma) = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j \tag{3.69}$$

Where the first sum is over pairs of adjacent spins counting every pair only once. And we use $< ij >$ to indicate that i and j are nearest neighbors. μ indicates the magnetic moment. The

negative sign on the second term is there by convention [13]. The configuration probability is given by the Boltzmann distribution with inverse temperature $\beta \geq 0$

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta} \tag{3.70}$$

where $\beta = (k_B T)^{-1}$ and the normalization constant

$$Z_\beta = \sum_\sigma e^{-\beta H(\sigma)} \tag{3.71}$$

is the partition function. For a function f of the spins, which is the observable here, we denote

$$< f >_\beta = \sum_\sigma f(\sigma) P_\beta(\sigma) \tag{3.72}$$

the expectation value of f. The configuration probabilities $P_\beta(\sigma)$ represent the probability that the system in in a state with configuration σ in equilibrium.

The minus sign on each term of the Hamiltonian function $H(\sigma)$ is conventional. Using this sign convention, the Ising models can be classified according to the sign of the interaction: if, for all pairs i, j

$$J_{ij} \begin{cases} > 0, \text{ ferromagnetic interaction} \\ < 0, \text{ anti-ferromagnetic interaction} \\ = 0, \text{ non-interacting spins} \end{cases} \tag{3.73}$$

otherwise the system is called non-ferromagnetic.

In a ferromagnetic Ising model, spins tend to be aligned, meaning, the configurations in which adjacent spins are of the same sign have higher probability. In an anti-ferromagnetic model, adjacent spins tend to have opposite signs.

The sign convention of $H(\sigma)$ also explains how a spin site j interacts with the external field. Namely, the spin site wants to line up with the external field.

$$h_j \begin{cases} > 0, \text{ the spin site } j \text{ desires to line up in the positive direction} \\ > 0, \text{ the spin site } j \text{ desires to line up in the negative direction} \\ = 0, \text{ no external influence on the spin site} \end{cases} \tag{3.74}$$

(a) all are in spin up state (b) only one site is in spin down state

Fig. 3.9 1 dimensional Ising model

Ising models are often examined without an external field interacting with the lattice, that is, $h = 0$ for all j in the lattice Λ. Using this simplification, our Hamiltonian becomes:

$$H(\sigma) = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j \tag{3.75}$$

When the external field is everywhere zero, $h = 0$, the Ising model is symmetric under switching the value of the spin in all the lattice sites; a non zero field breaks this symmetry.

Another common simplification is to assume that all of the nearest neighbors $< ij >$ have the same interaction strength. Then we can set $J_{ij} = J$ for all pairs i, j. In this case our Hamiltonian is further simplified to:

$$H(\sigma) = -J\sum_{<ij>} \sigma_i\sigma_j \tag{3.76}$$

Ising himself had provided the theory of his model for 1 dimensional case. He did not find any phase transition and concluded that phase transition is not possible in any dimension.

Consider an one dimensional lattice where all sites are in spin up state. Then according to Ising model their total energy E and entropy S is as follows

$$E = -NJ \tag{3.77}$$

$$S = 0 \tag{3.78}$$

Where N is the number of sites on the lattice. Now if one of the sites is fliped then

$$E = -(N-2)J \tag{3.79}$$

$$S = \log N \tag{3.80}$$

Therefore the cost is $\Delta E = 2J$ and change in entropy is $\Delta S = \log N$ for flipping spin of one site. The figure 3.9 shows this.

Therefore the change in free energy due to flipping one spin is,

$$\Delta F = \Delta E - T\Delta S \tag{3.81}$$

$$= 2J - T\log N \tag{3.82}$$

In the thermodynamic limit $N \to \infty$ the second term always dominates except for $T = 0$. Thus in one dimensional lattice there is phase transition at non zero temperature sice we cannot have $\Delta F = 0$ (the transition point).

Now interesting this happens in case of two dimensional lattice. Say we have a square lattice of size N where there is an island of $L = 3$ sites of different spins **??**.

$$\Delta E = 2LJ \tag{3.83}$$
$$\Omega = 3^L N \tag{3.84}$$
$$S = K \log \Omega \tag{3.85}$$
$$\Delta S = S - 0 = S \tag{3.86}$$

Therefore the free energy is

$$\begin{aligned} \Delta F &= \Delta E - T\Delta S && (3.87)\\ &= 2JL - KT \log(3^L N) && (3.88)\\ &= 2JL - TL\log 3 - KT \log N && (3.89) \end{aligned}$$

since at transition point $\Delta F = 0$ we get

$$0 = L(2J - T_c \log 3) \tag{3.90}$$
$$T_c = \frac{2J}{\log 3} \tag{3.91}$$

clearly $J \neq 0$ then $T_c \neq 0$. The exact solution is

$$T_c = \frac{2J}{\log(1+\sqrt{2})} \tag{3.92}$$

Thus we can see that spontaneous magnetizaion (phase transition) is possible in 2D for a non zero T. And any higher dimensional lattice undergoes a transition for a non zero temperature.

Chapter 4

Percolation Theory

Percolation theory potentially has been of great interest as it can describe many phenomena [87]. New models and variants of existing model is always welcome due to its importance and of wide interdisciplinary interests. In recent decades there has been a surge of research activities in studying percolation thanks to the emergence of network which has been used as the skeleton for percolation which can mimic structure of many natural and man-made systems.

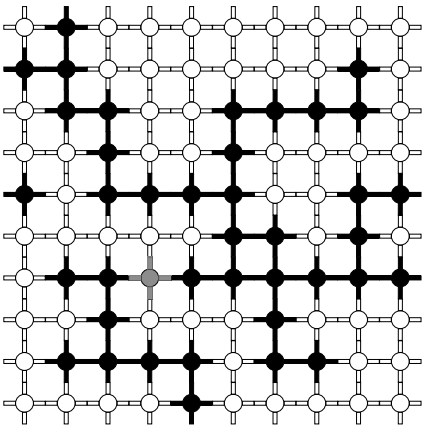
There are several reason to study percolation. First, it is easy to formulate and simple to implement as there is only one control parameter, called occupation probability p 4.4.1. Second, scientists use it as a theoretical model for phase transition, just like architects use geometric model before building large expensive structure, because of its simplicity. Third, it is well endowed with beautiful features and conjectures like finite-size scaling, universality just like its thermal counterpart. Fourth, besides being the paradigmatic model for phase transition, it has been found that the notion of percolation is omnipresent in a wide range of many seemingly disperate systems 4.9.

To study percolation theoretically, the first thing that one need is to choose a skeleton or playground, namely an empty lattice (or a graph/network), consisting of sites (or nodes) and bonds (or links). The definition of the percolation model is then so simple that it merely needs a sentence to define it. Each site or bond of the chosen skeleton, depending on whether we want to study site or bond type percolation, is either occupied with probability p or remains empty with probability $1 - p$ independent of the state of its neighbors. Recently, percolation has received a renewed attention due to widening scope for using complex networks as a skeleton and due to widening extent of using various variants as a rule. In percolation most observable quantities this way or another is connected to clusters, group of contiguous

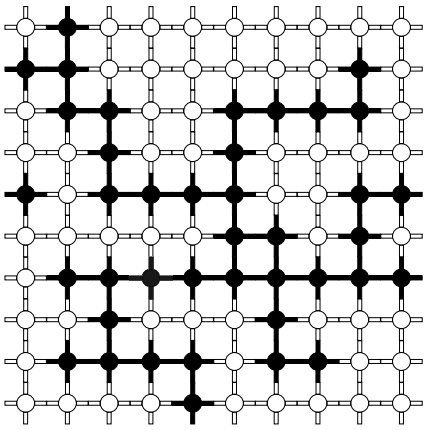
occupied sites form a cluster, or to their distribution function. As the occupation probability p is tuned starting from $p = 0$, one finds that at certain value of $p = p_c$ the observable quantities undergoes a sudden and sharp change which is always regarded as a sign of phase transition. Indeed, the value at which such change occurs is called threshold or critical value which is equivalent to critical temperature of its thermal counterpart. The phase transition that percolation describes is purely geometrical in nature. It requires no consideration of quantum and many particle interaction effects and hence we can use it as a model for thermal Continuous Phase Transition (CPT) like artichect use model before constructing large and complicated structure

4.1 Percolation Phenomena

The word 'Percolation' comes from the coffee percolator but it has nothing to do with coffee brewing. The only connection might be in the concept that lies behind the name. Let's start explaining the phenomena by example. Let's consider a square grid made of conductor of size $L \times L$ containing L^2 sites (insulator).Now we set up an arrangement to put a potential difference across the square grid and measure the effective resistance of the grid as well as the current. Suppose now we start taking of the sites one by one at a random and place a conductor there. We define a parameter called Occupation Probability, p, which is the fraction of the sites replaced as conductor to the total number of sites. We visit all the sites and generate a random number and only if $r <= p$ we replace the site with a conductor. We observe that the electric conductance of the grid will be found to increase with increasing sites being replaced by conductors. As the sites are being turned into insulators, the value of p changes. We see that at a certain value of p , the electricity starting flowing. This particular value is known as Percolation Threshold, p_c . This vanishing resistance occurs when a particular amount of sites turns into conductors from insulators that causes the system to get the connection between the two end across polarity. The exact value of p_c has been found to be close to 0.5927. One can never expect to get the value each time they perform this experiment, infact, the chance of getting this exact value at any experiment can be one in a million. So we do this same experiment a number of times and then average over the value to get a better result. This example shows a simple way of understanding the phenomenon that we call percolation. The theory which simulates this kind of phenomenon is known as Percolation Theory. It provides a quantitative description of the nature of continuous pathways through space. The usual objective of research implementing this phenomenon is to characterize some aspect of the critical phenomena of the phase transition between



(a) One step away to flow current from top to bottom only if the gray site is next to be occupied.



(b) Current flows from top to bottom for the first time, i.e. $p = p_c$.

Fig. 4.1 percolation phenomena in square structure. No current if $p < p_c$.

finite and infinite range connectivity. This is actually non-trivial when the space is randomly disordered and the connected regions acquire fractal properties [101, 72].

4.2 Historical Overview

In 1941, the idea of percolation was first conceived by Flory [44] in the context of gelation transition. But as a mathematical model, it was formulated in the late fifties, to understand the motion of gas molecules through the maze of pores in carbon granules filling a gas mask. This seminal work was done by Simon Broadbent and John Hammersley [24], an engineer and a mathematician respectively. Later on, percolation problem was popularized in physics community by Cyril Domb, Michael Fisher, John Essam and M.F. Skyes [40, 42]. Another remarkable work was the observation of percolation to be the limiting case of the general Potts model, which includes the Ising model and can be solved exactly which is done by Fortuin and Kasteleyn in 1969 [61]. This work paved the way to many exact results in percolation, and also allowed the usage of powerful re-normalization group ideas [27]. Finding percolation threshold both exactly and by simulation has been an enduring subject of research in this field [90], as well as the development of algorithms such as those by Hoshen and Kopelman [55], by Leath [65], and by Newman and Ziff [77] (which we have used in our research). Finding rigorous proofs of exact thresholds and bounds has also been an enduring area of research for mathematicians (Kesten [62], Wierman [97], Bollobas and Riordan [22] etc.) Another infusion of interest in percolation came from the surgin field of network theory which goes back to the study of random and complete graphs by Erdos-Renyi(1959). In ER

model, an observation of made of formation of a giant component, this giant component is exactly analogous to the formation pattern in percolation [1, 39]. It was then revitalized by interest in the small world phenomenon and Scale free networks. In 2000, Newman and Moore found the critical point for a random graph in the limit of large size, in which case the system is effectively a Bethe lattice, and this result connects to the early work of Flory, Fisher and Essam, but it was found with a general degree distribution [75]. In the field of random networks, the model of explosive percolation was first introduced by Achlioptas, D'Souza and Spencer [9], and this has been another fascinating problem which has led to a wave of new interest in percolation.

4.3 Classifications and Playground

Any percolation problem have two major parts, one is the rule which states how and what to occupy and connect and another is a playground on which we apply the rules. The term spanning cluster is the cluster that connects the opposite boundary of a playground. If, however, the system has no boundary then it is measured in terms of largest cluster and is called Giant Connected Component or GCC and it only appears if the system has reached or passed the threshold.

4.3.1 Types of Percolation

Since the first percolation model studied was Bernoulli percolation (In this model all bonds are independent. This model is called bond percolation by physicists) through time physicists have defined different types of percolation model in different types of skeleton or playground. Here we discuss some of the most used percolation types.

Bond Percolation

In bond (or edge, link) percolation we occupy the bonds with probability p and we use sites to connect the bonds together. The cluster size is measured in terms of the number of sites in the cluster. If p is below a critical value p_c then there is no spanning cluster (or GCC) and if $p \geq p_c$ then we will have a spanning cluster or GCC.

Site Percolation

In site (or vertex, node) percolation we occupy the sites. According to the definition of site percolation we use sites to measure the cluster size. But in order to keep it consistent with

the laws of thermodynamics we have changed the definition [84]. Now we use bonds to measure the cluster size while we occupy sites. This change of definition does not effect the exponent that describe the phase transition. Before the critical point where $p < p_c$ there is not spanning cluster and if $p = p_c$ the spanning cluster appears for the first time and it remains as the largest cluster of the system. All the property that describes the phase transition are present at $p = p_c$ and this is where we study them.

Explosive Percolation

In 2009 Achlioptas et al. proposed a biased occupation rule, known as the Achlioptas process (AP), that encourages slower growth of the larger clusters and faster growth of the smaller clusters instead of random occupation in classical percolation [9]. According to this rule a pair of links or, bonds are first picked uniformly at random from all possible distinct links. However, of the two, only the one that satisfies the pre-selected rule is finally chosen to occupy and the other one is discarded. The preset rule is usually chosen so that it discourages the growth of the larger clusters and encourages the growth of the smaller clusters. As a result, the percolation threshold is delayed and hence the corresponding p_c is always higher than the case where only one bond is always selected. Furthermore, it is natural to expect that close to p_c nearly equal sized clusters, waiting to merge, are so great in number that occupation of a few bonds results in an abrupt global connection and thus the name "Explosive Percolation" (EP). Investigation of Achlioptas processes on different types of substrate networks and with different choices of rules especially with the aim of developing rules that do not use global information about a graph is an active area of research.

K-Core Percolation

The K-core of an unweighted, undirected network is the maximal subset of nodes such that each node is connected to at least K other nodes [93]. Determining K-cores computationally is fast and they are insightful in many situations [37, 35]. Every undirected, unweighted network has a K-core decomposition. K-shell of a network is defined as the set of all nodes that belong to the K-core but not to the $(K+1)$- core. K-core is given by the union of all c-shells for $c >= K$ and the K-core decomposition is the set of all of its c-shells. One can examine the K-core of a network as the limit of a dynamical pruning process. Starting with the initial network we delete all nodes with fewer than k neighbors. After this pruning, the degree of some of the remaining nodes will have been reduced. Repeating this process to delete nodes will give a network which will have fewer than K remaining neighbors. Iterating this process until no further pruning is possible leaves the K-core of the network [83].

Bootstrap Percolation

Bootstrap percolation is an infection-like process in which nodes becomes infected if sufficiently many of their neighbors are infected [10]. In bootstrap percolation, sites on an empty lattice are first randomly occupied and then all occupied sits with less than a given number m of the occupied neighbors are successively removed until a stable configuration reached. On any lattice for sufficiently large m, the ensuing clusters can only be infinite. On a Bethe lattice for $m \geq 3$, the fraction of the lattice occupied by infinite clusters discontinuously jumps from zero at the percolation threshold. From an analysis of stable and metastable ground state of the dilute Blume-Capel model [18], it is concluded that the effects like bootstrap percolation may occur in some real magnets [29].

Other

Apart from the type of percolation process described briefly above there are numerous other types of percolation. In *Limited Path Percolation*, one construes "connectivity" as implying that sufficiently short path still exists after some network components have been removed [67]. The percolation of K-cliques (completely connected sub-graphs of K nodes) has been used to study the algorithmic detection of dense sets of nodes known as "communities" [81]. Various percolation processes have also been studied in several different types of multi-layer networks (e.g. multiplex networks and interdependent networks) [20, 64]. Another class of models results if we remove the restriction of a lattice and allow particles to occupy positions which vary continuously in space. *Continuum Percolation* [51, 82, 21], as it is called, suffers from the added complication that tricks which can sometimes be used on lattice models cannot be applied. A quite different process as *Invasion Percolation* [49, 70, 99]; its invention was prompted by attempts to understand flow in porous media. Random numbers are assigned to each site of a lattice. Choose a site, or sites, on one side of the lattice and draw a bond to the neighbor which has the lower random number assigned to it. (The growing cluster represents the invading fluid with the remainder of the sites representing the initial, or defending, fluid). This process continues until the cluster reaches the other side [66].

4.3.2 Types of Playground

Apart from the rules we need a playground to study percolation. Most used playground is described in the following.

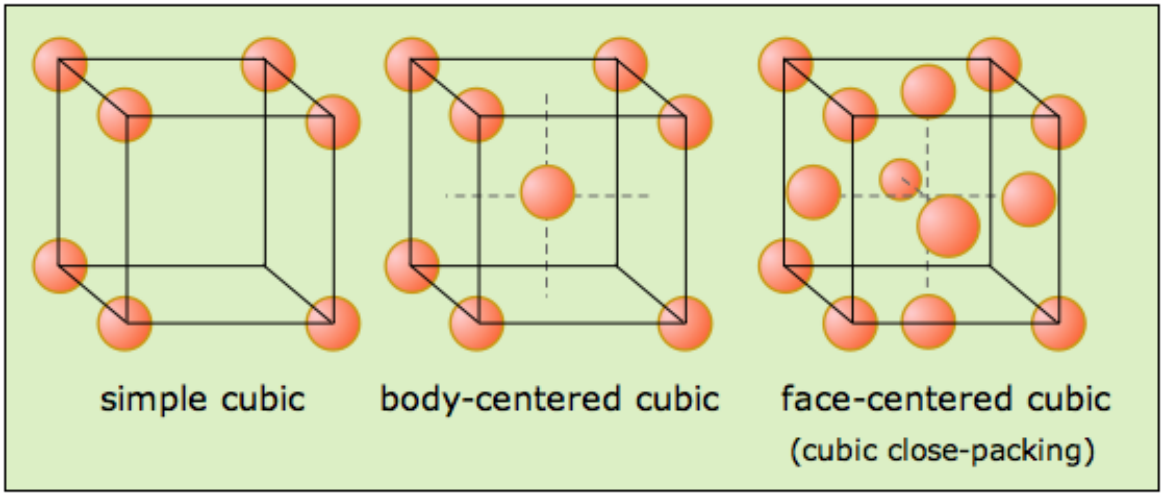
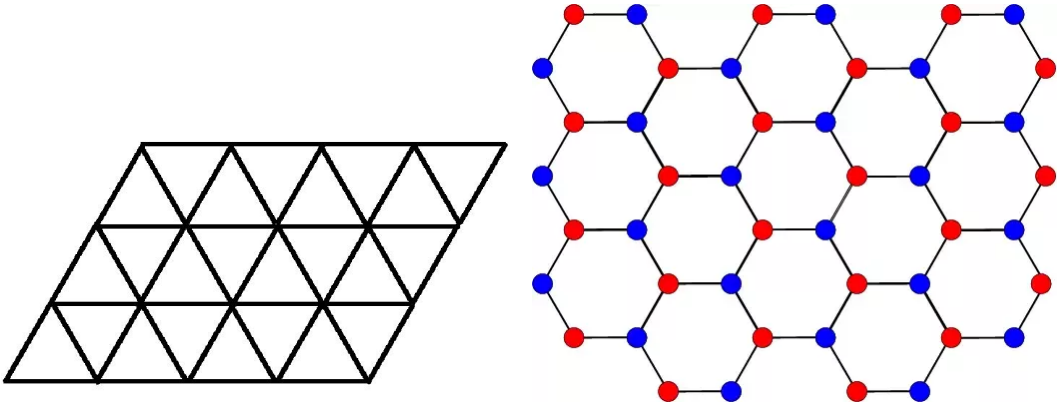


Fig. 4.2 Different types of cubic lattice [2]



(a) Triangular Lattice [2] (b) Honeycomb Lattice [4]

Fig. 4.3 Different types of cubic lattice

Lattice

Percolation was mainly studied on different types of lattice. For example, Honeycomb lattice, Bethe lattice, Simple Cubic lattice, Body-Centered-Cubic lattice, Face-Centered-Cubic lattice. In 1998 Christian D. Lorenz et al. did extensive Monte Carlo simulation to study bond percolation on the simple cubic, face-centered-cubic and body-centered-cubic lattices using epidemic approach. There simulations provide very precise values of the critical thresholds [68]. They calculated Fisher exponent, τ, the finite-size correction exponent, Ω and the scaling function exponent, σ confirmed to be universal. They also did percolation on the HCP (hexagonal closed packed) lattice [69]. Before that in 1981 JC Wireman studied bond percolation on honeycomb and triangular lattices [98].

Furthermore, an exact solution on Bethe lattice for high density percolation was done by G. R. Reich and P. L. Leath in 1978 [85] and J. Chalupa et al. did bootstrap percolation on Bethe lattice in the following year [29].

Graph or Network

A new playground was added to the world of percolation in 1959 when two prominent mathematicians of all time, Paul Erdos and Alfred Renyi introduced Random Graphs []. Before that, it was mostly popular among the mathematicians but not that much fascinating for most of the physicists because of its abstraction. But with the advent of scale free networks [8] which mimics the real life networks such as citation network, social network, protein-protein interaction, in 1999, physicists became much more interested in random networks. The difference in the terminology like graphs and networks are just graphs are mostly used by mathematicians and computer scientists and networks is mainly referred by physicists to the same concept. Duncan S. Callaway and his group did percolation study to find robustness and fragility [26]. Clique percolation is also studied on random networks [36]. A critical phenomenon analysis on random networks for core percolation is done by Bauer [16]. In early 80's, before the birth of scale free networks, C McDiarmid did two significant works which you can find in the references [].

Reuvan Cohen et al. studied scale free networks close to the percolation threshold [32]. N. Schwartz et al. worked on percolation problem in directed scale free networks [91]. Filippo Radicchi and Santo Fortunato studied scale-free networks constructed via a cooperative Achlioptas Growth Process [9]. They showed that networks constructed via this biased procedure show a percolation transition which strongly differes from the one observed in standard percolation, where links were introduced just randomly.

4.4 Basic Elements

In this section we discuss some of the basic elements of percolation. All the observable quantities depends on these elements.

4.4.1 Occupation Probability

The probability at which each site (bond) is occupied is called occupation probability in site (bond) percolation and it is denoted as p. In section 4.7 we discuss who we determine p in

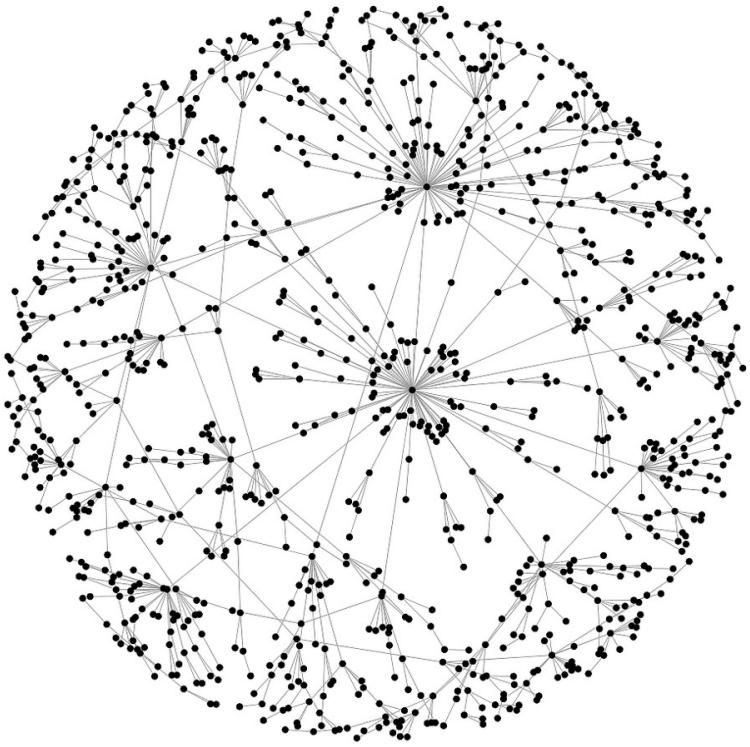


Fig. 4.4 Scale Free Network [5]

percolation. Simply saying, instead of fixing p for one experiment we can find all quantity for each values of p using the famous Ziff algorithm [76, 77].

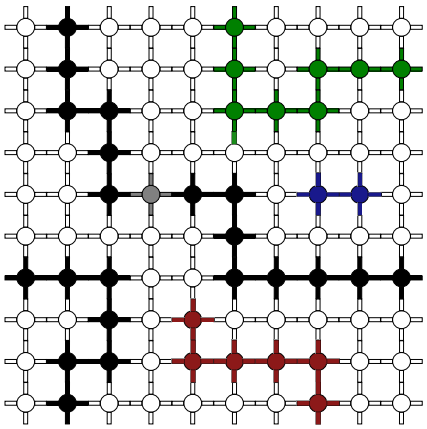
4.4.2 Cluster

Cluster is a collection of sites and bonds. In bond percolation we occupy bond and measure cluster size in terms of the number of sites in it. And following this idea we measure the cluster size in terms of the number of bonds in it. Which is the new definition of site percolation [84]. Measuring cluster size in terms of the number of bonds in it in site percolation reproduces all known results and it is consistent with laws of thermodynamics.

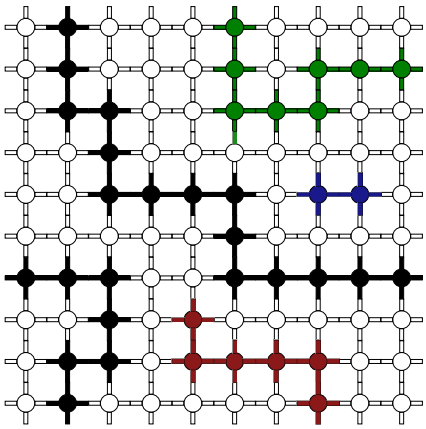
4.4.3 Spanning cluster

4.5 Observable Quantities

In percolation we study formation of clusters, their properties such as how they are distributed as a function of control parameter p. A cluster is a group of occupied bonds (sites) in site (bond) percolation [84] With no gap or unoccupied object between them. In a network cluster



(a) One step away from threshold. Since the gray site is not occupied. The moment it gets occupied we reach percolation threshold



(b) The gray site gets occupied and a wrapping cluster appears for the first time. We have reached percolation threshold

Fig. 4.5 A square lattice of length $L = 10$. Demonstrating the appearance of the wrapping cluster

is defined as a group of nodes that connects the links. In this section we discuss some of the most used observable quantities in percolation.

4.5.1 Percolation Threshold, p_c

The idea of percolation threshold is a mathematical concept that deals with formation of long range connectivity in random systems. While there are no existence of a giant connected component that are talked about below the threshold, its existence is well present above it. As the occupation probability increases from 0 toward 1, average cluster size also increases and among all cluster one cluster pops up to be the spanning cluster at p_c. Hence p_c is the percolation threshold or critical point. In the thermodynamic limit this cluster becomes infinitely large. Thus for $p < p_c$ there is no spanning cluster and for $p \geq p_c$ there is one. The spanning cluster is a special type of cluster which spans the entire lattice. In periodic case we call it wrapping cluster. A figure illustrating this process is given here 4.5. Percolation threshold has been determined for different types of lattices. The table 4.1 shows some of them.

One simple way of obtaining p_c is to perform M number of independent experiment for a particular L and them take the average

$$p_{c_avg} = \lim_{M\to\infty} \frac{1}{M} \sum_i p_{c_i} \tag{4.1}$$

Lattice	p_c, site percolation	p_c, bond percolation
Body Centered	0.246	0.1803
Face Centered	0.198	0.119
Simple Cubic	0.3116	0.2488
Diamond	0.43	0.388
Honeycomb	0.6962	0.65271
Triangular	0.50	0.34729
Square	0.592746	0.50

Table 4.1 Percolation Threshold for Some Regular Lattices

But performing infinite number of experiment is not possible. So we use another approach which is described in section 4.5.2 and 5.4.1

4.5.2 Spanning Probability, $w(p,L)$

The best quantity for finding the critical exponent ν is the spanning probability $W(p,L)$. It describes the likelihood of finding a cluster that spans across the entire system of length L either horizontally or vertically at a given occupation probability p. To find $W(p,L)$ we perform say M independent realizations under the same identical conditions. In each realization for a given finite system size we take record of the p_c value at which there appears a spanning cluster for the first time. If there is a spanning cluster at $p = p_{c_i}$ then it means that there exists a spanning cluster for all $p_{c_i} \leq p \leq 1$. To find a regularity or a pattern among all the M numbers of p_c values recorded, one usually looks at the relative frequency of occurrence within a class or width Δp. To find $W(p,L)$, we can process the data containing M number of p_c values to plot histogram displaying normalized relative frequency as a function of class of width Δp chosen as per convenience [84]. Figure 5.1 shows spanning probability $w(p,L)$ as a function of p and L. Clearly all curves meet at a specific point regardless of system length L. Thus we can say if $L \to \infty$ the curve would still go through that point and that's how we get the p_c value. Then if we apply scaling on the x-axis by $(p-p_c)L^{1/\nu}$ we would get a perfect data collapse for a specific $1/nu$ that is our exponent. This process is discussed further in section 5.4.1 and 5.4.2.

4.5.3 Entropy, $H(p,L)$

Entropy in one of the key feature of a phase transition model. But thermodynamic entropy, e.g. Boltzmann entropy or Clausius entropy, cannot be calculated for any model that depends on a probabilistic theory such as our percolation on a square lattice model. So we take

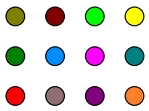
our approach in another way. Information entropy or the *Shanon entropy* is best suited for our model. The concept of Shannon entropy in information theory describes how much information there is in a signal or event. This concept of information entropy was introduced by Claude Shannon in his 1948 [95]. The seminal work of Shannon based on papers by Nyquist [78, 79] and Hartley [53]. He rationalized these early efforts into a coherent mathematical theory of communication.

The Defition of Shannon entropy is

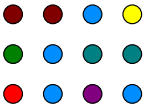
$$H = -\sum_i \mu_i \log \mu_i \tag{4.2}$$

where, μ_i is the probability of getting i-th element.
As we have seen in section 3.2.1 that the entropy measures disorderness of a system. It is also easy to understand order and disorder in solid to liquid transition. But it is not that easy in percolation since the idea of order and disorder in percolation is not yet clear. To understand disorder, let us consider that at $p = 0$ we have 12 isolated sites and each has different color to identify them visually, figure 4.6. Thus each color corresponds to one distinct cluster. Occupation of a bond means merging of two colors into one. If one of the components is bigger in size than the other then the newly merged cluster will take the color of the bigger cluster and if they are equal then we choose one at random. If we now continue to occupy all the frozen bonds then we will finally have one cluster of one color. Initially at $p = 0$ we have 12 different colors and hence it can easily be regarded as the most disordered state. On the other hand, at the other extreme we will have only one cluster represented by one color which can be regarded as the ordered state. We can easily extend the problem to a system that contains N number of sites but colored with 12 colors only such that $n_1, n_2, \ldots, n_{12}$ of them are red, orange, ..., violet respectively and hence we can define $\mu_i = n_i/N$. We now make M number of independent attempts to pick one site at each attempt from N sites at random with uniform probability. Say, that we found n_1' times red, n_1' times orange, and so on such that $\sum_{i=1}^{m} n_i' = M$. We assume that both N and M are sufficiently large and $M \approx N$. The total number of ways we could have M outcomes are

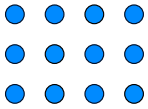
$$\Omega = \frac{M!}{\left(M_{\mu_1}\right)!\left(M_{\mu_2}\right)!\ldots\left(M_{\mu_m}\right)!} \tag{4.3}$$



(a) Entropy of this system is in minimum



(b) Entropy of this system is in between maximum and minimum



(c) All distinct cluster. A system of maximum entropy

Fig. 4.6 A system of 12 cluster

since $n_i' \approx M_{\mu_i}$. Taking log on both side of the above equation and using the String's approximation $\log(M!) = M\log M - M$ for very large M we get

$$\begin{aligned}
\log\Omega &= \log M! - \log\left(\prod_i M_{\mu_i}\right) \\
&= M\log M - M - \sum_i \log\left(M_{\mu_i}!\right) \\
&= M\log M - M - \sum_i \left[M_{\mu_i}\log M_{\mu_i} - M_{\mu_i}\right] \\
&= M\log M - \sum_i M_{\mu_i}\log M_{\mu_i} \\
&= M\log M - M\sum_i \frac{M_{\mu_i}}{M}\left[\log\left(\frac{M_{\mu_i}}{M}\right) + \log M\right] \\
&= M\log M - M\sum_i \mu_i \log\mu_i + M\sum_i \frac{M_{\mu_i}}{M}\log M
\end{aligned} \tag{4.4}$$

Finally we have,

$$\log\Omega = -M\sum_{i=1}^{m}\mu_i\log\mu_i = MH(\mu) \tag{4.5}$$

where $H(\mu)$ is nothing but the Shannon entropy $H(p)$ and clearly it is the degree of uncertainty per attempt. Total entropy or information is therefore equal to NH if we consider $M = N$. In the case when each site has distinct color then each site will have the equal chance of being picked. It means $\mu_i = 1/N \forall i$ and hence $H(\mu) = N\log(N)$ which is the average entropy or degree of disorder and the total entropy is $NH(\mu)$. Now initially if we had N distinct color then the system would have the maximum entropy $S = N\log N$. On the other hand, if all the sites had the same color then the system would have minimum entropy $S = 0$. Thus percolation is indeed an order-disorder transition where disorder is equivalent to degree of confusion [84]. Now recall the definition of Boltzmann entropy in equation 3.19. If we consider $K_B = 1$ then we get Shannon entropy to represent Boltzmann entropy.

worked out example

Say we have a coin with a head and a tail. If the coin is unbiased then the probability of getting the head or the tail is 50% or 0.5. Now what's the entropy of this system? The Shanon entropy is the one that can be used here. For convenience $\log_2$ will be used for evaluating logarithms here, after all $\log_2 = const.\log_{10} = const.\log_e$. Here, $\mu_i = 0.5$ and $\log_2(0.5) = -1$, Therefore we have

$$\begin{aligned} H &= -(0.5\log_2(0.5) + 0.5\log_2(0.5)) \\ &= -(0.5 \times (-1) + 0.5 \times (-1)) \\ &= 1 \end{aligned}$$

so in this system entropy is 1.
Now take a new system where there is 4 identical object. Since all objects are identical, each have probability $\mu_i = 1/4$ and $\log_2(1/4) = -2$. Then the total entropy of that system is 2. So this is clear that the entropy increses with the increase of the system size. Here system size is determined by the number of particles in it. Now, let's take a non-uniform system, where there are total 8 particles and there are 4 cluster. Cluster 1 has 4 particles and cluster 2 has 2 particles and other 2 cluster of 1 particle each. Probability of getting cluster 1 is $\mu_1 = 4/8$ and for cluster 2 it is $\mu_2 = 2/8$ and for other clusters it is $\mu_3 = \mu_4 = 1/8$. Now the entropy of the system becomes,

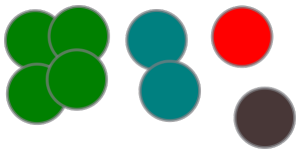
$$\begin{aligned} H &= -\sum_i \mu_i \log_2 \mu_i \\ &= -(4/8\log_2(4/8) + 2/8\log_2(2/8) + 1/8\log_2(1/8) + 1/8\log_2(1/8) \\ &= -(-1/2 - 1/2 - 3/8 - 3/8) \\ &= 7/4 \end{aligned}$$

which is less then the entropy of a system where all 8 particles are disconnected, i.e., $H = 3$. So we can see that as the particles are joined together entropy reduces, which is in agreement with the experimental results.

4.5.4 Specific Heat, $C(p,L)$

According to the definition of specific heat in thermodynamics 3.27 we can find specific heat if we know the temperature and entropy. In percolation theory we measure the Shannon

(a) Free particles. $H = 3$



(b) Some Free and Some Bound Particles. $0 < H < 3$

(c) Bount particles. $H = 0$

Fig. 4.7 entropy of a system of 8 particles

entropy, $H(p,L)$. And we use $(1-p)$ as the analogue of temperature which gives

$$C = (1-p)\frac{dH}{d(1-p)} \tag{4.6}$$

$$= -(1-p)\frac{dH}{dp} \tag{4.7}$$

using this definition we can easily find the specific heat of the percolating system. And from specific heat we obtain the critical exponent α.

4.5.5 Order Parameter, $P(p,L)$

From above discussion we can say that if $p \geq p_c$ the spanning cluster exists but we still cannot say if a randomly chosen site belongs to the spanning cluster. Therefore we need to quantify the strength of the spanning cluster. Percolation strength or P is defined as the probability to find the site that belongs to the spanning cluster, meaning randomly pick a site and what is the probability that the selected site will belong to the spanning cluster. And this quantity should depend on occupation probability p and system size L. We call it Percolation Strength or sometimes Order Parameter as it describes the measure of order in the system. Order means the likeliness of not getting confused. If all clusters of same size, i.e. identical, we will get confused which cluster we have chosen ($p = 0$ case) but if there is only one cluster there is no chance of confusion ($p = 1$ case).

We define the percolation strength as

$$P = \frac{\text{number of sites in the spanning cluster}}{\text{total number of sites in the lattice}} \tag{4.8}$$

But in a system where there are no boundary, e.g. a network or Bethe lattice, the idea of spanning cluster is not valid. Then we use the largest cluster to define the percolation strength

$$P = \frac{\text{number of nodes in the largest cluster}}{\text{total number of nodes in the network}} \tag{4.9}$$

Both definition, though looks a bit different when plotted, gives the same critical exponent β. How to find this exponent is shown in section 5.4.4.

Mathematically

$$P(p,L) = \frac{K}{\sum_i k_i} \tag{4.10}$$

where K is the size of the spanning cluster and k_i is the size of the $i-th$ cluster. Percolation strength is the Order parameter of the system which is the measure of Order of a system. Note that, with periodic boundary condition we have

$$\sum_i k_i = L^2 \tag{4.11}$$

and without periodic boundary condition

$$\sum_i k_i = L(L-1) \tag{4.12}$$

4.5.6 Susceptibility, $\chi(p,L)$

4.5.7 Mean Cluster Size, S

4.5.8 Cluster Size Distribution Function, n_s

$$n_s(p_c) \sim s^{-\tau} \tag{4.13}$$

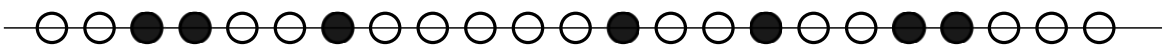


Fig. 4.8 One Dimensional Lattice. Empty ones are white and filled ones are black.

4.5.9 Correlation Function, $g(r)$

4.5.10 Correlation length, ξ

4.5.11 Fractal Dimension, d_f

4.6 Exact Solutions

Percolation problem can be solved exactly in 1 and ∞ dimension. In dimension $1 < d < \infty$ there is not analytical solution, it can only be solved approximately using simulations. Analytic solution in dimension greater than 1 and less than ∞ is a still to be solved problem. Interestingly, many of the features found in one dimension seem to be valid for higher dimensions too. Thus using the insight of these exact solutions in 1 and ∞ dimension we get a window into the world of phase transitions, scaling and critical exponents.

4.6.1 One Dimension

Threshold

The simplest lattice one can think of is the one dimensional lattice. It consists of many sites arranged at an equidistant positions along a line. Each site of the lattice can either be occupied with probability p or remain empty with probability $1-p$. Thus there are only two possible states of each site. A cluster is a group of neighboring occupied sites which contains no empty sites in between. A single empty sites splits a cluster into two clusters. If we find n successive occupied sites, we say that it forms a cluster of size n. We want to find the probability at which an infinite cluster appears for the first time, i.e., the critical occupation probability.

Let $\omega(p,L)$ is the probability that a linear chain of size L has percolating cluster at probability p. Note that, if two sites form one cluster, the probability that we find such cluster is p^2. Similarly if we want a cluster containing L sites the probability is $\omega(p,L) = p^L$, means L successive sites are occupied independent of each other.

$$\lim_{L\to\infty} omega(p,L) = \begin{cases} 0\ ,\ \forall p < 1 \\ 1 \text{only if p = 1} \end{cases} \tag{4.14}$$

For $p = 1$ all sites of the lattice are occupied and a percolating cluster spans from $-\infty$ to ∞ so that each and every and every sites of the lattice belong to the percolating cluster.For $p < 1$ we will have on the average $(1-p)^L$ empty sites. So if $L \to \infty$, we have $(1-p)^L \to const.$ revealing that there will be at least one, if not more, empty site somewhere in the chain. Which proves that as long as $p < 1$ there is no spanning cluster. Thus the percolation threshold or the critical occupation probability in one dimension is

$$p_c = 1 \tag{4.15}$$

Cluster Size

A cluster of size s,a.k.a. s-cluster, is formed when s successive sites are occupied and they are surrounded by two empty sites. Probability of s successive sites are being occupied is p^s and 2 sites are unoccupied is $(1-p)^2$. Thus the probability of picking a cluster at random that belongs to an s-cluster is

$$n_s = p^s(1-p)^s \tag{4.16}$$

n_s is also the number of s-clusters per lattice site. Note that the state of one particular site is independent of any other sites, that's why we multiply probabilities. Further manipulation of equation 4.16 gives

$$n_s = (1-p)^2 \exp(s \ln p) = (1-p)^2 \exp(-s/\xi) \tag{4.17}$$

where ξ is the correlation length and defined as

$$\xi = -\frac{1}{\ln p} = -\frac{1}{\ln(p_c - (p_c - p))} \sim (p - p_c)^{-1} = (p - p_c)^{\nu} \tag{4.18}$$

in the limit $p \to p_c$ and since $p_c = 1$.

Mean Cluster Size

The probability that an arbitrary site is in s-cluster is larger by a factor of s. This site can be any of the sites in the s-cluster. The probability that an arbitrary chosen site belongs to a cluster of size s is $n_s s$, since n_s is known to be the number of s-clusters per lattice site. Every occupied site must belong to one cluster even if it is a cluster of only one site, i.e., a cluster of size unity. The probability that an arbitrary site belongs to a cluster is therefore proportional

to the probably p that it is occupied.

$$\sum_{s=1}^{\infty} sn_s = \frac{numberoftotaloccupiedsites}{numberoftotallatticesites} = p \tag{4.19}$$

A quick check of the validity of equation 4.19 can be performed using equation 4.16.

$$\begin{aligned}
\sum_{s=1}^{\infty} sn_s &= \sum_s s(1-p)^2 p^s \\
&= (1-p)^2 \sum_s sp^s \\
&= (1-p)^2 \sum_s p\frac{d(p^s)}{dp} \\
&= (1-p)^2 p\frac{d\sum_s p^s}{dp} \\
&= (1-p)^2 p\frac{dp(1-p)^{-1}}{dp} \\
&= (1-p)^2 p\left(\frac{1}{1-p} + \frac{p}{(1-p)^2}\right) \\
&= p
\end{aligned} \tag{4.20}$$

Here we have used the series sum 4.21.

$$\begin{aligned}
\sum_s p^s &= p + p^2 + p^3 + \ldots \\
&= p(1 + p + p^2 + \ldots) \\
&= p(1-p)^{-1}
\end{aligned} \tag{4.21}$$

An important question one can ask is that what is average size of the cluster that we are hitting. Since $n_s s$ is the probability that an arbitrary site belongs to an s-cluster and $\sum_s n_s s$ is the probability that it belongs to any cluster. Thus we define w_s as

$$w_s = \frac{n_s s}{\sum_s n_s s} \tag{4.22}$$

w_s is the probability that the cluster to which an arbitrary occupied site belongs contain exactly s sites. The average cluster size S is therefore

$$S = \sum_s w_s s \tag{4.23}$$

This equation is very much similar to

$$\bar{x} = \int xp(x)dx \tag{4.24}$$

using equation 4.22 we get

$$\begin{aligned}
S &= \frac{\sum_s n_s s^2}{\sum_s n_s s} \\
&= \sum_{s=1}^{\infty} \frac{s^2 n_s}{p} \\
&= \frac{(1-p)^2}{p} \sum_{s=1}^{\infty} s^2 p^s \\
&= \frac{(1-p)^2}{p} \left(p\frac{d}{dp} \right)^2 \left(\sum_{s=1}^{\infty} p^s \right) \\
&= \frac{(1-p)^2}{p} \left(p\frac{d}{dp} \right)^2 (p(1-p)^{-1}) \\
&= p(1-p)^2 \frac{d^2}{dp^2}(p(1-p)^{-1}) \\
&= p(1-p)^2 \frac{d}{dp}(1-p)^{-2} \\
&= p(1-p)^2 2(1-p)^{-3} \\
&= \frac{2p}{1-p} \\
&= \frac{1+p}{1-p}
\end{aligned} \tag{4.25}$$

we can write

$$S(p) = \frac{1-p}{1+p} = \frac{p_c + p}{p_c - p} \tag{4.26}$$

using the fact that $p_c = 1$ in 1D lattice. This equation reveals that the mean cluster size diverges for $p \to p_c$ where the minus sign signifies that we are approaching from below p_c. This is in sharp contrast with higher dimensional ones where we can approach to p_c from either end while in one dimension we cannot have access to the state $p > p_c$. We thus find the mean cluster size diverges following power law as we have [54]

$$S(p) \sim (p_c - p)^{-1} \tag{4.27}$$

We encounter the similar behaviour in the higher dimensions also.

Correlation Function and Correlation Length

The correlation function or pair connectivity $g(r)$ is the probability that a site at position r from an occupied site belongs to the same finite cluster. We are not including the contribution of the infinite cluster. This is valid infinite cluster does not exists as long as $p < 1$. Let $r = 0$ then $g(r = 0) = 1$ since the site at $r = 0$ is the selected occupied site by definition. For 1D case a site at r to be occupied and belongs to the same finite cluster, we will need r subsequent sites and the probability of getting this is p^r. Therefore

$$g(r) = p^r \tag{4.28}$$

It can also be expressed in terms of correlation length ξ

$$g(r) = \exp(\ln(p^r)) = \exp(-r/\xi) \tag{4.29}$$

where ξ is the correlation length 4.18.
Now that we have correlation function, we can define mean cluster size in terms of it

$$S = 1 + \sum_{r=1}^{\infty} g(r) \tag{4.30}$$

At this point it is evident that the cutoff cluster size s_ξ , mean cluster size $S(p)$, and correlation length ξ diverges at the percolation threshold. The divergence has the form of a simple power law of the distance from the critical occupation probability. In higher dimensional percolation problem this observation is also valid.

4.6.2 Infinite Dimension

Apart from one dimension percolation problem can be solved in infinite dimension. For this we need a suitable playground such as Bethe lattice. Bethe lattice lattice is a special type of lattice where each site has z neighbors and each branch gives rise to $(z-1)$ other branches. Figure 4.9 shows the Bethe lattice for $z = 3$. Note that for $z = 2$ we have nothing but the one dimensional lattice.

Properties of infinite dimensional object

For a 3D object the surface area is has dimension to L^2 and volume as dimension L^3. The same pattern is true of object in any dimension. If we denote area by A and volume by V for

any dimension we have

$$A \propto V^{1-1/d} \tag{4.31}$$

now as $d \to \infty$ we have

$$A \propto V \tag{4.32}$$

Therefore if we find that the area of any object is proportional to its volume we can say it is an infinite dimensional object.

Bethe Lattice

In order to construct Bethe lattice for any z we start with a central point which will be connected to z sites. For example if $z = 3$ then we will have a central site connected to 3 sites by a branch and when we go to next layer each branch will be divided to 2 more branches and this process will be continued up to r layers 4.9. Only at the surface of the lattice, where the branching is stopped, is only one bond or branch connecting the surface site to the interior. There is only open loops in this structure, which means that if we never change direction always reach new site if we never go back.Number of sites in the Bethe lattice increases exponentially with the distance from the origin, whereas in any d-dimensional lattice structure it would increase with distance d . In the case of Bethe lattice with $z = 3$, the origin is surrounded by a shell of three sites ("first generation"), in the second shell we have six sites followed by a third generation of twelve sites, etc. After r generation the total number of sites in the Bethe lattice is

$$1 + 3 \times (1 + 2 + \ldots + 2^{r-1}) = 3.2^r - 2 \tag{4.33}$$

The number $3 \times 2^{r-1}$ is the number of sites at the surface. Here we have used the following finite series sum

$$1 + 2 + 2^2 + 2^3 + \ldots + 2^r = 2^{r+1} - 1 \tag{4.34}$$

And if we measure the surface to volume ratio we get

$$\frac{A}{V} = \frac{number of sites in the surface}{total number of sites} = \frac{3 \times 2^{r-1}}{3 \times 2^r - 2} \tag{4.35}$$

as $r \to \infty$ we get

$$\frac{A}{V} \sim \frac{3 \times 2^{r-1}}{3 \times 2^r} = \frac{1}{2} = constant \tag{4.36}$$

Therefore Bethe lattice is indeed an infinite dimensional lattice.

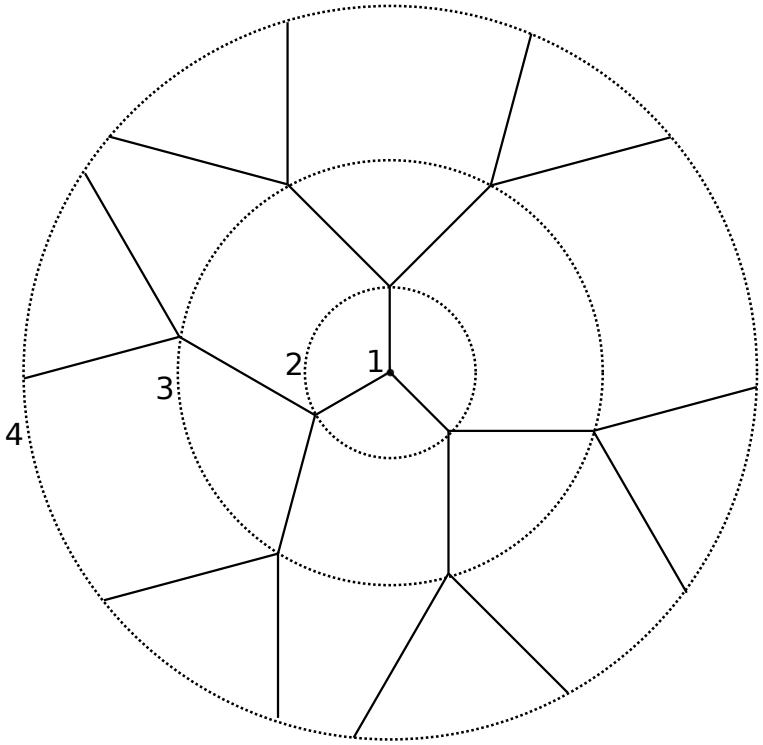


Fig. 4.9 Bethe Lattice for $z = 3$

Percolation Threshold

Percolation threshold of Bethe lattice is the occupation probability at which an infinite cluster appears for the first time. To find it we start walking from the origin and after one step we have $z-1$ new bonds that is connected to $z-1$ new sites in those direction. On the average there will be $(z-1)p$ occupied sites. And for each site there will be another $z-1$ branch and those bonds are connected to $(z-1)p$ sites on the average and so on. After r step we will have an infinite cluster at probability $((z-1)p)^r$. Since $r \to \infty$ we have $((z-1)p)^r = 0$ if $(z-1)p < 1$. Thus we choose $(z-1)p = 1$ so that we will get an infinite cluster. That lead us to the desired critical occupation probability

$$\begin{aligned} (z-1)p_c &= 1 \\ p_c &= \frac{1}{z-1} \end{aligned} \tag{4.37}$$

For $z = 3$ we have $p_c = 1/2$.

Percolation Strength

Percolation strength of an infinite cluster is the probability of any arbitrary site to be the part of the infinite cluster. For the sake of calculation, for $p > p_c$ in the Bethe lattice, we introduce a new quantity Q as the probability that an arbitrary site is note connected to the infinite cluster through a fixed branch originating from this site. Restricting ourselves to the lattice with $z = 3$ and using basic probability theory, the strength

$$P(p) = p(1 - Q^3) \tag{4.38}$$

Here p is the probability that the site is occupied and $(1 - Q^3)$ is the probability that at least one branch is connected to infinity.
The probability that the two subbranches which start at the neighbor are not both leading infinity is Q^2. The quantity pQ^2 is the probability that this neighbor is occupied but not connected to infinity by any of its two subbranches. This neighbor is empty with probability $(1 - p)$, in which case even well connected subbranches do not help it. This gives us,

$$Q = (1 - p) + pQ^2 \tag{4.39}$$

This is the probability that this fixed branch does not lead to infinity, either because the connection is already broken at the first neighbor, or because later something is missing in the subbranch. So the solution of this quadratic equation is

$$Q = 1, \frac{1-p}{p} \tag{4.40}$$

For z neighbors, in general we have

$$Q = 1, 1 - \frac{2p(z-1) - 2}{p(z-1)(z-2)} \tag{4.41}$$

for $p < p_c$, there are no infinite clusters, fo with probability 1 there are no connection to infinity. Now we use Taylor expansion for $P(p)$ around $p = p_c = 1/2$

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p\left(1 - \left(\frac{1-p}{p}\right)^3\right) & \text{for } p \geq p_c \end{cases} \tag{4.42}$$

Let,

$$f(p) = \left(\frac{(1-p)}{p}\right)^3 \tag{4.43}$$

Then

$$\begin{aligned} f'(p) &= -3p^{-}4(1-p)^3 - 3p^{-}3(1-p)^2 \\ &= -\frac{3}{p}\left(\frac{(1-p)}{p}\right)^3 - \frac{3}{p}\left(\frac{(1-p)}{p}\right)^2 \end{aligned} \tag{4.44}$$

$$P(p) = P(p_c) + (p-p_c)P'(p_c) + \ldots \tag{4.45}$$
$$= 0 + (p-p_c)\left(1 - f(p_c) - pf'(p_c)\right) + \ldots \tag{4.46}$$
$$= 6(p-p_c) + \ldots \tag{4.47}$$
$$\tag{4.48}$$

Therefore we get

$$P(p) \propto (p-p_c) \text{ for} p \to p_c^+ \tag{4.49}$$

the critical exponent β is defined by

$$P(p) \propto (p-p_c)^\beta \tag{4.50}$$

Thus in Bethe lattice $\beta = 1$.

Mean Cluster Size

In case of Bethe lattice the mean cluster size is defined as the average number of sites to which the origin belongs. Let T be the mean cluster size for one branch, that is the average number of sites to which the origin is connected and which belongs to one branch. Again, subbranches have the same mean cluster T as the branch itself. If the neighbor is empty the cluster size for this branch is zero. If the neighbor is occupied, it contributes its own mass to the cluster which is unity and adds the mass T for each of its two subbranches. Thus,

$$T = (1-p) \times 0 + p(1+2T) \tag{4.51}$$

Solving this we get

$$T = \frac{p}{1-2p} \tag{4.52}$$

for $p < p_c$.
The total cluster size is zero if the origin is empty and $(1+3T)$ if the origin is occupied.

Therefore the mean cluster size $S(p)$ is

$$S(p) = 1 + 3T \tag{4.53}$$
$$= \frac{1+p}{1-2p}$$
$$= \frac{1+p}{2(p_c - p}$$
$$= \frac{1+p}{2}(p_c - p)^{-1} \tag{4.54}$$

Thus the critical exponent $\gamma = 1$ for Bethe lattice. This is the exact result for mean cluster size and we notice that it diverges for $p \to p_c$.

Correlation Function and Correlation Length

The radial correlation function $g(r)$ is the average number of occupied sites within the same cluster at a distance r from an arbitrary occupied site. The probability that a site at distance r from the origin is occupied and the sites in between are occupied too is equal to p^r. Now if we think about a shell of radius r then the number of all the sites enclosed by this shell is $z(z-1)^{r-1}$. Thus

$$g(r) = z(z-1)^{r-1}p^r \tag{4.55}$$
$$= \frac{z}{z-1}\left(p(z-1)\right)^r \tag{4.56}$$
$$= \frac{z}{z-1}\exp\left[\log\left[p(z-1)\right]\right] \tag{4.57}$$

The value of percolation threshold for Bethe lattice can be found by analyzing the behaviour of the correlation function at large distances, i.e. at r $\to \infty$. For $p(z-1) < 1$, $g(r)$ decreases exponentially, on the other hand for $p(z-1) > 1$, the correlation function diverges which signifies the existence of an infinite cluster. Mathematical treatment yields the correlation length from 4.18

$$\xi = \frac{-1}{\log[p(1-z)]}$$
$$= \frac{-1}{\log(p/p_c)}$$
$$= (p - p_c)^{-1} \tag{4.58}$$

as p approaches p_c, that is $\nu = 1$.
Clearly the 1D lattice and Bethe lattice exhibits power law while we approach a critical value which suggests the same phenomena in other variants of such problems.

4.7 Algorithm

In the classical Hosen-Kopelman algorithm for percolation model [55], one first choose an occupation probability p and then generate a number r for each site of the lattice. The site is occupied if $r \leq p$ and remain empty if $r > p$. One therefore create an entire new state of a given lattice size for every different value of p. Note that the number of occupied sites n for a given p may very in each realization. However, the expected or ensemble average over M experiments will give $n = pM$ in the limit $M \rightarrow$. Thus the number of occupied bonds or sites is also a measure of p. Using this idea Ziff and Newman [77] proposed an algorithm which generate states for each value of n from zero up to some maximum value $n = L^2$ for site percolation on $L \times L$ square lattice for instance. In this way, one can save some effort by noticing the fact that a new state with $n+1$ occupied sites or bonds can be created by adding one extra randomly chosen site or bond to the state containing n sites or bonds. The first step of their algorithm is to decide an order in which the bonds or sites are to be occupied. That is, every attempt to occupy a bond/site is successful.

4.8 Relation of Phase Transition with Percolation

4.9 Application

Ever since the percolation phenomena was discovered it has been extensively used in wide range of science. Some of it is discussed here. Though limited, this discussion gives us the significance of percolation and enables us to appreciate it.

4.9.1 Epidemiology

Many diseases spread through human populations via close physical interactions. The interpersonal contact patterns that underlie disease transmission can naturally be thought to form a network, where links join individuals who interact with each other. During an outbreak, disease then spreads along these links. All epidemiological models make assumptions about the underlying network of interactions, often without explicitly stating them.

Percolation has long been an important tool in infectious disease epidemiology [15]. L Meyers gave a wonderful insight of contact network epidemiology, a more powerful approach that applies bond percolation on random graphs to model the spread of infectious disease through heterogeneous populations [73].

Before that in 2000, Moore et al. studied some simple models of disease transmission on small-world networks [75]. They showed that the resulting models display epidemic behavior when the infection or transmission probability rises above the threshold for site or bond percolation on the network, and they gave exact solutions for the position of this threshold in a variety of cases.

Alessandro Vespignani and his team studied wifi networks and malware epidemiology. They developed an epidemiological model that takes into consideration prevalent security flaws on these routers.They simulated spread of such a contagion on real-world data for georeferenced wireless routers [57].

Sander et al. considered a spatial model related to bond percolation for the spread of a disease that includes variation in the susceptibility to infection. They worked on a lattice with random bond strengths and showed that with strong heterogeneity, i.e. a wide range of variation of susceptibility, patchiness in the spread of the epidemic is very likely, and the criterion for epidemic outbreak depends strongly on the heterogeneity. Their results were qualitatively different from those of standard models in epidemiology, but correspond to real effects [88].

After the birth of scale free network the study of epidemics has become even more popular among statistical physicists.

4.9.2 Neural Network and Cognitive Psychology

Percolation is used to understand the way activation and diffusion of neural activity occur within neural networks [48]. Iian Breskin's team in 2006 studied living neural networks by measuring the neurons' response to a global electrical stimulation. They showed through analysis that neural connectivity is lowered by reducing the synaptic strength, chemically blocking neurotransmitter receptors. They used a graph-theoretic approach to show that the connectivity undergoes a percolation transition. This occurs as the giant component disintegrates, characterized by a power law with an exponent $\beta \simeq 0.65$ [23].

It is easiest to understand percolation theory by explaining its use in epidemiology [75]. Individuals that are infected with a disease can spread it knowingly or unknowingly via social or physical interaction. It's easy to say that the more social a person is the more it is likely that he will spread more disease than the unsocial one. Therefore some factors, e.g.,

occupation, size of social circle etc, influence the rate of infection.

Now, if one were to think of neurons as the individuals and synaptic connections as the social bonds between people, then one can determine how easily messages between neurons will spread [48] When a neuron fires, the message is transmitted along all synaptic connections to other neurons until it can no longer continue.

Synaptic connections are considered either open or closed (like a social or unsocial person) and messages will flow along any and all open connections until they can go no further. Just like occupation and sociability play a key role in the spread of disease, so does the number of neurons, synaptic plasticity [58] and long-term potentiation when talking about neural percolation. Percolating clusters are a single large group of neurons that are all connected by open bonds and take up the majority of the network. Any signals that originate at any point within the percolating cluster will have a great impact and diffusion across the network than signals that original outside of the cluster. This is much like how a teacher is more likely to spread an infection to a whole community through contact with the students and subsequently with the families than an isolated businessman that works from home.

4.9.3 Ferromagnetism

One of the most studied phase transition phenomena of physics is that para-magnetic to ferromagnetic transition. The magnetic spins of a magnetic material, e.g., nickel, interact with each other: the energy is lower if the two spins on adjacent nickel atoms are parallel than if they are anti-parallel. This lower energy tends to cause the spins to be parallel and below a temperature called the Curie temperature,T_c , most of the spins in the nickel are parallel, their magnetic moments then add up constructively and the piece of nickel has a net magnetic moment: it is a ferromagnetic. Above the Curie temperature on average half the spins point in one direction and the other half in the opposite direction. Then their magnetic moments cancels out, and the nickel has no net magnetic moment. It is then a para-magnet. Thus at T_c the nickel goes from having no magnetic moment to having a magnetic moment. This is a sudden qualitative change and when this happens we say that a phase transition has occurred. Here the phase transition occurs when the magnetic moment goes from zero to non-zero. It is from the para-magnetic phase to the ferromagnetic phase. So, this critical value T_c of the temperature marking the borderline between the existence and non-existence of so called spontaneous magnetization. A standard mathematical model for this phenomenon is the Ising model [30]. It turns out that there are two parameters which specify the conditional probabilities: the 'external magnetic field' h, and the strength J of interaction between neighbors. If $J = 0$, the states of different vertices are independent,

Fig. 4.10 NGC 4414, a typical spiral galaxy in the constellation Coma Berenices, is about 55,000 light-years in diameter and approximately 60 million light-years away from Earth.

and the process is equivalent to site percolation [34]. The relationship between the Ising model and bond percolation is rather strong. It turns out that they are linked via a type of 'generalized percolation' called the other considerations [33, 92]. Studing the random-cluster model, one can obtain conclusions valid simultaneously for percolation and the Ising model. This discovery was made in 1970 by Fortuin and Kastelyn [47, 45, 46], and it has greatly influenced part of the current view of disordered physical systems

4.9.4 Cosmology

We know mass distribution and motions of the components of a galaxy are determined by gravity, it has not been clear what is responsible for the striking morphology of a spiral galaxy such as shown in the figure. The spiral arms extend over 16,000 parsecs (1 parsecs equals 3.26 light-years), and the traditional view is that it is necessary to have a long-range interaction like gravity, which interacts with object that have mass, to create such long-range order. However, in condensed matter physics it is well known that long-range order can be induced by a short-range interaction, and this is a characteristic feature of a continuous phase transition [48].

The structural features of spiral galaxies arises from a percolation phase transition that underlies the phenomenon of propagating star formation. According to this view, the

appearance of spiral arms is a consequence of the differential rotation of the galaxy and the characteristic divergence of correlation lengths for continuous phase transitions.

Other structural properties of spiral galaxies, such as the distribution of the gaseous components and the luminosity, arise directly from a feedback mechanism that pins the star formation rate close to the critical point of the phase transition. At least for some galaxies, morphological and other features are already fixed by general properties of phase transitions, irrespective of detailed dynamic or other considerations [92, 33].

Definitions of some quantities used in percolation. Basic Algorithm

4.9.5 Square Lattice

A square lattice is an ideal playground for percolation. If it has length L then number of sites in the lattice is L^2 and number of bonds in the lattice is $2L^2$. All sites are equally separated from each other at a certain distance. And all sites have exactly four neighbor. Since with the periodic boundary condition the sites in the left edge are connected with the sites in the right edge and same rule for sites in the top and bottom edges. If the sites are densely spaced the experiment will be accurate, meaning, the larger the size of the lattice the accurate the results will be. It implies that a lattice of infinite size should be used which is practically impossible. The simple solution to this problem is to use number of large lengths, (say $L = \{L_1, L_2, \ldots L_n\}$, where n is a finite number and $L_1 < L_2 < \ldots < L_n$), and extrapolate the results for infinite lattice. The visual structure of the square lattice is as follows 4.11. This is and empty lattice structure. Filled circles are for occupied site and filled bonds are for occupied bonds 4.12.

4.9.6 Site Percolation

The algorithm for site percolation is as follows,

1. take a square lattice of length L.
2. fill all $2L^2$ bonds initially.
3. occupy a randomly chosen site and it will join some clusters.
4. each time a site is occupied, it will get connected to four neighboring bonds and will form a cluster of size 4. Note that we define cluster size by number of bonds in it.
5. if a site is occupied and right next to it there is another occupied site and a cluster of size 7 will be formed.

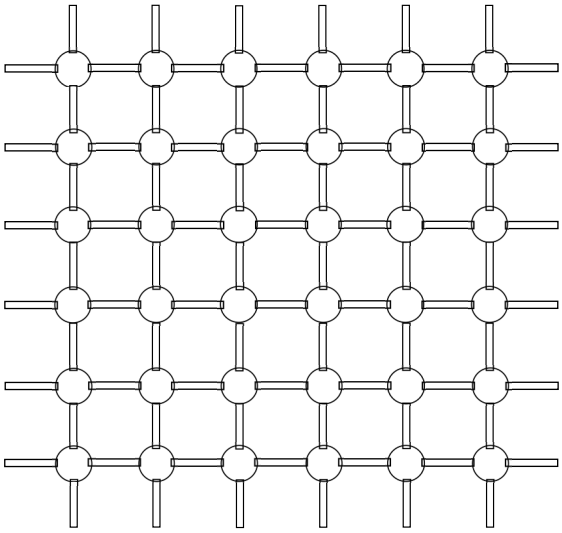
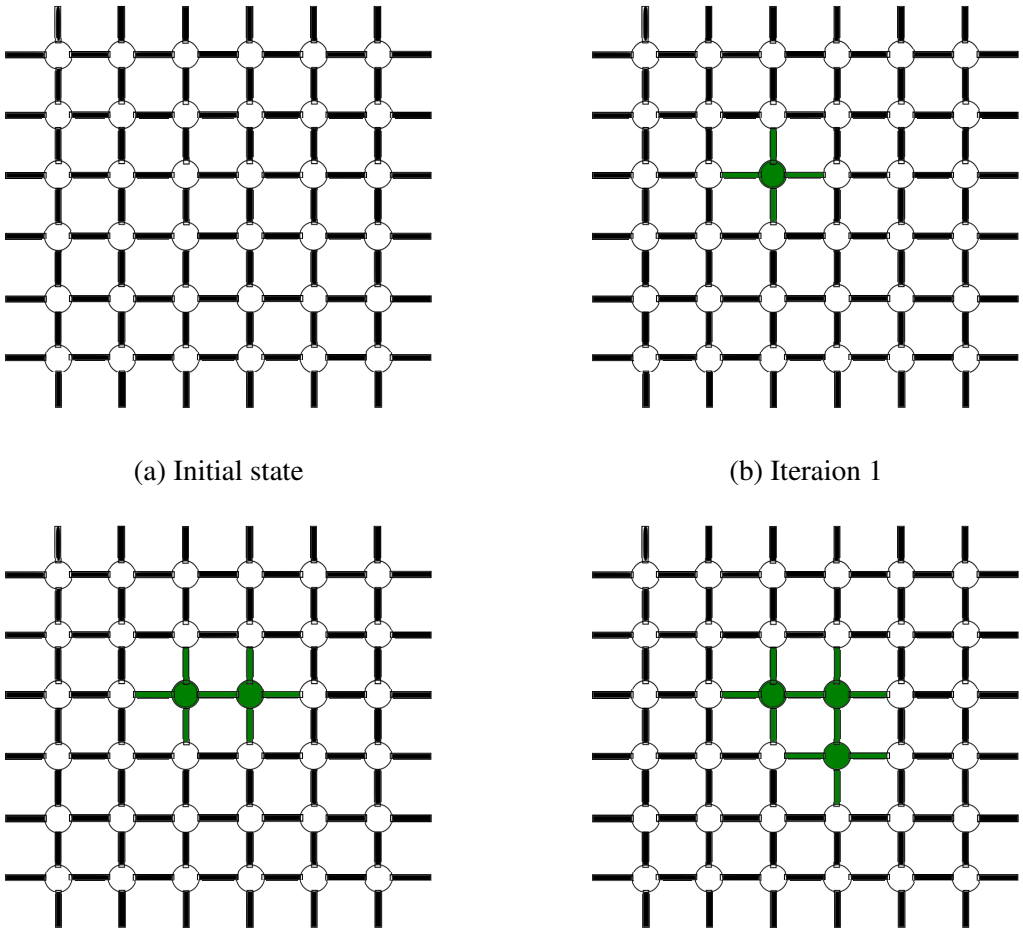


Fig. 4.11 Square Lattie (empty) of length 6

Fig. 4.12 Site and Bond symbol (empty and occupied).



(a) Initial state (b) Iteraion 1

(c) Iteraion 2 (d) Iteraion 3

Fig. 4.13 Growth of a Cluster in Site Percolation on square Lattice

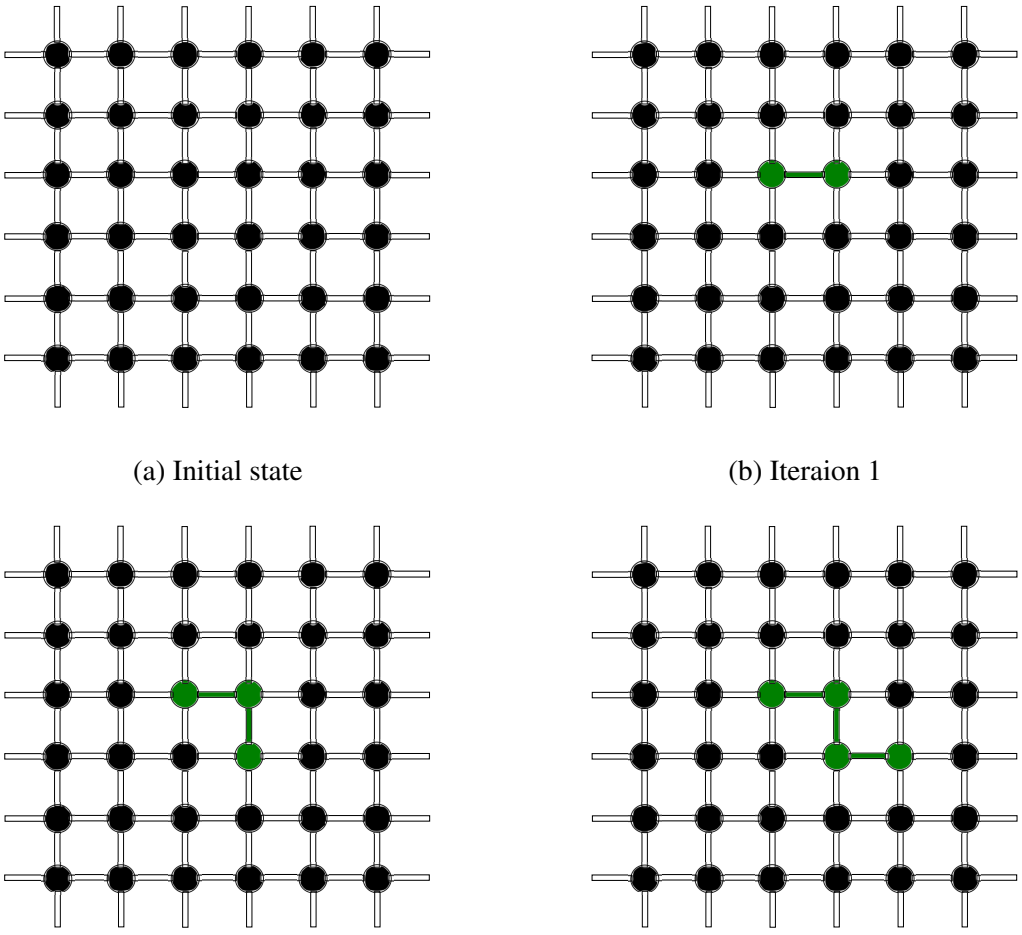
6. this process is repeated until all the sites are occupied and only one cluster remains

The formation of cluster is visualized in the figure 4.13.

4.9.7 Bond Percolation

The algorithm for bond percolation is as follows,

1. take a square lattice of length L.
2. fill all L^2 the sites initially.
3. occupy a randomly chosen bond and it will join some clusters.



(a) Initial state

(b) Iteraion 1

(c) Iteraion 2

(d) Iteraion 3

Fig. 4.14 Growth of a Cluster in Bond Percolation on square Lattice

4. each time a bond is occupied, it will get connected to two neighboring sites and will form a cluster of size 2. Here cluster size by number of sites in it.

5. if a bond is occupied and right next to it there is another occupied bond and they are connected by a site and a cluster of size 3 will be formed.

6. this process is repeated until all the bonds are occupied and only one cluster remains

The formation of cluster is visualized in the figure 4.14.

Chapter 5

Ballistic Deposition on Square Lattice

We investigate percolation by random sequential ballistic deposition (RSBD) on a square lattice with interaction range upto second nearest neighbors. The critical points p_c and all the necessary critical exponents α, β, γ, ν etc. are obtained numerically for each range of interactions. Like in its thermal counterpart, we find that the critical exponents of RSBD depend on the range of interactions and for a given range of interaction they obey the Rushbrooke inequality. Besides, we obtain the exponent τ which characterizes the cluster size distribution function $n_s(p_c) \sim s^{-\tau}$ 4.5.8 and the fractal dimension d_f that characterizes the spanning cluster at p_c 4.5.11. Our results suggest that the RSBD for each range of interaction belong to a new universality class which is in sharp contrast to earlier results of the only work that exhist on RSBD.

Imagine a spherical shaped object, say marble, is thrown on top of a 2D square lattice structure. First possible scenario is that the marble will be deposited in the first encountered site in the lattice . Now if the first encountered site is not empty, the possible scenario is that the marble will go in any of the four direction, $+x$, $-x$, $+y$ or $-y$, assuming no other direction in between is allowed in the lattice. Now if the first neighbor is not empty then the marble will continue to go on in the previously selected direction and choose the next neighbor. This is the main theme of this thesis.

In our experiment, we occupy a randomly chosen site if it is empty else we select one of its four neighbor to occupy if it is empty else select next neighbor in that direction and occupy that site if it is empty else ignore current iteration and choose another site randomly. This process is repeated until there is no empty site in the lattice. We call this process the ballistic deposition on the square lattice. We introduce 1st and 2nd nearest neighbor interaction in this way.

5.1 Site Percolation Redefined

5.2 Structure and Algorithm

Random percolation (RP) model can also be seen as a random sequential adsorption (RSA) process of particles on a given substrate to form monolayers of clusters of complex shape and structures. In RSA, a site is first picked at random and it is occupied if it is empty and the trial attempt is rejected if it is already occupied. We shall first show that this process too reproduce all the existing results of the CRP including the p_c value. We can modify the rejection criterion. First, we assume that the adsorbing particles are hard sphere and impenetrable. Then we assume that if a particle fall onto an already adsorbed particle it is not straightaway rejected. Instead, it is allowed to roll down over the already deposited particle to one of its nearest neighbours at random following the steepest descent path. The particle is then adsorbed permanently if the nearest neighbour is empty else the trial attempt is rejected. This is known as the ballistic deposition (BD) model for $l = 1$. We also consider the case that if the nearest neighbour is occupied then the incoming particle attempt to push the neighbour to its next neighour site along the same line to make room for itself. However, the trial attempt of pushing the neighbour is successful if the next neibhouring site along the same line is empty else the trial attempt is discarded. We regard it as BD model for $l = 2$ while the classical percolation correspond to BD model with $l = 0$. Our primery goal is to prove that the critical exponents of percolation changes as changes as we increase the range of interaction like we find in its thermal counterpart. We numerically find the various necessary critical exponents and find that BD for each different range of interaction belong to different universality class and each universality class obeys the Rusbrooke inequality.

Percolation is all about configuration of clusters of deposited particles and the investigation of the emergence of a large-scale connected path created by clusters formed by contiguous diposoted particles. We use extensive Monte Carlo simulation on a square lattice with the usual periodic boundary condition to study site percolation according to RSBD rule.

The algorithm of the percolation by RSBD can be described as follows. We first label all the sites row by row from left to right starting from the top left corner. That is, we first label the first row from left to right as $i = 1, 2, ..., L$, the second row again from left to right as $i = L+1, L+2, ..., 2L$ and we continue this till we reach the bottom row which we label as $i = (L-1)L+1, ..., L^2$. Then at each step we pick a discrete random number R from $1, 2, ..., L^2-1, L^2$ using uniform random number generator and check if the site it represents

is already occupied or not. If it is empty we occupy it straightaway and move on to the next step. Else we pick one of its neighbours at random. The second attempt in the same step, that mimic the roll over mechanism, is successul if the neighbour it picks is empty and if not the trial attempt to deposit is rejected permanently and we move on to the next step anyway. This process is repeated over and over again till we want it to stop. We call it RSBD of degree one. We also consider the case of RSBS of degree two where the trial attempt is made to occupy the second nearest neighbour too. In this case if the incoming particle that fall onto an already occupied site and find its neighbour is ocupied too but the next nearest neighbour site is empty then the neighbour move to the empty site to make space for the incoming perticle to be deposited there.

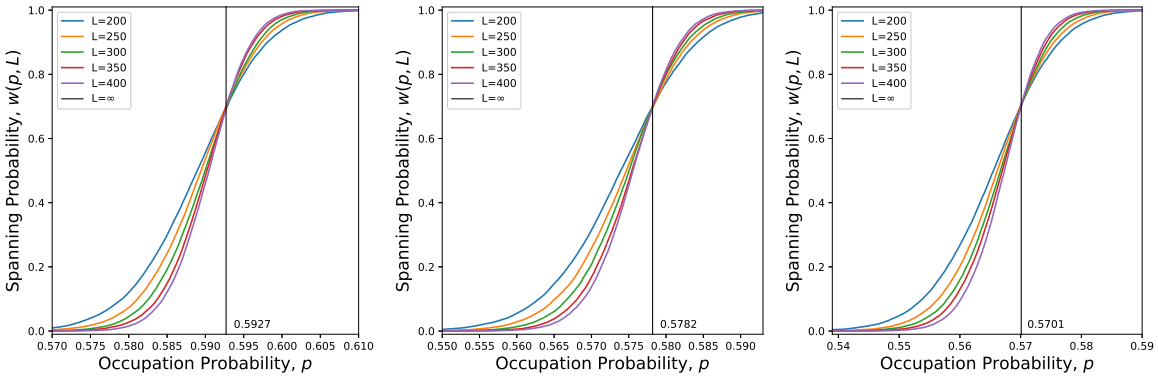
1. take a square lattice of length L.
2. choose a site randomly
3. if the chosen site is empty then occupy it else choose one of the four neighbor randomly
4. if the chosen neighbor is empty then occupy it else choose second nearest neighbor in that direction
5. if the second nearest neighbor is empty then occupy the site else ignore this step

5.3 Finite Size Scaling in Percolation Theory

5.4 Finding Numerical Values

5.4.1 Critical occupation probability, p_c

When we occupy sites of the square lattice, initially, there are only cluster of size 1. As we keep occupying different size of clusters starts to appear. At a certain point a special cluster appears which spans the entire lattice. We call this cluster the *Spanning Cluster*. It should be noted that the spanning cluster is a special property of the lattice and the appearance of the spanning cluster is the result of phase transition. At the point where the spanning cluster first appears is called the critical point and denoted by p_c, meaning the occupation probability at the critical point. The figure 5.1 shows the graph of the spanning probability, $w(p,L)$, versus the occupation probability p for different interactions $(L0,L1,L2)$ for different lengths. We have found that p_c is $0.5927, 0.5782, 0.5701$ for $L0,L1,L2$ respectively.Thus for long range interaction p_c is smaller than for short range interaction. The quantity $w(p,L)$ is called



(a) L0 (b) L1 (c) L2

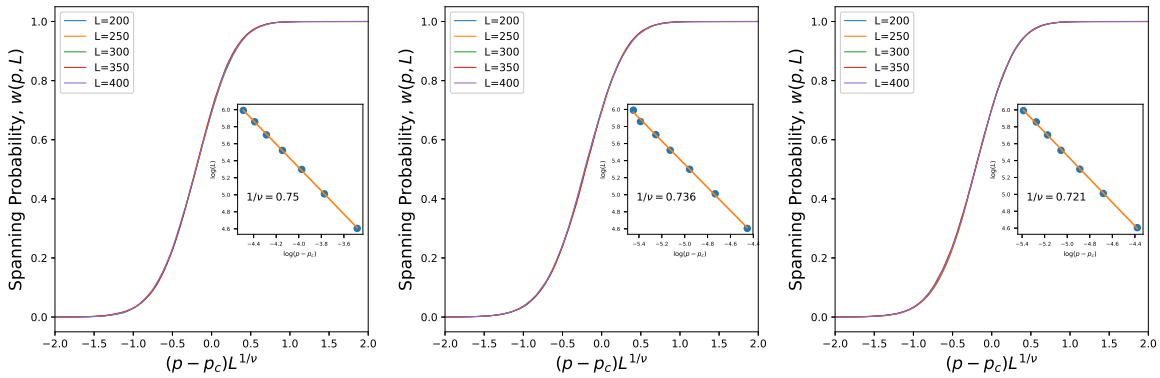
Fig. 5.1 Spanning Probability, $w(p,L)$ vs Occupation Probability, p

the spanning probability in a non periodic case and wrapping probability in a periodic case. The question is how do we find the wrapping probability, given that we have a list of p_c for different length. Note that for a certain length L, in each realization the p_c is not exact value, instead it is a range of values that contains the p_c. For example, say we have a lattice of length 200 and for that we will have different p_c at each realization. After an infinite number of experimentation we will have to take an average and that will give the exact value of p_c. But since it is practically impossible, we can find $p_{c_{avg}}$ for different lattice size then from the graph we can extrapolate the exact value of p_c for infinite lattice. Here $p_{c_{avg}}$ is calculated from a finite set of p_c for a certain length. This process is not good enough. Since it requires $p_{c_{avg}}$'s for a number of lattice size which is very costly to obtain. But from the data, list of p_c's for different length, we can find the cumulative frequency distribution. It is astonishing that for all length the wrapping probability coincide at a specific point. This implies that if we could have an infinite system, the wrapping probability for that system would have gone through this same point. This means we got our critical point, p_c, as the intersection of the $w(p,L)$ for different lengths.

5.4.2 Spanning Probability and finding $1/\nu$

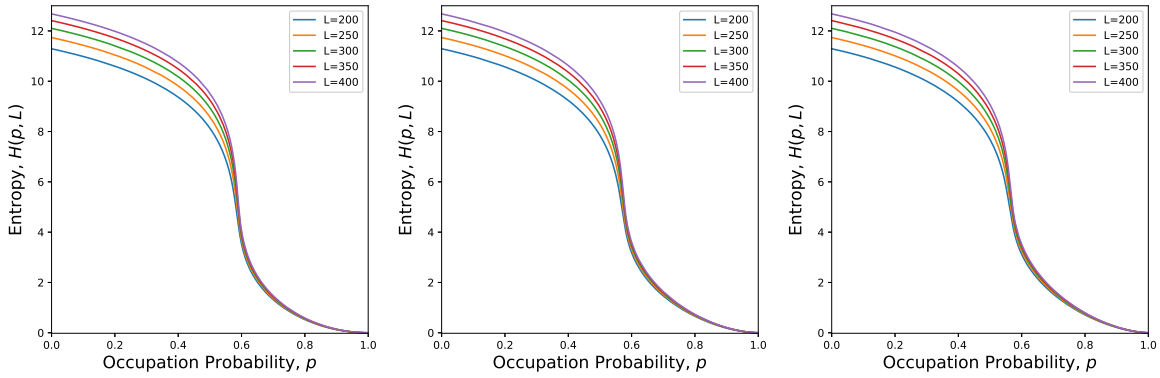
From the figure 5.1 we can see that, as we increase the length of the lattice the wrapping probability $w(p,L)$ moves closer and closer to the critical point. And if we draw a horizontal line at a certain height, say $y = 0.1$, and find the intersection of this line with $w(p,L)$ for each length and note the p and if we plot $\log(L)$ vs $\log(p - p_c)$ we get the slope $1/\nu$. If we now use the finite size scaling (FSS) hypothesis

$$w = (p - p_c)L^{1/\nu} \tag{5.1}$$



(a) L0 (b) L1 (c) L2

Fig. 5.2 $w(p,L)$ vs $(p-p_c)L^{1/\nu}$



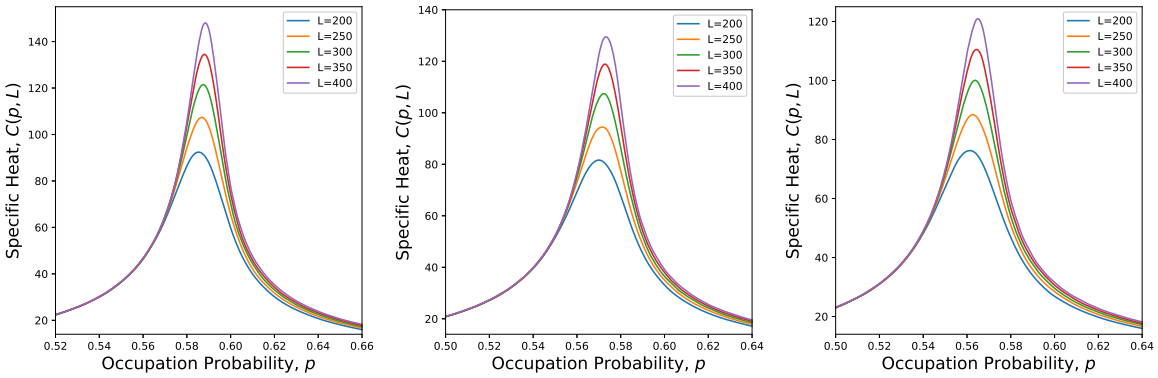
(a) L0 (b) L1 (c) L2

Fig. 5.3 Entropy, $H(p,L)$ vs Occupation Probability, p

we get a very good data collapse for $L0, L1, L2$ and got $1/\nu$ as $0.75, 0.736, 0.721$ respectively which is shown in figure 5.2. That is they are self-similar **??**.

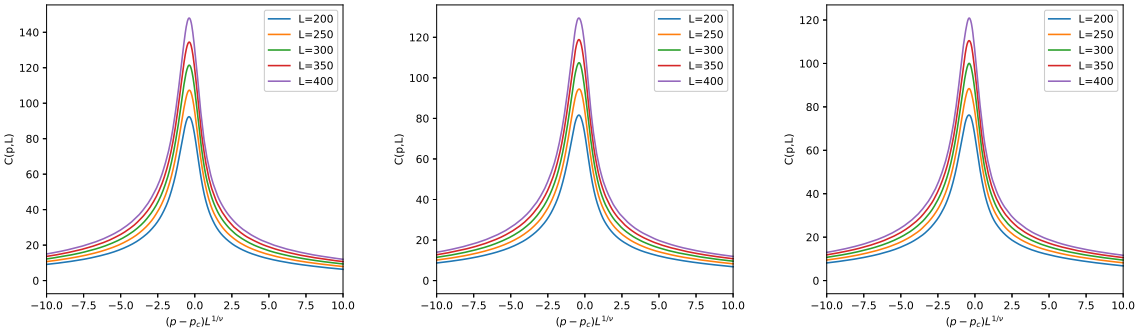
5.4.3 Entropy, Specific Heat and finding α

For any phase transition model the entropy is crucial. In percolation theory we use Shannon Entropy [95]. Using the definition **??** we get the figure 5.3 And since the specific heat $C(p,L)$ is nothing but the derivative of entropy, by simply differentiating entropy we get the specific heat (although we need to perform convolution**??** in order to get a smooth curve) shown in figure 5.4. From specific heat we can find the exponent α. To do this first we need to scale the x-values of the specific heat data using the exponent $1/\nu$ obtained from 5.4.2 and get the graph as in figure **??**. From this graph we will not the height of each line and call it C_h. Since each line corresponds to a specific length L we can plot $\log(C_h)$ versus $\log(L)$ and the



(a) L0 (b) L1 (c) L2

Fig. 5.4 Specific Heat, $C(p,L)$ vs Occupation Probability, p



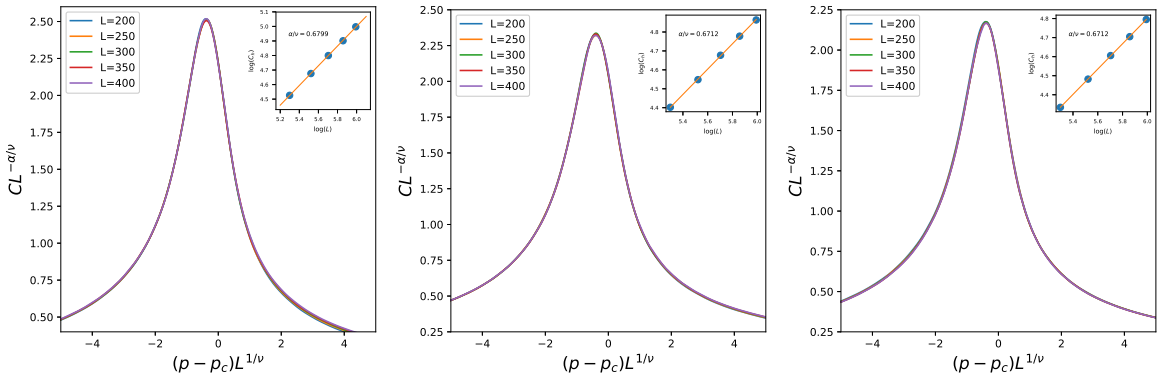
(a) L0 (b) L1 (c) L2

Fig. 5.5 $C(p,L)$ vs $(p-p_c)L^{1/\nu}$

absolute value of the graph will give α/ν and from that we can find the exponent α simply by dividing α/ν by $1/\nu$. We get α values $0.906, 0.911, 0.919$ for $L0, L1, L2$ correspondingly. and using this value we can apply FSS hypothesis to get data collapse. If we plot $CL^{-\alpha/\nu}$ vs $(p-p_c)L^{1/\nu}$ we get perfect data collapse for $L0, L1, L2$ and it is shown in figure 5.6

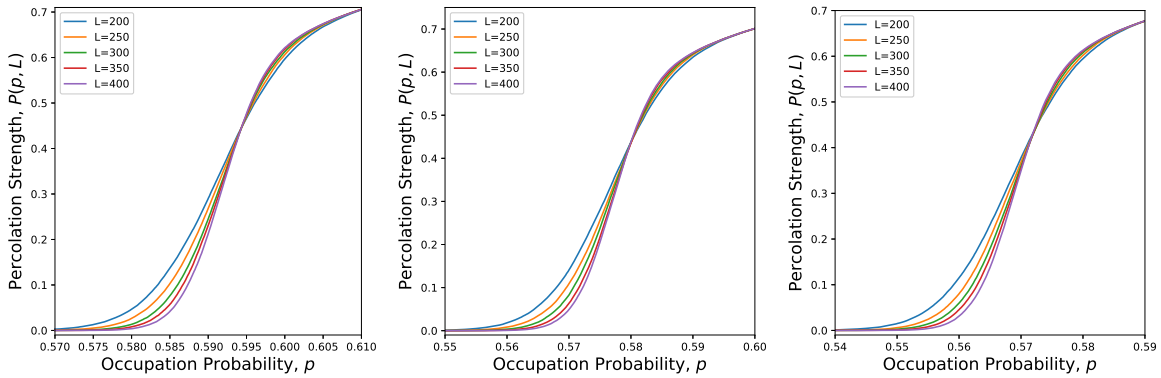
5.4.4 Order Parameter and finding β

Order parameter, also knows as the percolation strength, is ,along with entropy, an important quantity in the study of phase transition. It is denoted as $P(p,L)$. Using the definition **??** we obtain the order parameter for our system and it is shown in the figure 5.7. Since using spanning cluster and the largest cluster gives the same exponent, it really does not matter which one we use. But in our case there is a boundary of the system, which we define as periodic. Hence using spanning cluster is appropriate. Using the exponent $1/\nu$ obtained in



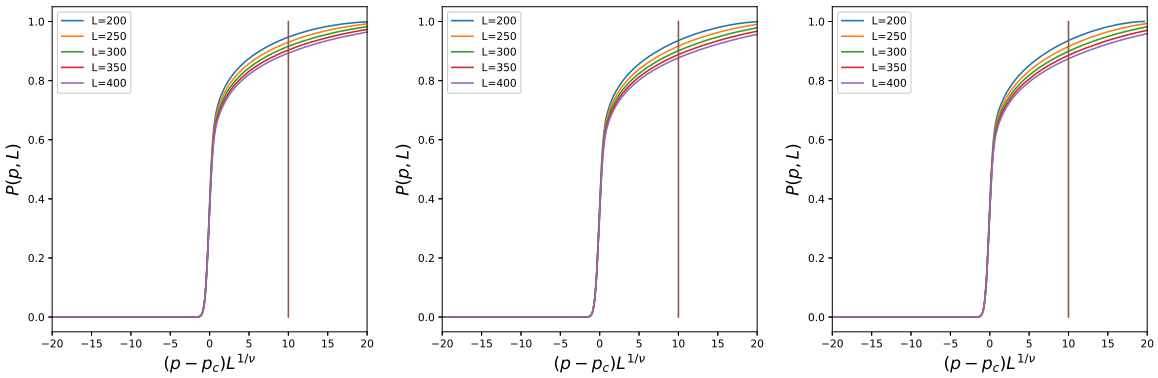
(a) L0 (b) L1 (c) L2

Fig. 5.6 $CL^{-\alpha/\nu}$ vs $(p-p_c)L^{1/\nu}$



(a) L0 (b) L1 (c) L2

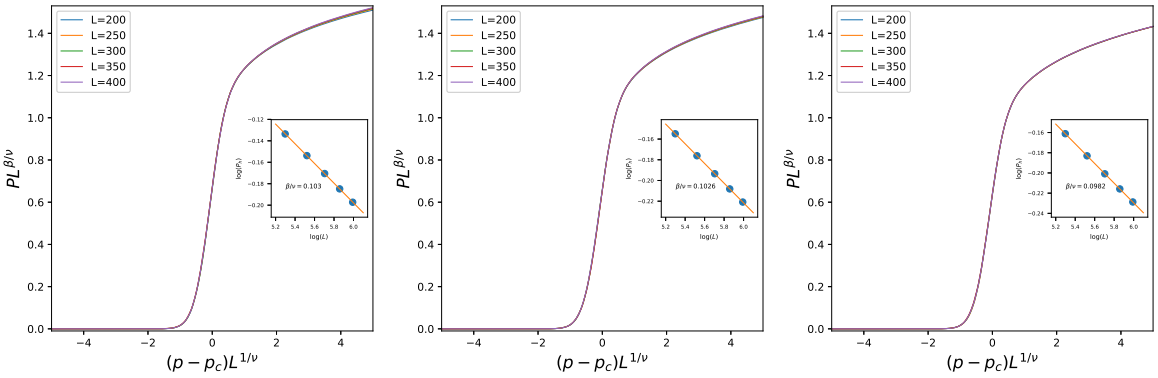
Fig. 5.7 Order Parameter, $P(p,L)$ vs Occupation Probability, p



(a) L0 (b) L1 (c) L2

Fig. 5.8 Order Parameter, $P(p,L)$ vs Occupation Probability, p

Fig. 5.9 $P(p,L)$ vs $(p-p_c)L^{1/\nu}$



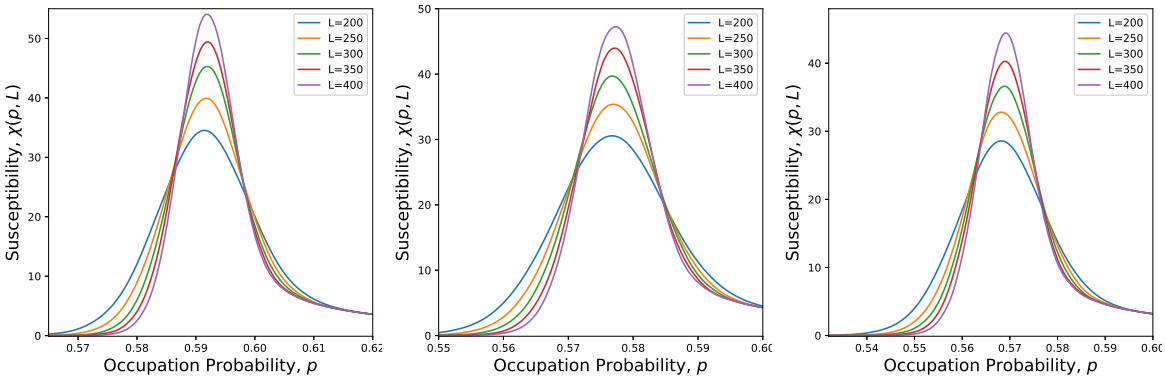
(a) L0 (b) L1 (c) L2

Fig. 5.10 $PL^{\beta/\nu}$ vs $(p-p_c)L^{1/\nu}$

section 5.4.2 we scale the x-values as $(p-p_c)L^{1/\nu}$ and get the following figure 5.8. Then in figure 5.8 we draw a vertical line where there are several horizontal lines. We measure the height of the lines and call it P_h and after plotting $\log(P_h)$ vs $\log(L)$ (inset of figure 5.10)we get the exponent β/ν from it's slope and obtain exponent β by dividing β/ν by $1/\nu$. Using the FSS hypothesis 2.4.2 we plot $PL^{\beta/\nu}$ versus $(p-p_c)L^1/\nu$ and get a good data collapse which is shown in figure 5.10.

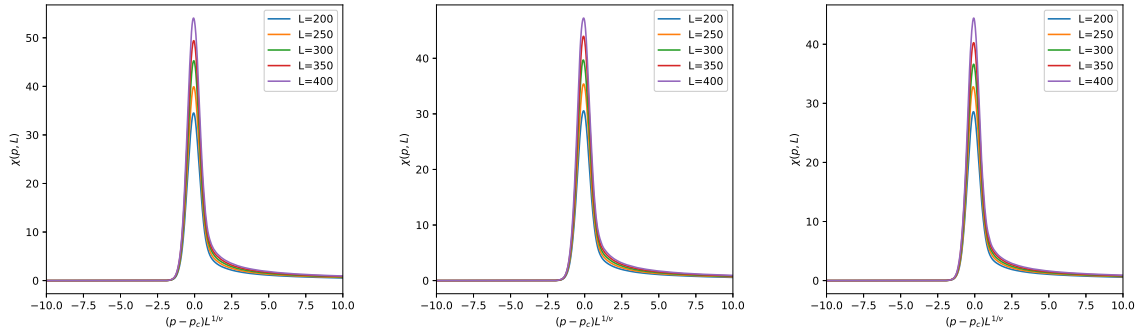
5.4.5 Susceptibility and finding γ

Susceptibility is defined as the derivative of the order parameter $P(p,L)$ with respect to the control parameter p,i.e., $\chi = \frac{dP}{dp}$. Using this definition we obtain the graph of susceptibility 5.11. And if we scale the x values and plot χ vs $(p-p_c)L^{1/\nu}$ we get all the peak point



(a) L0 (b) L1 (c) L2

Fig. 5.11 Susceptibility, $\chi(p,L)$ vs Occupation Probability, p



(a) L0 (b) L1 (c) L2

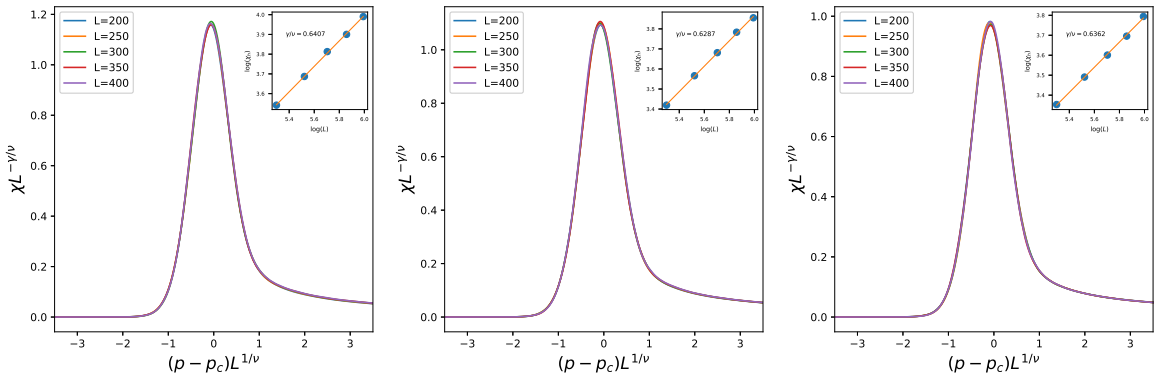
Fig. 5.12 $\chi(p,L)$ vs $(p-p_c)L^{1/\nu}$

aligned (figure 5.12). Note that the value of $1/\nu$ is known from section 5.4.2. Then we take the reading of the height of each line and call it χ_h. Since each line represents a different lattice size, plotting $\log(\chi_h)$ vs $\log(L)$ gives the slope γ/ν. And using the FSS hypothesis we plot $\chi L^{-\gamma/\nu}$ vs $(p-p_c)L^{1/\nu}$ and obtain a perfect data collapse. It is shown in figure 5.13. We obtain the values of γ to be $0.8543, 0.8542, 0.882$.

5.4.6 Cluster Size Distribution

Cluster size S is related to n_S by the relation

$$n_S \sim S^{-\tau} \tag{5.2}$$



(a) L0 (b) L1 (c) L2

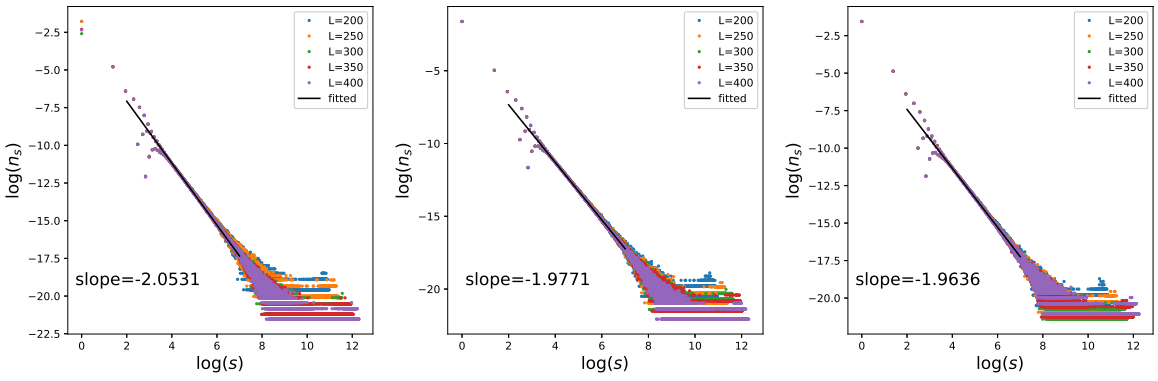
Fig. 5.13 $\chi L^{\gamma/\nu}$ vs $(p-p_c)L^{1/\nu}$

Fig. 5.14 Number of cluster of size s, n_s vs size of the cluster s

taking log on both sides gives us

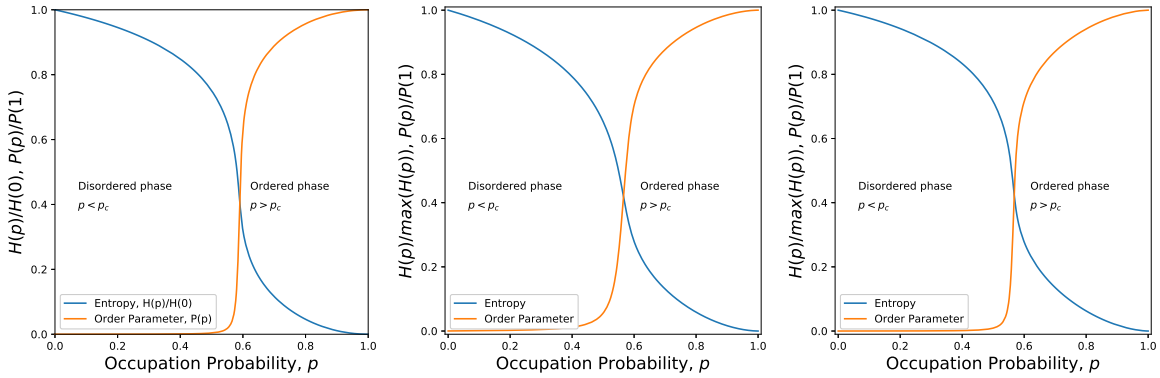
$$\log n_S = -\tau \log S \tag{5.3}$$

Thus the exponent τ gives us the information of the average cluster size. At the critical point all the cluster (apart from the largest ones and smallest ones) follows a pattern. Their size is related to the number times of they appear. n_s vs s graph



(a) L0 (b) L1 (c) L2

Fig. 5.15 $\log(n_s)$ vs $\log(s)$

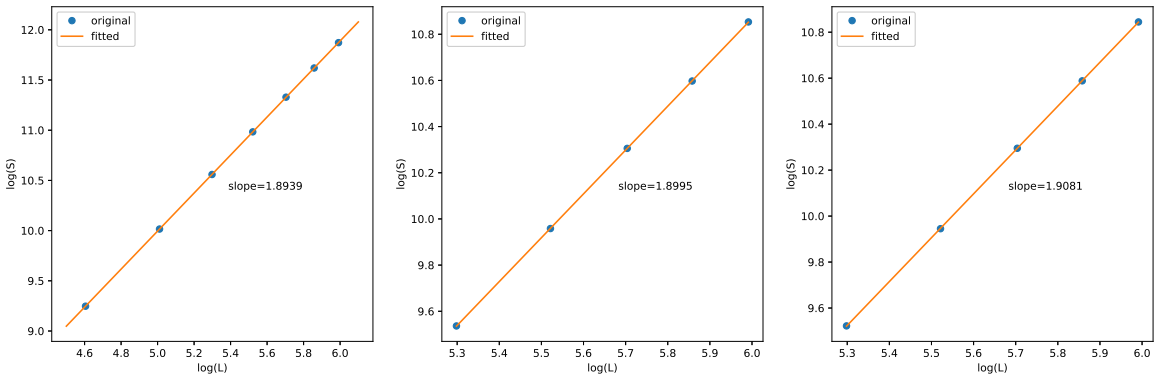


(a) L0 (b) L1 (c) L2

Fig. 5.16 $H(p,L)/H(0,L)$ or $P(p,L)/P(1,L)$ vs p

5.4.7 Order-Disorder Transition

Phase transition is an order-disorder transition. There is a critical point which separates the two regions. Before the critical point the system is in disordered phase and after it is in ordered phase when we increase temperature in thermodynamics. Behavior of two phases are completely different. It's astonishing how the behavior changes. In percolation theory, this order disorder transition is different than in thermodynamics. Here disordered means uncertainty, since we are dealing with a system where probability is the control parameter (the occupation probability p). When p is minimum all clusters are disconnected and have size of unity. This means that we can to pick a cluster with probability $\frac{1}{2L^2}$, where L is the lattice size and $2L^2$ is the number of bonds in the lattice. That's why entropy is maximum and order parameter is minimum in this region. Now as we keep occupying the lattice clusters of different size arises, and at some point a miracle happens. It is the critical point where the transition occurs. A cluster appears for the first time which spans the entire lattice either horizontally or vertically. And in case of periodic condition the cluster wraps the lattice all the way around it. This cluster is called the spanning (wrapping) cluster in non-periodic (periodic) condition. The probability of picking this cluster at random is always larger than picking any other clusters. Thus system goes to the ordered state. And if we keep occupying the lattice at some point all cluster are joined to form one cluster. Thus picking this cluster at random has no uncertainty, meaning we have reached the entirely ordered phase. Here entropy is minimum and ordered parameter is maximum. A graph **??** containing both entropy and order parameter can show this process. We have normalized the entropy (figure 5.3) to match with the order parameter (figure 5.7).



(a) L0 (b) L1 (c) L2

Fig. 5.17 $\log(S)$ vs $\log(L)$

5.4.8 Fractal Dimension

At critical point the square lattice shows the property of a fractal. A fractal is an object which occupies less space than it is embedded. For example a piece of cheese is a 3D fractal, since there are holes in the cheese which is empty. We use the relation

$$S \sim L^{d_f} \tag{5.4}$$

taking log we get

$$\log(S) = d_f \log(L) \tag{5.5}$$

Here S is the average size of the spanning cluster at critical point. Using this we get the figure **??**. And we obtain fractal dimension d_f for $L0, L1, L2$ which is listed in **??**. Fractal dimension gives us the information about the size of the spanning(wrapping) cluster. If the lattice size is known we can estimate the average size of the spanning cluster using d_f and 5.4.

Chapter 6

Summary and Discussion

We have investigated percolation by random sequential ballistic deposition (RSBD) on a square lattice with interaction range upto second nearest neighbors. The critical points p_c and all the necessary critical exponents α, β, γ, ν etc. are obtained numerically for each range of interactions. Like in its thermal counterpart, we find that the critical exponents of RSBD depend on the range of interactions and for a given range of interaction they obey the Rushbrooke inequality. Besides, we obtain the exponent τ which characterizes the cluster size distribution **??** and the fractal dimension d_f that characterizes the spanning cluster at p_c. Our results suggest that the RSBD for each range of interaction belong to a new universality class which is in sharp contrast to earlier results of the only work that exhist on RSBD.

We denote $L0, L1, L2$ for expressing direct, first nearest neighbor and second nearest neighbor interaction respectively. Up until now we knew the exponents for $L0$ for old definition of site percolation. We have found same exponents for the thermodynamically consistent new definition of site percolation and we also have investigated for short and long range interactions and we call this $L1$ and $L2$ respectively. Note that $L1$ is the case where we can choose the first nearest neighbor and $L2$ is the case where we can chose 2nd nearest neighbor in the direction of first nearest neighbor. We can use new feature of $L1$ only if the feature of $L0$ is unavailable, i.e., the selected site is already occupied. Similarly we can use new feature of $L2$ only if the feature of $L0$ and $L1$ is unavailable. Using this in mind we perform simulation and we obtain the critical exponents which agree with the laws of thermodynamics and the Rushbrooke inequality is satisfied in all cases.
The combined exponents are listed below
The critical exponents found in all cases are listed below,

Interaction	p_c	$1/\nu$	α/ν	β/ν	γ/ν
l0	0.5927	0.75	0.6799	0.103	0.64071
l1	0.5782	0.736	0.6712	0.1026	0.6287
l2	0.5701	0.721	0.6631	0.0982	0.6362

Table 6.1 List of combined exponents

Interaction	α	β	γ	$\alpha+2\beta+\gamma$
l0	0.906	0.137	0.8543	2.0347
l1	0.911	0.139	0.8542	2.044
l2	0.919	0.136	0.882	2.07

Table 6.2 Exponents Satisfying Rushbrooke Inequality

Here we notice that the critical point decreases as we increase the range of interaction. But the fractal dimension increases. This is reasonable since my occupying nearest and second nearest neighbor we are increasing the change of any individual cluster to grow faster. This is the reason for the p_c value to decrease. But it grows in area not in length average meaning when the spanning cluster appears it will contain more sites and bonds than in regular percolation which is evident from the fractal dimension d_f.
All other exponents changes a bit but their shape is not different. That's why change is not visible to the naked eye and it requires a thorough investigation.

Interaction	d_f	τ
l0 (standard)	91/48	187/91
l0 (obtained)	1.8939	2.0531
l1	1.8994	1.9771
l2	1.9081	1.9636

Table 6.3 Exponents giving cluster information

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Appendix A

Percolation

A.1 Algorithm

The UML diagram for the program is

A.2 Code

Each header file starts with a directive *#ifndef* and *#define*, which is necessary because one header file is needed multiple times and including it more than once results in error. These directive prevents it. Of course this directive must be closed by *#endif*.

A.2.1 Index

Here the notion of index of site and index of bond is defined. Site index has two element which determine row and column. Bond Index had three element describing bond type, row, column. Bond type can be horizontal or vertical.

the **src/index/index.h** file

```
#ifndef SITEPERCOLATION_INDEX_H
#define SITEPERCOLATION_INDEX_H

#include <ostream>
#include <iostream>
#include <sstream>
#include <vector>

#include "../types.h"
#include "../exception/exceptions.h"
```

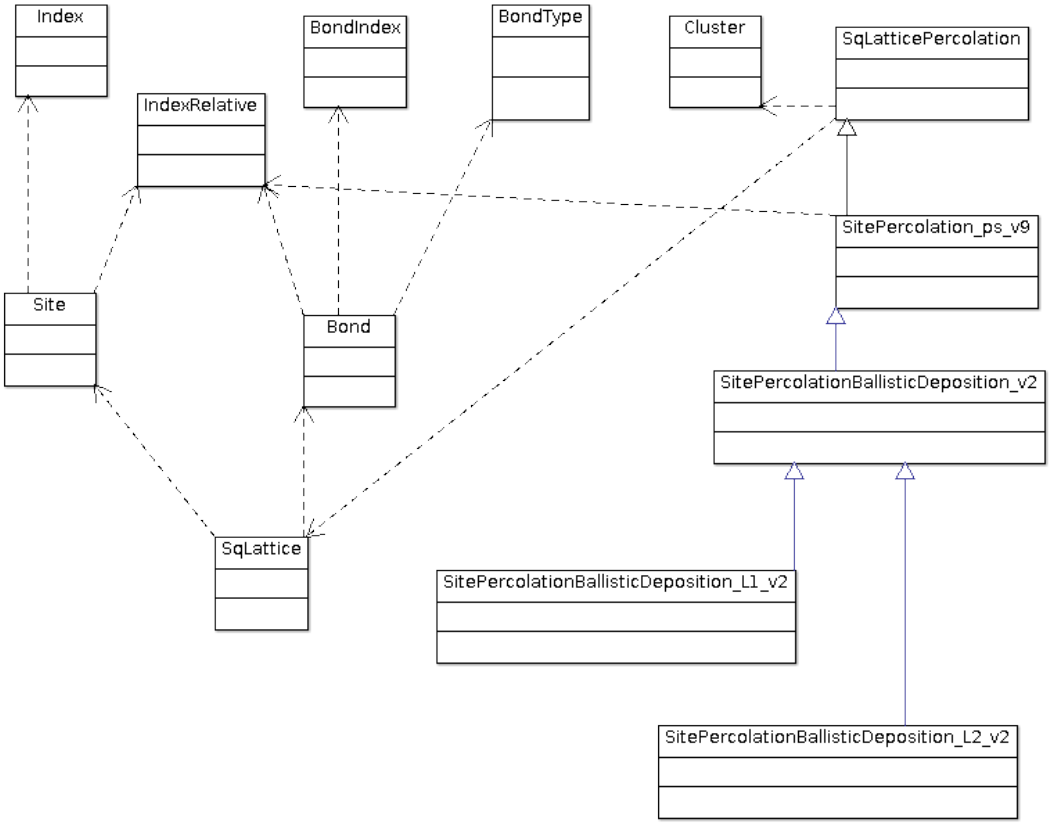

Fig. A.1 Schematic UML diagram for Site Percolation Ballistic Deposition program. This figure shows the dependencies and inheritance os the Classes and Structs in the program.

```
#include "../lattice/bond_type.h"


struct Index{
value_type row_{};
value_type column_{};

~Index()                        = default;
Index()                         = default;

Index(value_type x, value_type y) : row_{x}, column_{y} {}

};


class IndexRelative{
public:
int x_{};
int y_{};

~IndexRelative()                          = default;
IndexRelative()                           = default;

IndexRelative(int x, int y) : x_{x}, y_{y} {}

};

struct BondIndex{
BondType bondType;

value_type row_;
value_type column_;

~BondIndex()                            = default;
BondIndex()                             = default;

BondIndex(BondType hv, value_type row, value_type column)
:  row_{row}, column_{column}
{
bondType = hv;
}

bool horizontal() const { return bondType == BondType::Horizontal;}
bool vertical() const { return bondType == BondType::Vertical;}
```

```
55
56 };
57
58
59 std::ostream& operator<<(std::ostream& os, const Index& index);
60 bool operator==(const Index& index1, const Index& index2);
61 bool operator<(const Index& index1, const Index& index2);
62
63 std::ostream& operator<<(std::ostream& os, const IndexRelative& index);
64
65 std::ostream& operator<<(std::ostream& os, const BondIndex& index);
66 bool operator==(BondIndex index1, BondIndex index2);
67 bool operator<(BondIndex index1, BondIndex index2);
68
69
70 /**
71 *  Get 2nd nearest neightbor / sin the direction of 1st nearest neighbor
      , while @var center is the center
72 */
73 Index get_2nn_in_1nn_direction(Index center, Index nn_1, value_type
      length);
74 std::vector<Index> get_2nn_s_in_1nn_s_direction(Index center, const std
      ::vector<Index> &nn_1, value_type length);
75
76 #endif /* SITEPERCOLATION_INDEX_H */
```

The **src/index/index.cpp** file

```
1 #include <iomanip>
2 #include "index.h"
3
4 using namespace std;
5
6 ostream& operator<<(ostream& os, const Index& index)
7 {
8 return os <<'(' << index.row_ << ',' << index.column_ << ')';
9 }
10
11 ostream& operator<<(ostream& os, const IndexRelative& index)
12 {
13 return os << '(' << std::setw(3) << index.x_ << ',' << std::setw(3) <<
      index.y_ << ')';
14 }
15
16 bool operator==(const Index& index1, const Index& index2){
```

```
17 return (index1.row_ == index2.row_) && (index1.column_ == index2.column_
       );
18 }
19
20 bool operator<(const Index& index1, const Index& index2){
21 if(index1.row_ < index2.row_)
22 return true;
23 if(index1.row_ == index2.row_){
24 return index1.column_ < index2.column_;
25 }
26 return false;
27 }
28
29 ostream& operator<<(ostream& os, const BondIndex& index){
30 if(index.horizontal()){
31 // horizontal bond
32 os << "<->" ;
33 }
34 if (index.vertical()){
35 // vertical bond
36 os << "<|>" ;
37 }
38 return os << '(' << index.row_ << ',' << index.column_ << ')';
39 }
40
41 bool operator==(BondIndex index1, BondIndex index2){
42 if(index1.horizontal() ==  index2.horizontal() || index1.vertical() ==
       index2.vertical()){
43 // horizontal or vertical
44 return index1.row_ == index2.row_ && index1.column_ == index2.column_;
45 }
46 return false;
47 }
48
49
50 bool operator<(BondIndex index1, BondIndex index2){
51 cout << "not yet defined : line " << __LINE__ << endl;
52 return false;
53 }
54
55
56 /**
57 * Get the 2nd nearest nearest neighbor in the direction of 1st nearest
       neighbor.
```

```
58 * Periodicity is not considered here.
59 */
60 Index get_2nn_in_1nn_direction(Index center, Index nn_1, value_type
       length){
61 int delta_c = int(nn_1.column_) - int(center.column_);
62 int delta_r = int(nn_1.row_) - int(center.row_);
63 if (delta_c == 0 && delta_r == 0){
64 cout << "Both indices are same : line " << __LINE__ << endl;
65 }
66 else if(delta_c > 1 || delta_r > 1){
67 // meaning, the sites are on the opposite edges
68 //        cout << "2nd index is not the First nearest neighbor : line "
       << __LINE__ << " : file " << __FILE__ << endl;
69 }
70
71 return Index{(nn_1.row_ + delta_r + length) % length, (nn_1.column_ +
       delta_c + length) % length};
72 }
73
74
75 /**
76 * Get all second nearest neighbors based on the first nearest neighbors.
77 * Periodicity is not considered here
78 */
79 vector<Index> get_2nn_s_in_1nn_s_direction(Index center, const vector<
       Index> &nn_1, value_type length){
80 vector<Index> nn_2(nn_1.size());
81
82 for(size_t i{}; i != nn_1.size() ; ++i){
83 int delta_c = int(nn_1[i].column_) - int(center.column_);
84 int delta_r = int(nn_1[i].row_) - int(center.row_);
85 if (delta_c == 0 && delta_r == 0){
86 cout << "Both indices are same : line " << __LINE__ << endl;
87 }
88 else if(delta_c > 1 || delta_r > 1){
89 // meaning, the sites are on the opposite edges
90 //            cout << "center " << center << " nn " << nn_1 << endl;
91 //            cout << "2nd index is not the First nearest neighbor :
       line " << __LINE__ << " : file " << __FILE__ << endl;
92 }
93
94 nn_2[i] =  Index{(nn_1[i].row_ + delta_r + length) % length, (nn_1[i].
       column_ + delta_c + length) % length};
95 }
```

```
96 return nn_2;
97 }
```

A.2.2 Site

The site class contains all information about a site, e.g., if it is active or not and if it is then what is it's group id or relative index.

The **src/lattice/site.h** file

```
1  #ifndef SITEPERCOLATION_SITE_H
2  #define SITEPERCOLATION_SITE_H
3
4  #include <array>
5  #include <set>
6  #include <vector>
7  #include <iostream>
8  #include <memory>
9
10 #include "../index/index.h"
11 #include "../types.h"
12
13
14 /**
15 * single Site of a lattice
16 */
17 struct Site{
18 /**
19 * if true -> site is placed.
20 * if false -> the (empty) position is there but the site is not (
       required for site percolation)
21 */
22 bool _status{false};
23 int _group_id{-1};
24 Index _id{};
25
26 //relative distance from the root site. {0,0} if it is the root site
27 //for detecting wrapping
28 IndexRelative _relative_index{0,0};
29
30
31 public:
32
33 ~Site()                    = default;
```

```
Site()                  = default;
Site(const Site&)             = default;
Site(Site&&)            = default;
Site& operator=(const Site&)  = default;
Site& operator=(Site&&) = default;

Site(Index id, value_type length){
// I have handle _neighbor or corner points and edge points carefully
if(id.row_ >= length || id.column_ >= length){
std::cout << "out of range : line " << __LINE__ << std::endl;
}
_id.row_ = id.row_;
_id.column_ = id.column_;
}


bool isActive() const { return _status;}
void activate(){ _status = true;}
void deactivate() {
_relative_index = {0,0};
_group_id = -1;
_status = false;
}
Index ID() const { return  _id;}
/*
* Group get_ID is the set_ID of the cluster they are in
*/
int      get_groupID() const {return _group_id;}
void     set_groupID(int g_id) {_group_id = g_id;}

std::stringstream getSite() const {
std::stringstream ss;
if(isActive())
ss << _id;
else
ss << "(*)";
return ss;
}


void relativeIndex(IndexRelative r){
_relative_index = r;
}

```

```
78 void relativeIndex(int x, int y){
79 _relative_index = {x,y};
80 }
81
82 IndexRelative relativeIndex() const {return _relative_index;}
83 };
84
85 std::ostream& operator<<(std::ostream& os, const Site& site);
86 bool operator==(Site& site1, Site& site2);
87 #endif
```

The **src/lattice/site.cpp** file

```
1 #include <iomanip>
2 #include "site.h"
3
4 std::ostream& operator<<(std::ostream& os, const Site& site)
5 {
6 if(site.isActive())
7 return os << site._id;
8 else
9 return os << "(*)";
10 }
11
12
13 bool operator==(Site& site1, Site& site2){
14 return (site1.ID().row_ == site2.ID().row_) && (site1.ID().column_ ==
      site2.ID().column_);
15 }
```

A.2.3 Bond

The bond class contains all information about a bond, e.g., if it is active or not and if it is then what is it's group id.

The **src/lattice/bond.h** file

```
1 #ifndef SITEPERCOLATION_BOND_H
2 #define SITEPERCOLATION_BOND_H
3
4
5 #include <ostream>
6 #include <iostream>
7 #include <sstream>
8
```

```
#include "../index/index.h"
#include "../types.h"


/**
* A bond has two end
* say a 5x5 lattice bond between end1 (0,0) and end2 (0,1)
* if _status is false -> bond is not there
*
*/
struct Bond{
// check if active or not
bool _status{false};
value_type _length;
int _group_id{-1};

BondType bondType;
//relative distance from the root site. {0,0} if it is the root site
IndexRelative _relative_index{0,0};
Index _end1;
Index _end2;
BondIndex _id;

~Bond() = default;
Bond() = default;
Bond(Index end1, Index end2, value_type length){
_end1.row_ = end1.row_;
_end1.column_ = end1.column_;
_end2.row_ = end2.row_;
_end2.column_ = end2.column_;

_length = length;
// check if the bond is valid
if(_end1.row_ == _end2.row_){
bondType = BondType::Horizontal;
// means x_ values are equal
if(_end1.column_ > _end2.column_){
if(_end1.column_ == _length-1 && _end2.column_ ==0){
// do nothing
}
else{
// sort them out
_end1.column_ = end2.column_;
_end2.column_ = end1.column_;
```

```
53 }
54 }
55 else if(_end1.column_ < _end2.column_){
56 if(_end1.column_ == 0 && _end2.column_ == _length-1){
57 _end1.column_ = end2.column_;
58 _end2.column_ = end1.column_;
59 }
60 }
61 }
62 else if(_end1.column_ == _end2.column_){
63 bondType = BondType::Vertical;
64 // means y_ values are equal
65 if(_end1.row_ > _end2.row_){
66 if(_end1.row_ == _length-1 && _end2.row_ ==0){
67 }
68 else{
69 // sort them out
70 _end1.row_ = end2.row_;
71 _end2.row_ = end1.row_;
72 }
73 }
74 else if(_end1.row_ < _end2.row_){
75 if(_end1.row_ == 0 && _end2.row_ == _length-1){
76 _end1.row_ = end2.row_;
77 _end2.row_ = end1.row_;
78 }
79 }
80 }
81 else{
82 std::cout << '(' << _end1.row_ << ',' << _end1.column_ << ')' << "<->"
83 << '(' << _end2.row_ << ',' << _end2.column_ << ')'
84 << " is not a valid bond : line " << __LINE__ << std::endl;
85 }
86
87 _id = BondIndex(bondType, _end1.row_, _end1.column_);  // unsigned long
88 }
89
90 std::vector<Index> getSites() const { return {_end1, _end2};}
91
92 Index id() const {
93 return _end1;
94 }
95
96 BondIndex ID() const {
```

```
97  return _id;
98  }
99
100 void activate() {_status = true;}
101 void deactivate() {
102 _relative_index = {0,0};
103 _group_id = -1;
104 _status = false;
105 }
106 bool isActive() const { return _status;}
107 /*
108 * Group get_ID is the set_ID of the cluster they are in
109 */
110 int get_groupID() const {return _group_id;}
111 void set_groupID(int g_id) {_group_id = g_id;}
112
113 std::stringstream getBondString() const {
114 std::stringstream ss;
115 if(isActive()) {
116 // place '-' for horizontal bond and '|' for vertical bong
117 if(bondType == BondType::Horizontal) {
118 ss << '(' << _end1 << "<->" << _end2 << ')';
119 }
120 else {
121 ss << '(' << _end1 << "<|>" << _end2 << ')';
122 }
123 }
124 else
125 ss << "(**)";
126 return ss;
127 }
128
129 bool isHorizontal() const { return bondType == BondType::Horizontal;}
130 bool isVertical()   const { return bondType == BondType::Vertical;}
131
132 void relativeIndex(IndexRelative r){
133 _relative_index = r;
134 }
135
136 void relativeIndex(int x, int y){
137 _relative_index = {x,y};
138 }
139
140 IndexRelative relativeIndex() const {return _relative_index;}
```

```
141 };
142
143
144 std::ostream&   operator<<(std::ostream& os, const Bond& bond);
145 bool            operator==(Bond a, Bond b);
146 bool            operator<(const Bond& bond1, const Bond& bond2);
147 bool            operator>(const Bond& bond1, const Bond& bond2);
148
149 #endif //SITEPERCOLATION_BOND_H
```

The **src/lattice/bond.cpp** file

```
1  #include "bond.h"
2
3  /**
4  * use '-' and '|' in between '<>' to indicate horizontal or vertical
       bond
5  * ((0,1)<->(0,0)) for horizontal bond
6  * ((1,1)<|>(0,1)) for vertical bond
7  * @param os
8  * @param bond
9  * @return
10 */
11 std::ostream& operator<<(std::ostream& os, const Bond& bond)
12 {
13 if(bond.isActive()) {
14 // place '-' for horizontal bond and '|' for vertical bong
15 if(bond.isHorizontal()) {
16 return os << '(' << bond._end1 << "<->" << bond._end2 << ')';
17 }
18 return os << '(' << bond._end1 << "<|>" << bond._end2 << ')';
19 }
20 else
21 return os << "(**)";
22 }
23
24 bool operator==(Bond a, Bond b)
25 {
26 if(a.isHorizontal() && b.isHorizontal())
27 {
28 return (a.id().row_ == b.id().row_) && (a.id().column_ == b.id().column_
       );
29 }
30 if(a.isVertical() && b.isVertical()){
```

```
return (a.id().row_ == b.id().row_) && (a.id().column_ == b.id().column_
    );
}

return false;
}

bool  operator<(const Bond& bond1, const Bond& bond2){
if(bond1.isHorizontal() && bond2.isHorizontal()){
return bond1._end1.column_ < bond2._end1.column_;
}
if(bond1.isVertical() && bond2.isVertical()){
return bond1._end1.row_ < bond2._end1.row_;
}
return bond1.isHorizontal();
}


bool  operator>(const Bond& bond1, const Bond& bond2){
if(bond1.isHorizontal() && bond2.isHorizontal()){
return bond1._end1.column_ > bond2._end1.column_;
}
if(bond1.isVertical() && bond2.isVertical()){
return bond1._end1.row_ > bond2._end1.row_;
}
return bond1.isVertical();
}
```

The **src/lattice/bond_type.cpp** file

```
#ifndef PERCOLATION_BOND_V2_H
#define PERCOLATION_BOND_V2_H
/**
* Only two type bonds in 2D lattice
*/
enum class BondType{
Horizontal,
Vertical
};
#endif //PERCOLATION_BOND_V2_H
```

A.2.4 Lattice

The lattice class consists of array of sites and bonds. This class contains information about lattice size. And contains functions to view the lattice differently in the console.

the **src/lattice/lattice.h** file

```
#ifndef SITEPERCOLATION_LATTICE_H
#define SITEPERCOLATION_LATTICE_H

#include <vector>
#include <cmath>

#include "../percolation/cluster.h"
#include "../types.h"
#include "site.h"
#include "bond.h"


/**
* The square Lattice
* Site and Bonds are always present But they will not be counted unless they are activated
* always return by references, so that values in the class itself is modified
*/
class SqLattice {
std::vector<std::vector<Site>> _sites;  // holds all the sites
std::vector<std::vector<Bond>> _h_bonds;  // holds all horizontal bonds
std::vector<std::vector<Bond>> _v_bonds;  // holds all vertical bonds

bool _bond_resetting_flag=true; // so that we can reset all bonds
bool _site_resetting_flag=true; // and all sites

value_type _length{};

private:
void reset_sites();
void reset_bonds();
public:
~SqLattice() = default;
SqLattice() = default;
SqLattice(SqLattice&) = default;
SqLattice(SqLattice&&) = default;
SqLattice& operator=(const SqLattice&) = default;
```

```
37 SqLattice& operator=(SqLattice&&) = default;
38
39 SqLattice(value_type length, bool activate_bonds, bool activate_sites,
       bool bond_reset, bool site_reset);
40
41 void reset(bool reset_all=false);
42
43
44 /*************************************
45 * I/O functions
46 *************************************/
47 void view_sites();
48 void view_sites_extended();
49 void view_sites_by_id();
50 void view_sites_by_relative_index();
51 void view_bonds_by_relative_index_v4();
52 void view_by_relative_index();
53 void view(); // view lattice bonds and sites together
54
55 void view_h_bonds();
56 void view_v_bonds();
57
58 void view_bonds(){
59 view_h_bonds();
60 view_v_bonds();
61 }
62
63
64 void view_bonds_by_id();
65
66 /*********************************
67 * Activation functions
68 *********************************/
69 void activate_site(Index index);
70 void activateBond(BondIndex bond);
71
72 void deactivate_site(Index index);
73 void deactivate_bond(Bond bond);
74
75 value_type length() const { return  _length;}
76
77 Site& getSite(Index index);
78 Bond& getBond(BondIndex);
79
```

```
80  const Site& getSite(Index index) const ;
81  const Bond& getBond(BondIndex index) const ;
82
83  void setGroupID(Index index, int group_id);
84  void setGroupID(BondIndex index, int group_id);
85  const int getGroupID(Index index)const;
86  const int getGroupID(BondIndex index)const;
87
88
89  /*
        ************************************************************************
90  * Get Neighbor from given index
91  ************************************************************************
        */
92  std::vector<Index> get_neighbor_site_indices(Index site);    // site
        neighbor of site
93  std::vector<BondIndex> get_neighbor_bond_indices(BondIndex site); //
        bond neighbor of bond
94  std::vector<Index> get_neighbor_indices(BondIndex bond);    // two site
        neighbor of bond.
95
96  static std::vector<Index> get_neighbor_site_indices(size_t length, Index
         site);    // 4 site neighbor of site
97  static std::vector<BondIndex> get_neighbor_bond_indices(size_t length,
        BondIndex site); // 6 bond neighbor of bond
98  static std::vector<Index> get_neighbor_indices(size_t length, BondIndex
        bond);    // 2 site neighbor of bond.
99
100 };
101
102
103 #endif //SITEPERCOLATION_LATTICE_H
```

The **src/lattice/lattice.cpp** file

```
1  //
2  // Created by shahnoor on 10/2/2017.
3  //
4
5  #include <iomanip>
6  #include "lattice.h"
7  #include "../util/printer.h"
8
9  using namespace std;
```

```
10
11
12 /**
13 *
14 * @param length         -> length of the lattice
15 * @param activate_bonds -> if true all bonds are activated by default
16 *                          and will not be deactivated as long as the
       object exists,
17 *                          even if SLattice::reset function is called.
18 * @param activate_sites -> if true all sites are activated by default
19 *                          and will not be deactivated as long as the
       object exists,
20 *                          even if SLattice::reset function is called.
21 */
22 SqLattice::SqLattice(
23 value_type length,
24 bool activate_bonds, bool activate_sites,
25 bool bond_reset, bool site_reset)
26 : _length{length}, _bond_resetting_flag{bond_reset},
       _site_resetting_flag{site_reset}
27 {
28 cout << "Constructing Lattice object : line " << __LINE__ << endl;
29 _sites = std::vector<std::vector<Site>>(_length);
30 _h_bonds = std::vector<std::vector<Bond>>(_length);
31 _v_bonds = std::vector<std::vector<Bond>>(_length);
32 if(!activate_bonds && !activate_sites) {     // both are deactivated by
       default
33 for (value_type i{}; i != _length; ++i) {
34 _sites[i] = std::vector<Site>(_length);
35 _h_bonds[i] = std::vector<Bond>(_length);
36 _v_bonds[i] = std::vector<Bond>(_length);
37 for (value_type j{}; j != _length; ++j) {
38 _sites[i][j] = Site(Index(i, j), _length);
39 _h_bonds[i][j] = {Index(i, j), Index(i, (j + 1) % _length), _length};
40 _v_bonds[i][j] = {Index(i, j), Index((i + 1) % _length, j), _length};
41 }
42 }
43 }
44 else if(activate_bonds && !activate_sites) {     // all bonds are
       activated by default
45 for (value_type i{}; i != _length; ++i) {
46 _sites[i] = std::vector<Site>(_length);
47 _h_bonds[i] = std::vector<Bond>(_length);
48 _v_bonds[i] = std::vector<Bond>(_length);
```

```
49 for (value_type j{}; j != _length; ++j) {
50 _sites[i][j] = Site(Index(i, j), _length);
51 _h_bonds[i][j] = {Index(i, j), Index(i, (j + 1) % _length), _length};
52 _v_bonds[i][j] = {Index(i, j), Index((i + 1) % _length, j), _length};
53 _h_bonds[i][j].activate();
54 _v_bonds[i][j].activate();
55 }
56 }
57 }
58 else if(!activate_bonds && activate_sites) {     // all sites are
       activated by default
59 for (value_type i{}; i != _length; ++i) {
60 _sites[i] = std::vector<Site>(_length);
61 _h_bonds[i] = std::vector<Bond>(_length);
62 _v_bonds[i] = std::vector<Bond>(_length);
63 for (value_type j{}; j != _length; ++j) {
64 _sites[i][j] = Site(Index(i, j), _length);
65 _sites[i][j].activate();
66 _h_bonds[i][j] = {Index(i, j), Index(i, (j + 1) % _length), _length};
67 _v_bonds[i][j] = {Index(i, j), Index((i + 1) % _length, j), _length};
68 }
69 }
70 }
71 else {
72 for (value_type i{}; i != _length; ++i) {    // all bonds and sites are
       activated by default
73 _sites[i] = std::vector<Site>(_length);
74 _h_bonds[i] = std::vector<Bond>(_length);
75 _v_bonds[i] = std::vector<Bond>(_length);
76 for (value_type j{}; j != _length; ++j) {
77 _sites[i][j] = Site(Index(i, j), _length);
78 _sites[i][j].activate();
79 _h_bonds[i][j] = {Index(i, j), Index(i, (j + 1) % _length), _length};
80 _v_bonds[i][j] = {Index(i, j), Index((i + 1) % _length, j), _length};
81 _h_bonds[i][j].activate();
82 _v_bonds[i][j].activate();
83 }
84 }
85 }
86
87 }
88
89 /*****************************************************************
90 * Activation and Deactivation
```

```
91 ************************************************************/
92
93
94 void SqLattice::activate_site(Index index) {
95 _sites[index.row_][index.column_].activate();
96 }
97
98
99 void SqLattice::activateBond(BondIndex bond) {
100 // check if the bond is vertical or horizontal
101 // then call appropriate function to activate _h_bond or _v_bond
102 if(bond.horizontal()){ // horizontal
103 if(_h_bonds[bond.row_][bond.column_].isActive()){
104 cout << "Bond is already activated : line " << __LINE__ << endl;
105 }
106 _h_bonds[bond.row_][bond.column_].activate();
107 }
108 else if(bond.vertical()) // vertical
109 {
110 if(_v_bonds[bond.row_][bond.column_].isActive()){
111 cout << "Bond is already activated : line " << __LINE__ << endl;
112 }
113 _v_bonds[bond.row_][bond.column_].activate();
114 }
115 else{
116 cout << bond << " is not a valid bond : line " << __LINE__ << endl;
117 }
118
119 }
120
121
122 void SqLattice::deactivate_site(Index index){
123 _sites[index.row_][index.column_].deactivate();
124 }
125
126
127 void SqLattice::deactivate_bond(Bond bond) {
128 // check if the bond is vertical or horizontal
129 // then call appropriate function to activate _h_bond or _v_bond
130 if(bond.isHorizontal()){
131 if(_h_bonds[bond.id().row_][bond.id().column_].isActive()){
132 cout << "Bond is already activated : line " << __LINE__ << endl;
133 }
134 _h_bonds[bond.id().row_][bond.id().column_].deactivate();
```

```
135 }
136 else if(bond.isVertical())
137 {
138 if(_v_bonds[bond.id().row_][bond.id().column_].isActive()){
139 cout << "Bond is already activated : line " << __LINE__ << endl;
140 }
141 _v_bonds[bond.id().row_][bond.id().column_].deactivate();
142 }
143 else{
144 bond.activate();
145 cout << bond << " is not a valid bond : line " << __LINE__ << endl;
146 }
147 }
148
149
150 /*********************************************************
151 * Viewing methods
152 *********************************************************/
153 /**
154 *  View the sites of the lattice
155 *  place (*) if the site is not active
156 */
157 void SqLattice::view_sites()
158 {
159 std::cout << "view sites" << std::endl;
160 std::cout << '{';
161 for(value_type i{} ; i != _length ; ++i) {
162 if(i!=0) std::cout << "  ";
163 else std::cout << '{';
164 for (value_type j{}; j != _length; ++j) {
165 if(_sites[i][j].isActive()){
166 std::cout << _sites[i][j] ;
167 }
168 else{
169 std::cout << "(*)";
170 }
171 if(j != _length-1)
172 std::cout << ',';
173 }
174 std::cout << '}';
175 if(i != _length-1)
176 std::cout << std::endl;
177 }
178 std::cout << '}';
```

```
179 std::cout << std::endl;
180 }
181
182 /**
183 *  View the sites of the lattice
184 *  place (*) if the site is not active
185 *  Shows the group_id along with sites
186 *
187 *  Very good output format. Up to lattice size < 100
188 */
189 void SqLattice::view_sites_extended()
190 {
191 std::cout << "view sites" << std::endl;
192 std::cout << '{';
193 for(value_type i{} ; i != _length ; ++i) {
194 if(i!=0) std::cout << "  ";
195 else std::cout << '{';
196 for (value_type j{}; j != _length; ++j) {
197 std::cout << std::setw(3) << _sites[i][j].get_groupID() << ":";
198
199 if(_sites[i][j].isActive()) {
200 cout << '(' << std::setw(2) << _sites[i][j]._id.row_ << ','
201 << std::setw(2) << _sites[i][j]._id.column_ << ')';
202 }
203 else{
204 cout << std::setw(7) << "(*)";
205 }
206
207 if(j != _length-1)
208 std::cout << ',';
209 }
210 std::cout << '}';
211 if(i != _length-1)
212 std::cout << std::endl;
213 }
214 std::cout << '}';
215 std::cout << std::endl;
216 }
217
218
219
220 /**
221 * Displays group ids of sites in a matrix form
222 */
```

```
223 void SqLattice::view_sites_by_id() {
224 std::cout << "Sites by id : line " << __LINE__ << endl;
225 cout << "   ";
226 for(value_type j{}; j != _length; ++ j){
227 cout << " " << setw(3) << j;
228 }
229 cout << endl << " __|";
230 for(value_type j{}; j != _length; ++ j){
231 cout << "_ _ ";
232 }
233 cout << endl;
234 for(value_type i{} ; i != _length; ++i){
235 cout << setw(3) << i << "|";
236 for(value_type j{} ; j != _length ; ++ j){
237 cout << setw(3) << _sites[i][j].get_groupID() << ' ';
238 }
239 cout << endl;
240 }
241 }
242
243
244 /**
245 *
246 */
247 void SqLattice::view_sites_by_relative_index(){
248 std::cout << "Relative index : line " << __LINE__ << endl;
249 cout << "Format: \"id(x,y)\"" << endl;
250 cout << "   |";
251 for(value_type j{}; j != _length; ++ j){
252 cout << setw(4) << j << "         |";
253 }
254 cout << endl;
255 print_h_barrier(_length, "___|__", "___________|__");
256 for(value_type i{} ; i != _length; ++i){
257 cout << setw(3) << i << "|";
258 for(value_type j{} ; j != _length ; ++ j){
259 if(_sites[i][j].get_groupID() == -1){
260 // left blank
261 cout << setw(4) << _sites[i][j].get_groupID() << "         |";
262 continue;
263 }
264 cout << setw(4) << _sites[i][j].get_groupID() << _sites[i][j].
    relativeIndex() << "|";
265 }
```

```
266 cout << endl;
267 print_h_barrier(_length, "___|__", "__________|__");
268 }
269 //     print_h_barrier(_length, "___|__", "__________|_");
270 }
271
272
273
274
275
276 /**
277 * View bonds in the lattice by relative index. id of the site is showed
278 * format : id(relative index) for site and only id for bond
279 * if any site is isolated relative index is not shown
280 */
281 void SqLattice::view_bonds_by_relative_index_v4() {
282
283 std::cout << "Bonds by id : line " << __LINE__ << endl;
284 //cout << "site id -1 means isolated site and 0 means connected site in
       bond percolation(definition)" << endl;
285 print_h_barrier(15, "_", "___", "_\n");
286 cout << "|(site id) (horizontal bond id(relative index))|" << endl;
287 cout << "|(vertical bond id(relative index))           |" << endl;
288 print_h_barrier(15, "-", "---", "-\n");
289 // printing indices for columns
290 std::cout << "    | ";
291 for(value_type i{}; i != _length; ++i){
292 std::cout << i << "               | ";
293 }
294 std::cout << std::endl;
295
296 // pringing H,V label
297
298 print_h_barrier(_length, "    |  ", " V          H  |  ");
299 print_h_barrier(_length, "____|__", "_________________|__");
300
301 // for each row there will be two columns
302 for(value_type i{}; i != _length; ++i){
303 std::cout << i << ' ';
304 std::cout << "H |";
305 for(value_type j1{}; j1 != _length; ++j1){
306 int id = _sites[i][j1].get_groupID();
307 std::cout << std::setw(3) << id  ;
308 if(id != -1){
```

```
309 cout << _sites[i][j1].relativeIndex();
310 }else{
311 cout << "(-,-)    ";
312 }
313 std::cout << "   " << std::setw(3) << _h_bonds[i][j1].get_groupID() << "
    |";
314 }
315 std::cout << std::endl;
316 print_h_barrier(_length, "    |  ", "                |  "); // just to
    see a better view
317 std::cout << "  " << "V |";
318 for(value_type j2{}; j2 != _length; ++j2){
319 std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "
         |";
320 }
321 std::cout << std::endl;
322
323 // printing horizontal separator
324 print_h_barrier(_length, "____|__", "_________________|__");
325 }
326
327 std::cout << std::endl;
328 }
329
330
331
332 /**
333 * View lattice (sites and bonds) by relative index.
334 * format : id(relative_index)
335 */
336 void SqLattice::view_by_relative_index() {
337
338 std::cout << "Bonds by id : line " << __LINE__ << endl;
339 // printing indices for columns
340 std::cout << "    | ";
341 for(value_type i{}; i != _length; ++i){
342 std::cout << i << "                        | ";
343 }
344 std::cout << std::endl;
345
346 // pringing H,V label
347
348 print_h_barrier(_length, "    |  ", " V                  H   |  ");
349 print_h_barrier(_length, "____|__", "_________________________|__");
```

```
350
351 // for each row there will be two columns
352 for(value_type i{}; i != _length; ++i){
353 std::cout << i << ' ';
354 std::cout << "H |";
355 for(value_type j1{}; j1 != _length; ++j1){
356 std::cout << std::setw(3) << _sites[i][j1].get_groupID() << _sites[i][j1
    ].relativeIndex();
357 std::cout << "   " << std::setw(3) << _h_bonds[i][j1].get_groupID()
358 << _h_bonds[i][j1].relativeIndex() << "|";
359 }
360 std::cout << std::endl;
361 print_h_barrier(_length, "    |  ", "                          |  "); //
    just to see a better view
362 std::cout << "  " << "V |";
363 for(value_type j2{}; j2 != _length; ++j2){
364 std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID()
365 << _v_bonds[i][j2].relativeIndex() << "               |";
366 }
367 std::cout << std::endl;
368
369 // printing horizontal separator
370 print_h_barrier(_length, "____|__", "_________________________|__");
371 }
372
373 //        view_h_bonds_extended();
374 //        view_v_bonds_extended();
375 std::cout << std::endl;
376
377 }
378
379 /**
380 * View lattice (sites and bonds) by relative index.
381 * format : id(relative_index)
382 */
383 void SqLattice::view() {
384
385 std::cout << "Bonds by id : line " << __LINE__ << endl;
386 cout << "Structure " << endl;
387 print_h_barrier(10, "_", "___", "_\n");
388 cout << "|(site id) (horizontal bond id)|" << endl;
389 cout << "|(vertical bond id)            |" << endl;
390 print_h_barrier(10, "-", "---", "-\n");
391 // printing indices for columns
```

```
392 std::cout << "    | ";
393 for(value_type i{}; i != _length; ++i){
394 std::cout << i << "       | ";
395 }
396 std::cout << std::endl;
397
398 // pringing H,V label
399
400 print_h_barrier(_length, "    |  ", "V    H|  ");
401 print_h_barrier(_length, "____|__", "______|__");
402
403 // for each row there will be two columns
404 for(value_type i{}; i != _length; ++i){
405 std::cout << i << ' ';
406 std::cout << "H |";
407 for(value_type j1{}; j1 != _length; ++j1){
408 std::cout << std::setw(3) << _sites[i][j1].get_groupID() ;
409 std::cout << "  " << std::setw(3) << _h_bonds[i][j1].get_groupID() << "|
    ";
410 }
411 std::cout << std::endl;
412 print_h_barrier(_length, "    |  ", "       |  "); // just to see a
    better view
413 std::cout << "  " << "V |";
414 for(value_type j2{}; j2 != _length; ++j2){
415 std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "     |";
416 }
417 std::cout << std::endl;
418
419 // printing horizontal separator
420 print_h_barrier(_length, "____|__", "______|__");
421 }
422
423 //         view_h_bonds_extended();
424 //         view_v_bonds_extended();
425 std::cout << std::endl;
426
427 }
428
429
430 /**
431 *
432 */
433 void SqLattice::view_h_bonds()
```

```
{
std::cout << "view horizontal bonds" << std::endl;
std::cout << '{';
for(value_type i{} ; i != _length ; ++i) {
if(i!=0) std::cout << "  ";
else std::cout << '{';
for (value_type j{}; j != _length; ++j) {
std::cout << _h_bonds[i][j] ;
if(j != _length-1)
std::cout << ',';
}
std::cout << '}';
if(i != _length-1)
std::cout << std::endl;
}
std::cout << '}';
std::cout << std::endl;
}

/**
*
*/
void SqLattice::view_v_bonds()
{
std::cout << "view vertical bonds" << std::endl;
std::cout << '{';
for(value_type i{} ; i != _length ; ++i) {
if(i!=0) std::cout << "  ";
else std::cout << '{';
for (value_type j{}; j != _length; ++j) {
std::cout << _v_bonds[i][j] ;
if(j != _length-1)
std::cout << ',';
}
std::cout << '}';
if(i != _length-1)
std::cout << std::endl;
}
std::cout << '}';
std::cout << std::endl;
}


/**
```

```
478 *
479 */
480 void SqLattice::view_bonds_by_id(){
481 std::cout << "Bonds by id : line " << __LINE__ << endl;
482 cout << "Structure " << endl;
483 print_h_barrier(8, "__", "___", "_\n");
484 cout << "|      (horizontal bond id)|" << endl;
485 cout << "|(vertical bond id)        |" << endl;
486 print_h_barrier(8, "__", "___", "_\n");
487 // printing indices for columns
488 std::cout << "    | ";
489 for(value_type i{}; i != _length; ++i){
490 std::cout << i << "    | ";
491 }
492 std::cout << std::endl;
493
494 // pringing H,V label
495
496 print_h_barrier(_length, "    |  ", "V  H|  ");
497 print_h_barrier(_length, "____|__", "____|__");
498
499 // for each row there will be two columns
500 for(value_type i{}; i != _length; ++i){
501 std::cout << i << ' ';
502 std::cout << "H |";
503 for(value_type j1{}; j1 != _length; ++j1){
504 std::cout << "   " << std::setw(3) << _h_bonds[i][j1].get_groupID() << "
    |";
505 }
506 std::cout << std::endl;
507 std::cout << "  " << "V |";
508 for(value_type j2{}; j2 != _length; ++j2){
509 std::cout << std::setw(3) << _v_bonds[i][j2].get_groupID() << "   |";
510 }
511 std::cout << std::endl;
512
513 // printing horizontal separator
514 print_h_barrier(_length, "____|__", "____|__");
515 }
516
517 //        view_h_bonds_extended();
518 //        view_v_bonds_extended();
519 std::cout << std::endl;
520 }
```

```
521
522
523 Site& SqLattice::getSite(Index index) {
524 return _sites[index.row_][index.column_];
525 }
526
527
528 const Site& SqLattice::getSite(Index index) const {
529 return _sites[index.row_][index.column_];
530 }
531
532 const Bond& SqLattice::getBond(BondIndex index) const {
533 if (index.horizontal()) {
534 return _h_bonds[index.row_][index.column_];
535 }
536 if (index.vertical()) {
537 return _v_bonds[index.row_][index.column_];
538 }
539 throw InvalidBond{"Invalid bond : line " + to_string(__LINE__)};
540 }
541
542 void SqLattice::setGroupID(Index index, int group_id){
543 _sites[index.row_][index.column_].set_groupID(group_id);
544 }
545
546 void SqLattice::setGroupID(BondIndex index, int group_id){
547 if(index.horizontal()){
548 _h_bonds[index.row_][index.column_].set_groupID(group_id);
549 }
550 if(index.vertical()){
551 _v_bonds[index.row_][index.column_].set_groupID(group_id);
552 }
553 }
554
555 const int SqLattice::getGroupID(Index index)const{
556 return _sites[index.row_][index.column_].get_groupID();
557 }
558
559 const int SqLattice::getGroupID(BondIndex index)const{
560 if(index.horizontal()){
561 return _h_bonds[index.row_][index.column_].get_groupID();
562 }
563 if(index.vertical()){
564 return  _v_bonds[index.row_][index.column_].get_groupID();
```

```
565 }
566 return -1;
567 }
568
569
570 Bond& SqLattice::getBond(BondIndex index) {
571 if(index.horizontal())
572 return _h_bonds[index.row_][index.column_];
573 if(index.vertical())
574 return _v_bonds[index.row_][index.column_];
575 throw InvalidBond{"Invalid bond : line " + to_string(__LINE__)};
576 }
577
578 void SqLattice::reset(bool reset_all) {
579 if(reset_all){
580 reset_sites();
581 reset_bonds();
582 return;
583 }
584 // setting all group id to -1
585 if(_site_resetting_flag) {
586 reset_sites();
587 }
588 //    cout << "Bond resetting is disabled : line " << __LINE__ << endl;
589 if(_bond_resetting_flag) {
590 reset_bonds();
591 }
592
593 }
594
595 /**
596 *
597 */
598 void SqLattice::reset_bonds() {
599 for(value_type i{}; i != _h_bonds.size(); ++i){
600 for (int j{}; j != _h_bonds[i].size(); ++j) {
601 // deactivating. automatically set group id == - and relative index ==
    (0,0)
602 // setting group id = -1 and deactivating the bond
603 _h_bonds[i][j].deactivate();
604 _v_bonds[i][j].deactivate();
605
606
607 }
```

```
608 }
609 }
610
611 /**
612 *
613 */
614 void SqLattice::reset_sites() {
615 for(value_type i{}; i != _sites.size(); ++i){
616 for(value_type j{}; j != _sites[i].size(); ++j) {
617 // deactivating. automatically set group id == - and relative index ==
    (0,0)
618 // setting group id = -1 and deactivating the site
619 _sites[i][j].deactivate();
620 }
621 }
622 }
623
624
625 /*
    ****************************************************************************

626 * Get Neighbor from given index
627 ****************************************************************************
    */
628 /**
629 * Periodic case only.
630 * Each site has four neighbor sites.
631 * @param site
632 * @return
633 */
634 std::vector<Index> SqLattice::get_neighbor_site_indices(Index site){
635 std::vector<Index> sites(4);
636 sites[0] = {(site.row_ + 1) % _length, site.column_};
637 sites[1] = {(site.row_ - 1 + _length) % _length, site.column_};
638 sites[2] = {site.row_, (site.column_ + 1) % _length};
639 sites[3] = {site.row_, (site.column_ - 1 + _length) % _length};
640 return sites;
641 }
642
643 /**
644 * Periodic case only.
645 * Each bond has six neibhbor bonds.
646 * @param site
647 * @return
```

```
*/
std::vector<BondIndex> SqLattice::get_neighbor_bond_indices(BondIndex
    bond) {
value_type next_column = (bond.column_ + 1) % _length;
value_type prev_column = (bond.column_ - 1 + _length) % _length;
value_type prev_row = (bond.row_ - 1 + _length) % _length;
value_type next_row = (bond.row_ + 1) % _length;

vector<BondIndex> bonds(6);

// horizontal bond case
if (bond.horizontal()) {
// increase column index for the right neighbor

// left end of bond
bonds[0] = {BondType::Vertical, bond.row_, bond.column_};
bonds[1] = {BondType::Vertical, prev_row, bond.column_};
bonds[2] = {BondType::Horizontal, bond.row_, prev_column};

// right end bond
bonds[3] = {BondType::Vertical, prev_row, next_column};
bonds[4] = {BondType::Vertical, bond.row_, next_column};
bonds[5] = {BondType::Horizontal, bond.row_, next_column};

}
// vertical bond case
else if (bond.vertical()) {
// increase row index

// top end of bond
bonds[0] = {BondType::Horizontal, bond.row_, bond.column_};
bonds[1] = {BondType::Horizontal, bond.row_, prev_column};
bonds[2] = {BondType::Vertical, prev_row, bond.column_};

// bottom end of bond
bonds[3] = {BondType::Horizontal, next_row, bond.column_};
bonds[4] = {BondType::Horizontal, next_row, prev_column};
bonds[5] = {BondType::Vertical, next_row, bond.column_};

}


return bonds;
}
```

```
691
692 std::vector<Index> SqLattice::get_neighbor_indices(BondIndex bond) {
693 value_type r = bond.row_;
694 value_type c = bond.column_;
695 vector<Index> sites(2);
696 sites[0] = {r, c};
697 if(bond.horizontal()){
698 sites[1] = {r, (c+1) % _length};
699 }else{
700 sites[1] = {(r+1) % _length, c};
701 }
702 return sites;
703 }
704
705 /*************************************************************
706 * Static methods
707 */
708 std::vector<Index> SqLattice::get_neighbor_site_indices(size_t length,
    Index site){
709 std::vector<Index> sites(4);
710 sites[0] = {(site.row_ + 1) % length, site.column_};
711 sites[1] = {(site.row_ - 1 + length) % length, site.column_};
712 sites[2] = {site.row_, (site.column_ + 1) % length};
713 sites[3] = {site.row_, (site.column_ - 1 + length) % length};
714 return sites;
715 }
716
717 /**
718 * Periodic case only.
719 * Each bond has six neibhbor bonds.
720 * @param site
721 * @return
722 */
723 std::vector<BondIndex> SqLattice::get_neighbor_bond_indices(size_t
    length, BondIndex bond) {
724 value_type next_column = (bond.column_ + 1) % length;
725 value_type prev_column = (bond.column_ - 1 + length) % length;
726 value_type prev_row = (bond.row_ - 1 + length) % length;
727 value_type next_row = (bond.row_ + 1) % length;
728
729 vector<BondIndex> bonds(6);
730
731 // horizontal bond case
732 if (bond.horizontal()) {
```

```
733 // increase column index for the right neighbor
734
735 // left end of bond
736 bonds[0] = {BondType::Vertical, bond.row_, bond.column_};
737 bonds[1] = {BondType::Vertical, prev_row, bond.column_};
738 bonds[2] = {BondType::Horizontal, bond.row_, prev_column};
739
740 // right end bond
741 bonds[3] = {BondType::Vertical, prev_row, next_column};
742 bonds[4] = {BondType::Vertical, bond.row_, next_column};
743 bonds[5] = {BondType::Horizontal, bond.row_, next_column};
744
745 }
746 // vertical bond case
747 else if (bond.vertical()) {
748 // increase row index
749
750 // top end of bond
751 bonds[0] = {BondType::Horizontal, bond.row_, bond.column_};
752 bonds[1] = {BondType::Horizontal, bond.row_, prev_column};
753 bonds[2] = {BondType::Vertical, prev_row, bond.column_};
754
755 // bottom end of bond
756 bonds[3] = {BondType::Horizontal, next_row, bond.column_};
757 bonds[4] = {BondType::Horizontal, next_row, prev_column};
758 bonds[5] = {BondType::Vertical, next_row, bond.column_};
759
760 }
761
762
763 return bonds;
764 }
765
766 std::vector<Index> SqLattice::get_neighbor_indices(size_t length,
    BondIndex bond) {
767 value_type r = bond.row_;
768 value_type c = bond.column_;
769 vector<Index> sites(2);
770 sites[0] = {r, c};
771 if(bond.horizontal()){
772 sites[1] = {r, (c+1) % length};
773 }else{
774 sites[1] = {(r+1) % length, c};
775 }
```

```
776 return sites;
777 }
```

A.2.5 Exception

Different types of exceptions.

The **src/exception/exception.h** file

```
1  #ifndef PERCOLATION_EXCEPTIONS_H
2  #define PERCOLATION_EXCEPTIONS_H
3
4  #include <string>
5  #include <iostream>
6
7  /**
8   *
9   */
10 struct Mismatch{
11     std::string msg_;
12     size_t line_;
13     Mismatch(size_t line, std::string msg="")
14             :line_{line}, msg_{msg}  {}
15
16     void what() const {
17         std::cerr << msg_ << "\nId and index mismatch at line " << line_
       << std::endl;
18     }
19 };
20
21 /**
22  *
23  */
24 struct InvalidIndex{
25     std::string msg_;
26     InvalidIndex(std::string msg)  :msg_{msg}  {}
27
28     void what() const {
29         std::cerr << msg_ << std::endl;
30     }
31 };
32
33 /**
34  *
```

```
35  */
36 struct InvalidBond{
37     std::string msg_;
38     InvalidBond(std::string msg)  :msg_{msg}  {}
39 
40     void what() const {
41         std::cout << msg_ << std::endl;
42     }
43 };
44 
45 
46 /**
47  * When any neighor is occupied and no suitable neighbor is found, throw
        this exception
48  */
49 struct OccupiedNeighbor{
50     std::string msg_;
51     OccupiedNeighbor(std::string msg): msg_{msg}{}
52 
53     void what() const {
54         std::cout << msg_ << std::endl;
55     }
56 };
57 
58 /**
59  * If the 1st or the 2nd nearest neighbor is not valid
60  */
61 struct InvalidNeighbor{
62     std::string msg_;
63     InvalidNeighbor(std::string msg)  :msg_{msg}  {}
64 
65     void what() const {
66         std::cout << msg_ << std::endl;
67     }
68 };
69 
70 
71 #endif //PERCOLATION_EXCEPTIONS_H
```

A.2.6 Cluster

The cluster class contains all information about a cluster. Number of sites and bonds in a cluster and the id of the cluster is contained in a cluster.

The **src/percolation/cluster.h** file

```
#ifndef SITEPERCOLATION_CLUSTER_H
#define SITEPERCOLATION_CLUSTER_H

#include <vector>
#include <set>
#include "../lattice/bond.h"
#include "../types.h"
#include "../lattice/site.h"


/**
* Cluster of bonds and sites
* version 3
* final goal -> make a template cluster. so that we can use it for Bond cluster or Site cluster
* root site (bond) is the first site (bond) of the cluster. nedeed for (wrapping) site percolation
*/
class Cluster{
// contains bond and site
std::vector<BondIndex>  _bond_index; // BondIndex for indexing bonds
std::vector<Index>      _site_index; // Site index

int _creation_time{-1};  // holds the creation birthTime of a cluster object
int _id{-1};
public:
//    using iterator = std::vector<Bond>::iterator;

~Cluster()                              = default;
Cluster()                               = default;
Cluster(Cluster&)                   = default;
Cluster(Cluster&&)                  = default;
Cluster& operator=(const Cluster&)      = default;
Cluster& operator=(Cluster&&)     = default;

explicit Cluster(int id){

_id = id;        // may be modified in the program

/*
* Only readable, not modifiable.
```

```
40 * when time = 0 => only lattice exists and bonds in site percolation,
       not any sites
41 * When id = 0, time = 1 => we have placed the first site, hence created
       a cluster with size greater than 1
42 *       Only then Cluster constructor is called.
43 *
44 */
45 _creation_time = id + 1;        // only readable, not modifiable
46 }
47
48
49 void addSiteIndex(Index );
50 void addBondIndex(BondIndex );
51
52 Index lastAddedSite(){return _site_index.back();}
53 BondIndex lastAddedBond(){return _bond_index.back();}
54
55
56 void insert(const std::vector<BondIndex>& bonds);
57 void insert(const std::vector<Index>& sites);
58
59 void insert(const Cluster& cluster);
60 void insert_v2(const Cluster& cluster);
61 void insert_with_id_v2(const Cluster& cluster, int id);
62
63
64 friend std::ostream& operator<<(std::ostream& os, const Cluster& cluster
       );
65
66 const std::vector<BondIndex>&    getBondIndices()     {return _bond_index
       ;}
67 const std::vector<Index>&        getSiteIndices()     {return _site_index
       ;}
68
69 const std::vector<BondIndex>&    getBondIndices() const  {return
       _bond_index;}
70 const std::vector<Index>&        getSiteIndices() const  {return
       _site_index;}
71
72 value_type numberOfBonds() const { return _bond_index.size();}
73 value_type numberOfSites() const { return _site_index.size();}
74 int get_ID() const { return _id;}
75 void set_ID(int id) { _id = id;}
76
```

```
77 int birthTime() const {return _creation_time;}
78
79 Index getRootSite()const{return _site_index[0];} // for site percolation
80 BondIndex getRootBond()const{return _bond_index[0];} // for bond
       percolation
81 bool empty() const { return _bond_index.empty() && _site_index.empty();}
82 void clear() {_bond_index.clear(); _site_index.clear(); }
83 };
84
85 #endif //SITEPERCOLATION_CLUSTER_H
```

The **src/percolation/cluster.cpp** file

```
1
2 #include "cluster.h"
3
4 using namespace std;
5
6 // add Site index
7 void Cluster::addSiteIndex(Index index) {
8 _site_index.push_back(index);
9 }
10
11 void Cluster::addBondIndex(BondIndex bondIndex) {
12 _bond_index.push_back(bondIndex);
13 }
14
15
16
17 void Cluster::insert(const std::vector<BondIndex>& bonds){
18 _bond_index.reserve(bonds.size());
19 for(value_type i{} ; i != bonds.size() ; ++i){
20 _bond_index.push_back(bonds[i]);
21 }
22 }
23
24 void Cluster::insert(const std::vector<Index>& sites){
25 _site_index.reserve(sites.size());
26 for(value_type i{} ; i != sites.size() ; ++i){
27 _site_index.push_back(sites[i]);
28 }
29 }
30
31 /**
32 * Merge two cluster as one
```

```
33 * All intrinsic property should be considered, e.g., creation time of a
       cluster must be recalculated
34 * @param cluster
35 */
36 void Cluster::insert(const Cluster &cluster) {
37 if(_id > cluster._id){
38 cout << "_id > cluster._id : line " << __LINE__ << endl;
39 _id = cluster._id;
40 }
41 // older time or smaller time is the creation birthTime of the cluster
42 //     cout << "Comparing " << _creation_time << " and " << cluster.
       _creation_time;
43 _creation_time = _creation_time < cluster._creation_time ?
       _creation_time : cluster._creation_time;
44 //     cout << " Keeping " << _creation_time << endl;
45 _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
       cluster._bond_index.end());
46 _site_index.insert(_site_index.end(), cluster._site_index.begin(),
       cluster._site_index.end());
47 }
48
49
50 /**
51 * Merge two cluster as one
52 * All intrinsic property should be considered, e.g., creation time of a
       cluster must be recalculated
53 * @param cluster
54 */
55 void Cluster::insert_v2(const Cluster &cluster) {
56 // older time or smaller time is the creation birthTime of the cluster
57 //     cout << "Comparing " << _creation_time << " and " << cluster.
       _creation_time;
58 _creation_time = _creation_time < cluster._creation_time ?
       _creation_time : cluster._creation_time;
59 //     cout << " Keeping " << _creation_time << endl;
60 _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
       cluster._bond_index.end());
61 _site_index.insert(_site_index.end(), cluster._site_index.begin(),
       cluster._site_index.end());
62 }
63
64
65 void Cluster::insert_with_id_v2(const Cluster &cluster, int id) {
66 _id = id;
```

```
67 // older time or smaller time is the creation birthTime of the cluster
68 //     cout << "Comparing " << _creation_time << " and " << cluster.
       _creation_time;
69 _creation_time = _creation_time < cluster._creation_time ?
       _creation_time : cluster._creation_time;
70 //     cout << " Keeping " << _creation_time << endl;
71 _bond_index.insert(_bond_index.end(), cluster._bond_index.begin(),
       cluster._bond_index.end());
72 _site_index.insert(_site_index.end(), cluster._site_index.begin(),
       cluster._site_index.end());
73 }
74
75
76 std::ostream &operator<<(std::ostream &os, const Cluster &cluster) {
77 os << "Sites : size (" << cluster._site_index.size() << ") : ";
78 os << '{';
79 for(auto a: cluster._site_index){
80 os << a << ',';
81 }
82 os << '}' << endl;
83
84 os << "Bonds : size (" << cluster._bond_index.size() <<") : ";
85 os << '{';
86 for(auto a: cluster._bond_index){
87 os << a << ',';
88 }
89 os << '}';
90
91 return os << endl;
92 }
```

A.2.7 Percolation

The *SqLatticePercolation* class contains generic operation that to performed for percolation on square lattice. It's subclass *SitePercolation_ps_v9* is the class when all required method for general site percolation with our definition is defined. And it's subclass *SitePercolationBallisticDeposition_v2* contains some method for ballistic deposition for $l = \{1,2\}$ which extends to two new subclass *SitePercolationBallisticDeposition_L1_v2* and *SitePercolationBallisticDeposition_L2_v2* with detailed method for ballistic deposition $l = 1$ and $l = 2$ respectively.

The **src/percolation/percolation.h** file

```
#ifndef SITEPERCOLATION_PERCOLATION_H
#define SITEPERCOLATION_PERCOLATION_H

#include <vector>
#include <set>
#include <unordered_set>
#include <map>
#include <climits>
#include <fstream>


#include "../types.h"
#include "../lattice/lattice.h"
#include "../index/index.h"

#include <random>


/**
* The Square Lattice Percolation class
*/
class SqLatticePercolation{
// constants
value_type  _length;
value_type _max_number_of_bonds;
value_type _max_number_of_sites;
char type{'0'}; // percolation type. 's' -> site percolation. 'b' ->
    bond percolation
protected:

// structural variables of lattice
SqLattice _lattice;

value_type _index_sequence_position{};

std::vector<Cluster> _clusters;   // check and remove reapeted index
    manually
// every birthTime we create a cluster we assign an set_ID for them

double _occuption_probability {};
// entropy
double _entropy{};
double _entropy_current{};
size_t _cluster_count{};
```

```
43 value_type _bonds_in_cluster_with_size_two_or_more{0};   // total number
       of bonds in the clusters. all cluster has bonds > 1
44 bool _reached_critical = false; // true if the system has reached
      critical value
45
46 value_type _total_relabeling{};
47 double time_relabel{};
48 value_type _number_of_occupied_sites{};
49 value_type _max_iteration_limit{};
50 std::random_device _random_device;
51 std::mt19937 _random_generator;
52
53 void set_type(char t){type = t;} // setting percolation type
54 public:
55 static constexpr const char* signature = "SqLatticePercolation";
56
57 virtual ~SqLatticePercolation() = default;
58 SqLatticePercolation(value_type length);
59 void reset();
60
61
62 bool occupy();
63 value_type length() const { return _length;}
64 value_type maxSites() const {return _max_number_of_sites;}
65 value_type maxBonds() const { return _max_number_of_bonds;}
66
67 /*********
68 *  I/O functions
69 */
70 virtual void viewCluster();
71 virtual void viewClusterExtended();
72 virtual void view_bonds(){
73 _lattice.view_bonds();
74 }
75 virtual void viewLattice(){
76 _lattice.view_sites();
77
78 }
79
80 /**
81 * Also shows the cluster index of the sites
82 */
83 virtual void viewLatticeExtended(){
84 _lattice.view_sites_extended();
```

```
85 }
86
87 /**
88 * Displays group ids of sites in a matrix form
89 */
90 virtual void viewLatticeByID(){
91 _lattice.view_sites_by_id();
92 _lattice.view_bonds_by_id();
93 }
94
95 virtual void viewSiteByID(){
96 _lattice.view_sites_by_id();
97 }
98
99 virtual void viewBondByID(){
100 _lattice.view_bonds_by_id();
101 }
102
103 virtual void viewSiteByRelativeIndex(){
104 _lattice.view_sites_by_relative_index();
105 }
106 virtual void viewBondByRelativeIndex(){
107 _lattice.view_bonds_by_relative_index_v4();
108 }
109
110 virtual void viewByRelativeIndex(){
111 _lattice.view_by_relative_index();
112 }
113
114 virtual void view(){
115 _lattice.view();
116 }
117
118 virtual double occupationProbability() const { return
    _occuption_probability;}
119 virtual double entropy() { return _entropy_current;}
120 double entropy_by_site(); // for future convenience. // the shannon
    entropy. the full calculations. time consuming
121 double entropy_by_bond(); // for future convenience. // the shannon
    entropy. the full calculations. time consuming
122 size_t numberOfcluster() const {return _cluster_count;}
123
124 void get_cluster_info(
125 std::vector<value_type> &site,
```

```
126 std::vector<value_type> &bond
127 );
128
129 char get_type() const {return type;} // get percolation type
130 virtual value_type maxIterationLimit() {return _max_iteration_limit;};
131
132 double get_relabeling_time() const {return time_relabel;}
133 value_type relabeling_count() const {return _total_relabeling;}
134 };
135
136
137 /**
138 * Site Percolation by Placing Sites
139 *
140 * version 9
141 *
142 * First it randomizes the site index list then use it.
143 * Paradigm Shift:
144 * Does not delete cluster only makes it empty so that index and id
    remains the same.
145 * This way Searching for index of the cluster using id can be omitted.
146 *
147 * Feature :
148 * 1. Can turn on and off both horizontal and boundary condition
149 *
150 * 2. Uses class Cluster_v2 for storing clusters
151 *
152 * 3. Uses Group_ID for Bonds and Sites to identify that they are in the
    same cluster
153 *
154 * 4. Occupation probability is calculated by sites,
155 *      i.e., number of active sites divided by total number of sites
156 *
157 * 5. Spanning is calculated by number of bonds in a spanning clusters
    with periodicity turned off,
158 *      i.e., number of bonds in the spanning clusters divided by total
    number of bonds
159 *
160 * 6. Unweighted relabeling is ommited in this version ??
161 *
162 * 7. Runtime is significantly improved. For example, if L=200 program
    will take ~1 min to place all sites.
163 *
164 * 8. Unnecessary methods of previous version is eliminated
```

```
*
* 9. Checking spanning by keeping track of boundary sites is implemented
*
* 10. last modified cluster id can be obtained from @var
    _last_placed_site
*
*
*/
class SitePercolation_ps_v9 : public SqLatticePercolation{
protected:
// flags to manipulate method
bool _periodicity{false};

value_type min_index; // minimum index = 0
value_type max_index; // maximum index = length - 1

// index sequence
std::vector<Index> index_sequence;  // initialized once
std::vector<value_type> randomized_index;

// every birthTime we create a cluster we assign an set_ID for them
int _cluster_id{};
value_type _index_last_modified_cluster{};  // id of the last modified
    cluster

// order parameter calculation ingradiants
// id of the cluster which has maximum number of bonds. used to
    calculate order parameter
value_type _number_of_bonds_in_the_largest_cluster{};
value_type _number_of_sites_in_the_largest_cluster{};   // might be
    useful later

Index _last_placed_site;    // keeps track of last placed site

/*************
* Spanning variables
***********/
/*Holds indices on the edges*/
std::vector<Index> _top_edge, _bottom_edge, _left_edge, _right_edge;

std::vector<Index> _spanning_sites;
std::vector<Index> _wrapping_sites;
std::vector<value_type> number_of_sites_to_span;
std::vector<value_type> number_of_bonds_to_span;
```

```
205
206 value_type _total_relabeling{};
207
208 /*************************************
209 * Private Methods
210 *************************************/
211 void relabel_sites(const std::vector<Index> &sites, int id_a, int
        delta_x_ab, int delta_y_ab);
212
213 double time_relabel{};
214 public:
215 static constexpr const char* signature = "SitePercolation_ps_v8";
216
217 ~SitePercolation_ps_v9() = default;
218 SitePercolation_ps_v9() = default;
219 SitePercolation_ps_v9(SitePercolation_ps_v9 & ) = default;
220 SitePercolation_ps_v9(SitePercolation_ps_v9 && ) = default;
221 explicit SitePercolation_ps_v9(value_type length, bool periodicity=true)
        ;
222
223 SitePercolation_ps_v9& operator=(SitePercolation_ps_v9 & ) = default;
224 //     SitePercolation_ps_v8&& operator=(SitePercolation_ps_v8 && ) =
        default;
225 double get_relabeling_time() {return time_relabel;}
226 value_type relabeling_count() const {return _total_relabeling;}
227
228 virtual void reset();
229
230
231 bool periodicity() const {return _periodicity;}
232 std::string getSignature();
233
234
235 void add_entropy_for_bond(value_type index);
236 void subtract_entropy_for_bond(const std::set<value_type> &
        found_index_set, int base=-1);
237
238 /*************************************************
239 * Site placing methods
240 *************************************************/
241 virtual bool occupy();
242 value_type placeSite_weighted(Index site); // uses weighted relabeling
        by first identifying the largest cluster
243 value_type placeSite_weighted(Index site,
```

```
244 std::vector<Index>& neighbor_sites,
245 std::vector<BondIndex>& neighbor_bonds);
246
247 Index selectSite(); // selecting site
248
249 void connection_v2(Index site, std::vector<Index> &site_neighbor, std::
    vector<BondIndex> &bond_neighbor);
250
251 // applicable to weighted relabeling
252 void relabel_sites_v5(Index root_a, const Cluster& clstr_b); // relative
     index is set accordingly
253
254 /*******************************************
255 * Information about current state of Class
256 *******************************************/
257 double numberOfOccupiedSite() const { return _number_of_occupied_sites;}
258 double occupationProbability() const { return double(
    _number_of_occupied_sites)/maxSites();}
259 double entropy(); // the shannon entropy
260
261 value_type numberOfBondsInTheLargestCluster_v2();
262 value_type numberOfSitesInTheLargestCluster();
263
264 value_type numberOfSitesInTheSpanningClusters_v2()  ;
265 value_type numberOfBondsInTheSpanningClusters_v2()  ;
266
267 value_type numberOfSitesInTheWrappingClusters()  ;
268 value_type numberOfBondsInTheWrappingClusters()  ;
269
270 /*********************************
271 * Spanning Detection
272 *********************************/
273 bool detectSpanning_v6(const Index& site);
274
275 bool check_if_id_matches(Index site, const std::vector<Index> &edge);
276
277 bool detectWrapping();
278
279 /*********************************
280 *  Tracker
281 *  Must be called each time a site is placed
282 *********************************/
283 void track_numberOfBondsInLargestCluster();
284 void track_numberOfSitesInLargestCluster();
```

```
285
286 /*******************************
287 * I/O functions
288 * Printing Status
289 *******************************/
290 Index lastPlacedSite() const { return _last_placed_site;}
291
292 void spanningIndices() const;
293 void wrappingIndices() const;
294
295 /*********************************************
296 * Visual data for plotting
297 *********************************************/
298 // lattice visual data for python
299 void writeVisualLatticeData(const std::string& filename, bool
    only_spanning=true);
300
301 protected:
302 void initialize();
303 void initialize_index_sequence();
304 void randomize_v2(); // better random number generator
305
306 int find_cluster_index_for_placing_new_bonds(const std::vector<Index> &
    neighbors, std::set<value_type> &found_indices);
307
308 value_type manage_clusters(
309 const std::set<value_type> &found_index_set,
310 std::vector<BondIndex> &hv_bonds,
311 Index &site,
312 int base_id // since id and index is same
313 );
314
315 public:
316 // on test
317 IndexRelative getRelativeIndex(Index root, Index site_new);
318 };
319
320 /*
    ***************************************************************************

321 * Site Percolation Ballistic Deposition
322 * Extended from SitePercolation_ps_v9
323 * ********************************************************/
```

```
324 class SitePercolationBallisticDeposition_v2: public
        SitePercolation_ps_v9{
325 protected:
326 // elements of @indices_tmp will be erased if needed but not of @indices
327 std::vector<value_type> indices;
328 std::vector<value_type> indices_tmp;
329 public:
330 static constexpr const char* signature = "
        SitePercolation_BallisticDeposition_v2";
331 virtual ~SitePercolationBallisticDeposition_v2(){
332 indices.clear();
333 indices_tmp.clear();
334 };
335 SitePercolationBallisticDeposition_v2(value_type length, bool
        periodicity);
336
337 virtual bool occupy();
338
339 /**********************************
340 * Site selection methods
341 */
342 Index select_site(std::vector<Index> &sites, std::vector<BondIndex> &
        bonds);
343 Index select_site_upto_1nn(std::vector<Index> &sites, std::vector<
        BondIndex> &bonds);
344 Index select_site_upto_2nn(std::vector<Index> &sites, std::vector<
        BondIndex> &bonds);
345
346 void reset();
347 void initialize_indices();
348
349 virtual std::string getSignature() {
350 std::string s = "sq_lattice_site_percolation_ballistic_deposition_";
351 if(_periodicity)
352 s += "_periodic_";
353 else
354 s += "_non_periodic_";
355 return s;
356 }
357
358
359 /**********************************
360 * occupy upto 1st nearset neighbor.
```

```
361 * If the randomly selected site is occupied then select one of the
        nearest neighor randomly
362 * If it is also occupied skip the rest setps and start next iteration
        Else occupy it
363 */
364 value_type placeSite_1nn_v2();
365 /*******************************
366 * occupy upto 2nd nearest neighbor.
367 * If the randomly selected site is occupied then select one of the
        nearest neighor randomly
368 * If it is also occupied, select the next neighbor in the direction of
        motion Else occupy it.
369 * If the 2nd nearest neighbor in the direction of motion is also
        occupied then skip the rest of the steps
370 *       and start the next iteration
371 */
372 value_type placeSite_2nn_v1();
373
374 };
375
376 /***********
377 * Only L1
378 */
379 class SitePercolationBallisticDeposition_L1_v2: public
        SitePercolationBallisticDeposition_v2{
380 public:
381 ~SitePercolationBallisticDeposition_L1_v2() = default;
382 SitePercolationBallisticDeposition_L1_v2(value_type length, bool
        periodicity)
383 :SitePercolationBallisticDeposition_v2(length, periodicity){}
384
385 bool occupy() {
386 // if no site is available then return false
387 if(_number_of_occupied_sites == maxSites()){
388 return false;
389 }
390 try {
391 value_type v = placeSite_1nn_v2();
392 _occuption_probability = occupationProbability(); // for super class
393 return v != ULLONG_MAX;
394 }catch (OccupiedNeighbor& on){
395 //        on.what();
396 return false;
397 }
```

```
398
399 }
400
401 std::string getSignature() {
402 std::string s = "sq_lattice_site_percolation_ballistic_deposition_L1";
403 if(_periodicity)
404 s += "_periodic_";
405 else
406 s += "_non_periodic_";
407 return s;
408 }
409
410 };
411
412 /*********************
413 *
414 */
415 class SitePercolationBallisticDeposition_L2_v2: public
    SitePercolationBallisticDeposition_v2{
416 public:
417 ~SitePercolationBallisticDeposition_L2_v2() = default;
418 SitePercolationBallisticDeposition_L2_v2(value_type length, bool
    periodicity)
419 :SitePercolationBallisticDeposition_v2(length, periodicity){}
420
421 bool occupy() {
422 // if no site is available then return false
423
424 if(_number_of_occupied_sites == maxSites()){
425 return false;
426 }
427
428 try {
429
430 //            value_type v = placeSite_2nn_v0();
431 value_type v = placeSite_2nn_v1();
432 _occuption_probability = occupationProbability(); // for super class
433
434 return v != ULLONG_MAX;
435 }catch (OccupiedNeighbor& on){
436 //        on.what();
437 //        cout << "line : " << __LINE__ << endl;
438 return false;
439 }
```

```
440
441 }
442
443 std::string getSignature() {
444 std::string s = "sq_lattice_site_percolation_ballistic_deposition_L2";
445 if(_periodicity)
446 s += "_periodic_";
447 else
448 s += "_non_periodic_";
449 return s;
450 }
451
452 };
453
454 #endif //SITEPERCOLATION_PERCOLATION_H
```

The **src/percolation/percolation.cpp** file

```
1  #include "percolation.h"
2
3  using namespace std;
4
5  /**
6  *
7  * @param length
8  */
9  SqLatticePercolation::SqLatticePercolation(value_type length) {
10 if (length <= 2) {
11 /*
12 * Because if _length=2
13 * there are total of 4 distinct bond. But it should have been 8, i.e, (2
       * _length * _length = 8)
14 */
15 cerr << "_length <= 2 does not satisfy _lattice properties for
      percolation : line" << __LINE__ << endl;
16 exit(1);
17 }
18 _length = length;
19 value_type _length_squared = length * length;
20 _max_number_of_bonds = 2*_length_squared;
21 _max_number_of_sites = _length_squared;
22 _clusters = vector<Cluster>();
23
24 //     size_t seed = 0;
```

```
25 //    cerr << "automatic seeding is commented : line " << __LINE__ <<
       endl;
26 auto seed = _random_device();
27 _random_generator.seed(seed); // seeding
28 cout << "seeding with " << seed << endl;
29 }
30
31
32 /**
33 *
34 */
35 void SqLatticePercolation::viewCluster() {
36 cout << "clusters with numberOfBonds greater than 1" << endl;
37 value_type total_bonds{}, total_sites{};
38
39 for (value_type i{}; i != _clusters.size(); ++i) {
40 if(_clusters[i].empty()){
41 //            cout << "Empty cluster : line " << endl;
42 continue;
43 }
44 cout << "cluster [" << i << "] : " << '{' << endl;
45 cout << _clusters[i];
46 total_bonds += _clusters[i].numberOfBonds();
47 total_sites += _clusters[i].numberOfSites();
48
49 cout << '}' << endl;
50 }
51 cout << "Total bonds " << total_bonds << endl;
52 cout << "Total sites " << total_sites << endl;
53 }
54
55
56
57 /**
58 * Extended version of view_cluster
59 */
60 void SqLatticePercolation::viewClusterExtended() {
61 cout << "clusters with numberOfBonds greater than 1" << endl;
62 value_type total_bonds{}, total_sites{};
63
64 std::vector<Index> sites;
65 std::vector<BondIndex> bonds;
66 for (value_type i{}; i != _clusters.size(); ++i) {
67 if(_clusters[i].empty()){
```

```
68 //            cout << "Empty cluster : line " << endl;
69 continue;
70 }
71 cout << "cluster [" << i << "] : ID (" << _clusters[i].get_ID() << "){"
       << endl;
72 // printing sites
73 sites = _clusters[i].getSiteIndices();
74 cout << "Sites : size (" << sites.size() << ") : ";
75 cout << '{';
76 for (auto a: sites) {
77 cout << a << ',';
78 }
79 cout << '}' << endl;
80
81 bonds = _clusters[i].getBondIndices();
82 cout << "Bonds : size (" << bonds.size() << ") : ";
83 cout << '{';
84 for (auto a: bonds) {
85 if (a.horizontal()) {
86 // horizontal bond
87 cout << _lattice.getBond({BondType::Horizontal, a.row_, a.column_}) << '
       ,';
88 } else if (a.vertical()) {
89 // vertical bond
90 cout << _lattice.getBond({BondType::Vertical, a.row_, a.column_}) << ','
       ;
91 } else {
92 cout << '!' << a << '!' << ','; // bond is not valid
93 }
94 }
95 cout << '}';
96
97 cout << endl;
98
99 total_bonds += _clusters[i].numberOfBonds();
100 total_sites += _clusters[i].numberOfSites();
101
102 cout << '}' << endl;
103 }
104 cout << "Total bonds " << total_bonds << endl;
105 cout << "Total sites " << total_sites << endl;
106 }
107
108 /**
```

```
109 *
110 * @param site
111 * @param bond
112 * @param total_site
113 * @param total_bond
114 */
115 void
116 SqLatticePercolation::get_cluster_info(
117 vector<value_type> &site,
118 vector<value_type> &bond
119 ) {
120 value_type total_site{}, total_bond{};
121 site.clear();
122 bond.clear();
123
124 unsigned long size = _clusters.size();
125 site.reserve(size);
126 bond.reserve(size);
127
128 value_type s, b;
129
130 for(value_type i{}; i < size; ++i){
131 if(_clusters[i].empty()){
132 //            cout << "Empty cluster : line " << endl;
133 continue;
134 }
135 s = _clusters[i].numberOfSites();
136 b = _clusters[i].numberOfBonds();
137 site.push_back(s);
138 bond.push_back(b);
139 total_site += s;
140 total_bond += b;
141 }
142 if(site.size() != bond.size()){
143 cout << "Size mismatched : line " << __LINE__ << endl;
144 }
145 //    cout << "total bonds " << total_bond << endl;
146 //    cout << "tatal sites " << total_site << endl;
147 if(type == 's'){
148 for(value_type j{total_bond}; j < maxBonds(); ++j){
149 bond.push_back(1); // cluster of length 1
150 total_bond += 1;
151 }
152 }
```

```
153 if(type == 'b'){
154 for(value_type j{total_site}; j < maxSites(); ++j){
155 total_site += 1;
156 site.push_back(1); // cluster of length 1
157 }
158 }
159 }
160
161 void SqLatticePercolation::reset() {
162 _lattice.reset();
163 _clusters.clear();
164 _index_sequence_position = 0;
165
166 _occuption_probability = 0;
167 // entropy
168 _entropy=0;
169 _entropy_current=0;
170 _total_relabeling = 0;
171 time_relabel = 0;
172 _cluster_count = 0;
173 _reached_critical = false;
174 }
175
176
177 /**
178 * Entropy calculation is performed here. The fastest method possible.
179 * Cluster size is measured by site.
180 * @return current entropy of the lattice
181 */
182 double SqLatticePercolation::entropy_by_site() {
183 double H{}, mu ;
184
185 for(size_t i{}; i < _clusters.size(); ++i){
186 if(!_clusters[i].empty()){
187 mu = _clusters[i].numberOfSites() / double(_number_of_occupied_sites);
188 H += mu*log(mu);
189 }
190 }
191
192 return -H;
193 }
194
195 /**
196 * Entropy calculation is performed here. The fastest method possible.
```

```
197 * Cluster size is measured by site.
198 * @return current entropy of the lattice
199 */
200 double SqLatticePercolation::entropy_by_bond() {
201 double H{}, mu ;
202
203 for(size_t i{}; i < _clusters.size(); ++i){
204 if(!_clusters[i].empty()){
205 mu = _clusters[i].numberOfBonds() / double(maxBonds());
206 H += mu*log(mu);
207 }
208 }
209
210 double number_of_cluster_with_size_one = maxBonds() -
    _bonds_in_cluster_with_size_two_or_more;
211 //     cout << " _bonds_in_cluster_with_size_two_or_more " <<
    _bonds_in_cluster_with_size_two_or_more << " : line " << __LINE__ <<
    endl;
212 mu = 1.0/double(maxBonds());
213 H += number_of_cluster_with_size_one * log(mu) * mu;
214
215 return -H;
216 }
```

The **src/percolation/percolation_site_v9.cpp** file

```
1 #include <cstdlib>
2 #include <climits>
3 #include <unordered_set>
4 #include <mutex>
5
6 #include "percolation.h"
7
8 #include "../util/printer.h"
9 #include <omp.h>
10 #include <thread>
11 #include <algorithm>
12
13 #include "../util/time_tracking.h"
14
15 using namespace std;
16
17
18
19 /**
```

```
20 *
21 * @param length        : length of the lattice
22 * @param impure_sites : number of impure sites. cannot be greater than
       length*length
23 */
24 SitePercolation_ps_v9::SitePercolation_ps_v9(value_type length, bool
       periodicity)
25 :SqLatticePercolation(length)
26 {
27 std::cout << "Constructing SitePercolation_ps_v9 object : line " <<
       __LINE__ << endl;
28 SqLatticePercolation::set_type('s');
29
30 _periodicity = periodicity;
31 _index_sequence_position = 0;
32 _lattice = SqLattice(length, true, false, false, true);   // since it is
       a site percolation all bonds will be activated by default
33
34 min_index = 0;
35 max_index = length - 1;
36
37 index_sequence.resize(maxSites());
38 randomized_index.resize(maxSites());
39 _max_iteration_limit = maxSites();
40
41 initialize_index_sequence();
42 initialize();
43 randomize_v2();  // randomize the untouched_site_indices
44 }
45
46
47 /**
48 *
49 */
50 void SitePercolation_ps_v9::initialize() {
51
52 // to improve performence
53 number_of_sites_to_span.reserve(maxSites());
54 number_of_bonds_to_span.reserve(maxSites());
55
56 _top_edge.reserve(length());
57 _bottom_edge.reserve(length());
58 _left_edge.reserve(length());
59 _right_edge.reserve(length());
```

```
60
61 //     randomized_index_sequence = index_sequence;
62 }
63
64
65 /**
66 * Called only once when the object is constructed for the first time
67 */
68 void SitePercolation_ps_v9::initialize_index_sequence() {
69 value_type m{}, n{};
70 for (value_type i{}; i != index_sequence.size(); ++i) {
71 randomized_index[i] = i;
72 index_sequence[i] = Index(m, n);
73 ++n;
74 if (n == length()) {
75 n = 0;
76 ++m;
77 }
78 }
79 //for (value_type i{}; i != index_sequence.size(); ++i) {cout <<
    index_sequence[i] << endl;}
80 }
81
82
83 /**
84 * Reset all calculated values and then call initiate()
85 * to initiallize for reuse
86 *
87 * caution -> it does not erase _calculation_flags, for it will be used
    for calculation purposes
88 */
89 void SitePercolation_ps_v9::reset() {
90 SqLatticePercolation::reset();
91 // variables
92 _number_of_occupied_sites = 0;
93 _index_sequence_position = 0;
94 _cluster_id = 0;
95
96 // containers
97 number_of_sites_to_span.clear();
98 number_of_bonds_to_span.clear();
99 _spanning_sites.clear();
100 _wrapping_sites.clear();
101 _bonds_in_cluster_with_size_two_or_more = 0;
```

```
102 _index_last_modified_cluster = 0;  // id of the last modified cluster
103 _number_of_bonds_in_the_largest_cluster = 0;
104 _number_of_sites_in_the_largest_cluster = 0;
105 // clearing edges
106 _top_edge.clear();
107 _bottom_edge.clear();
108 _left_edge.clear();
109 _right_edge.clear();
110 initialize();
111 randomize_v2();
112 time_relabel = 0;
113 _total_relabeling = 0;
114 }
115
116
117 /**
118 * Randomize the indices
119 */
120 void SitePercolation_ps_v9::randomize_v2(){
121
122 std::shuffle(randomized_index.begin(), randomized_index.end(),
        _random_generator);
123 //     cout << "Index sequence : " << randomized_index_sequence << endl;
124 }
125
126
127 /*************************************************
128 * Calculation methods
129 *
130 **********************************/
131
132 /*
133 * Instead of calculating entropy for 1000s of cluster in every iteration
134 * just keep track of entropy change, i.e.,
135 * how much to subtract and how much to add.
136 */
137 /**
138 * Must be called before merging the clusters
139 * @param found_index_set
140 */
141 void SitePercolation_ps_v9::subtract_entropy_for_bond(const set<
        value_type> &found_index, int base){
142 double nob, mu_bond, H{};
143 if(base >= 0){
```

```
144 nob = _clusters[base].numberOfBonds();
145 mu_bond = nob / maxBonds();
146 H += log(mu_bond) * mu_bond;
147 }
148 for(auto x : found_index){
149 nob = _clusters[x].numberOfBonds();
150 mu_bond = nob / maxBonds();
151 H += log(mu_bond) * mu_bond;
152 }
153 _entropy -= -H;
154 }
155
156
157
158 /**
159 * Must be called after merging the clusters
160 * Cluster length is measured by bonds
161 * @param index
162 */
163 void SitePercolation_ps_v9::add_entropy_for_bond(value_type index){
164 double nob = _clusters[index].numberOfBonds();
165 double mu_bond = nob / maxBonds();
166 double H = log(mu_bond) * mu_bond;
167 _entropy += -H;
168 }
169
170
171
172 /**
173 * Condition: must be called each time a site is placed
174 */
175 void SitePercolation_ps_v9::track_numberOfBondsInLargestCluster() {
176
177 // calculating number of bonds in the largest cluster // by cluster
    index
178 // checking number of bonds
179 if(_clusters[_index_last_modified_cluster].numberOfBonds() >
    _number_of_bonds_in_the_largest_cluster){
180 _number_of_bonds_in_the_largest_cluster = _clusters[
    _index_last_modified_cluster].numberOfBonds();
181 }
182
183 }
184
```

```
185 /**
186 *
187 */
188 void SitePercolation_ps_v9::track_numberOfSitesInLargestCluster(){
189
190 // calculating number of bonds in the largest cluster // by cluster
    index
191 // checking number of bonds
192 if(_clusters[_index_last_modified_cluster].numberOfSites() >
    _number_of_sites_in_the_largest_cluster){
193 _number_of_sites_in_the_largest_cluster = _clusters[
    _index_last_modified_cluster].numberOfSites();
194 }
195 }
196
197
198 /**
199 *
200 * @param neighbors          :
201 * @param found_index_set    : index of the clusters that will be merged
    together.
202 *                             Does not contain the base cluster index or
    id.
203 * @return                   : id of the base cluster
204 */
205 int
206 SitePercolation_ps_v9::find_cluster_index_for_placing_new_bonds(
207 const vector<Index> &neighbors, std::set<value_type> &found_index_set
208 ){
209 found_index_set.clear();
210 value_type size{}, tmp{}, index, base{ULONG_MAX};
211 int base_id{-1};
212 int id;
213 for (auto n: neighbors) {
214 id = _lattice.getGroupID(n);
215 if(id >=0) {
216 index = value_type(id);
217 tmp = _clusters[index].numberOfSites();
218 if(tmp > size){
219 size = tmp;
220 base_id = id;
221 base = index;
222 }
223
```

```
224 found_index_set.insert(index);
225
226 }
227 }
228 found_index_set.erase(base);
229 return base_id;
230 }
231
232
233 /**
234 * Last placed site is added to a cluster. If this connects other
    clusters then merge all
235 * cluster together to get one big cluster. All sites that are part of
    the other clusters
236 * are relabled according to the id of the base cluster.
237 * @param found_index_set : index of the clusters that are neighbors of
    the last placed site
238 * @param hv_bonds        : bonds that connects the last placed site and
    its neighbors
239 *                          and which are not part of any cluster of size
     larger than one
240 * @param site            : last placed site
241 * @param base_id         : id of the base cluster
242 * @return
243 */
244 value_type SitePercolation_ps_v9::manage_clusters(
245 const set<value_type> &found_index_set,
246 vector<BondIndex> &hv_bonds,
247 Index &site,
248 int base_id
249 )
250 {
251
252
253 if (base_id != -1) {
254 value_type base = value_type(base_id); // converting here
255 _clusters[base].addSiteIndex(site);
256 int id_base = _clusters[base].get_ID();
257 vector<Index> neibhgors = _lattice.get_neighbor_site_indices(site);
258 // find which of the neighbors are of id_base as the base cluster
259 IndexRelative r;
260 for(auto n: neibhgors){
261 if(_lattice.getGroupID(n) == id_base){
262 // find relative index with respect to this site
```

```
263 r = getRelativeIndex(n, site);
264 break; // since first time r is set running loop is doing no good
265 }
266 }
267
268 // put_values_to_the_cluster new values in the 0-th found index
269 _clusters[base].insert(hv_bonds);
270 _lattice.getSite(site).relativeIndex(r);
271 _lattice.setGroupID(site, id_base); // relabeling for 1 site
272
273 // merge clusters with common values from all other cluster        //
    merge clusters with common values from all other cluster
274
275
276 for(value_type ers: found_index_set){
277
278 _total_relabeling += _clusters[ers].numberOfSites(); // only for
    debugging purposes
279 // perform relabeling on the sites
280 relabel_sites_v5(site, _clusters[ers]);
281
282 // store values of other found indices to the cluster
283 _clusters[base].insert_v2(_clusters[ers]);
284 _cluster_count--; // reducing number of clusters
285 _clusters[ers].clear(); // emptying the cluster
286
287 }
288 _index_last_modified_cluster = base;
289
290
291 } else {
292 // create new element for the cluster
293 _clusters.push_back(Cluster(_cluster_id));
294 value_type _this_cluster_index = _clusters.size() -1;
295 _lattice.setGroupID(site, _cluster_id); // relabeling for 1 site
296 _cluster_count++; // increasing number of clusters
297 _cluster_id++;
298 _clusters.back().insert(hv_bonds);
299 _clusters[_this_cluster_index].addSiteIndex(site);
300 _index_last_modified_cluster = _this_cluster_index;   // last cluster is
    the place where new bonds are placed
301
302 }
303 return _index_last_modified_cluster;
```

```
304 }
305
306
307
308
309
310 /**
311 * Relative index of site_new with respect to root
312 * @param root
313 * @param site_new
314 * @return
315 */
316 IndexRelative SitePercolation_ps_v9::getRelativeIndex(Index root, Index
    site_new){
317 //     cout << "Entry \"SitePercolation_ps_v9::getRelativeIndex\" : line
    " << __LINE__ << endl;
318 int delta_x = -int(root.column_) + int(site_new.column_); // if +1 then
    root is on the right ??
319 int delta_y = int(root.row_) - int(site_new.row_); // if +1 then root is
     on the top ??
320
321
322 // normalizing delta_x
323 if(delta_x > 1){
324 delta_x /= -delta_x;
325 }
326 else if(delta_x < -1){
327 delta_x /= delta_x;
328 }
329
330 // normalizing delta_y
331 if(delta_y > 1){
332 delta_y /= -delta_y;
333 }else if(delta_y < -1){
334 delta_y /= delta_y;
335 }
336
337 IndexRelative indexRelative_root = _lattice.getSite(root).relativeIndex
    ();
338 //     cout << "Relative index of root " << indexRelative_root << endl;
339 //     cout << "Delta x,y " << delta_x << ", " << delta_y << endl;
340 IndexRelative r =  {indexRelative_root.x_ + delta_x, indexRelative_root.
    y_ + delta_y};
341 //     cout << "Relative index of site_new " << r << endl;
```

```
342 return r;
343 }
344
345
346
347 /**
348 * Take a bond index only if the corresponding site is active
349 * takes longer? time than version 1?, i.e., connection()
350 * @param site
351 * @param site_neighbor
352 * @param bond_neighbor
353 */
354 void SitePercolation_ps_v9::connection_v2(Index site, vector<Index> &
        site_neighbor, vector<BondIndex> &bond_neighbor)
355 {
356
357 value_type prev_column  = (site.column_ + length() - 1) % length();
358 value_type prev_row     = (site.row_ + length() - 1) % length();
359 value_type next_row     = (site.row_ + 1) % length();
360 value_type next_column  = (site.column_ + 1) % length();
361
362 if(!_periodicity){
363 // without periodicity
364 if (site.row_ == min_index) { // top edge including corners
365 if(site.column_ == min_index){
366 // upper left corner
367
368 site_neighbor.resize(2);
369 site_neighbor[0] = {site.row_, next_column};
370 site_neighbor[1] = {next_row, site.column_};
371
372 bond_neighbor.reserve(2);
373 if(!_lattice.getSite(site_neighbor[0]).isActive()){
374 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
        ;
375 }
376 if(!_lattice.getSite(site_neighbor[1]).isActive()){
377 bond_neighbor.push_back({BondType::Vertical, site.row_, site.column_});
378 }
379
380 return;
381
382 }
383 else if(site.column_ == max_index){
```

```
384 // upper right corner
385
386 site_neighbor.resize(2);
387 site_neighbor[0] = {site.row_, prev_column};
388 site_neighbor[1] = {next_row, site.column_};
389
390 bond_neighbor.reserve(2);
391 if(!_lattice.getSite(site_neighbor[0]).isActive()){
392 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
393 }
394 if(!_lattice.getSite(site_neighbor[1]).isActive()){
395 bond_neighbor.push_back({BondType::Vertical, site.row_, site.column_});
396 }
397
398 return;
399 }
400 else{
401 // top edge excluding corners
402 site_neighbor.resize(3);
403 site_neighbor[0] = {site.row_, next_column};
404 site_neighbor[1] = {site.row_, prev_column};
405 site_neighbor[2] = {next_row, site.column_};
406
407 bond_neighbor.reserve(4);
408 if(!_lattice.getSite(site_neighbor[0]).isActive()) {
409 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
    ;
410 }
411 if(!_lattice.getSite(site_neighbor[1]).isActive()){
412 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
413 }
414 if(!_lattice.getSite(site_neighbor[2]).isActive()){
415 bond_neighbor.push_back({BondType::Vertical,    site.row_, site.column_
    });
416 }
417
418 return;
419
420 }
421 }
422 else if (site.row_ == max_index) { // bottom edge including corners
423 if (site.column_ == min_index) {
424 // lower left corner
425 site_neighbor.resize(2);
```

```
426 site_neighbor[0] = {site.row_, next_column};
427 site_neighbor[1] = {prev_row, site.column_};
428
429 bond_neighbor.reserve(2);
430 if(!_lattice.getSite(site_neighbor[0]).isActive()){
431 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
        ;
432 }
433 if(!_lattice.getSite(site_neighbor[1]).isActive()){
434 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
435 }
436
437
438 return;
439
440 } else if (site.column_ == max_index) {
441 // lower right corner
442 site_neighbor.resize(2);
443 site_neighbor[0] = {site.row_, prev_column};
444 site_neighbor[1] = {prev_row, site.column_};
445
446 bond_neighbor.reserve(2);
447 if(!_lattice.getSite(site_neighbor[0]).isActive()){
448 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
449 }
450 if(!_lattice.getSite(site_neighbor[1]).isActive()){
451 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
452 }
453
454 return;
455
456 } else {
457 // bottom edge excluding corners
458 //  bottom edge
459 site_neighbor.resize(3);
460 site_neighbor[0] = {site.row_, next_column};
461 site_neighbor[1] = {site.row_, prev_column};
462 site_neighbor[2] = {prev_row, site.column_};
463
464 bond_neighbor.reserve(3);
465 if(!_lattice.getSite(site_neighbor[0]).isActive()) {
466 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
        ;
467 }
```

```
468 if(!_lattice.getSite(site_neighbor[1]).isActive()){
469 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
470 }
471 if(!_lattice.getSite(site_neighbor[2]).isActive()){
472 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
473 }
474
475 return;
476 }
477 }
478 /* site.x_ > min_index && site.x_ < max_index &&  is not possible
    anymore*/
479 else if (site.column_ == min_index) { // left edge not in the corners
480 site_neighbor.resize(3);
481 site_neighbor[0] = {site.row_, next_column};
482 site_neighbor[1] = {next_row, site.column_};
483 site_neighbor[2] = {prev_row, site.column_};
484
485 bond_neighbor.reserve(3);
486 if(!_lattice.getSite(site_neighbor[0]).isActive()) {
487 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
    ;
488 }
489 if(!_lattice.getSite(site_neighbor[1]).isActive()){
490 bond_neighbor.push_back({BondType::Vertical,     site.row_, site.column_
    });
491 }
492 if(!_lattice.getSite(site_neighbor[2]).isActive()){
493 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
494 }
495
496 return;
497 }
498 else if (site.column_ == max_index) {
499 // right edge no corners
500
501 site_neighbor.resize(3);
502 site_neighbor[0] = {site.row_, prev_column};
503 site_neighbor[1] = {next_row, site.column_};
504 site_neighbor[2] = {prev_row, site.column_};
505
506 bond_neighbor.reserve(3);
507 if(!_lattice.getSite(site_neighbor[0]).isActive()){
508 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
```

```
509 }
510 if(!_lattice.getSite(site_neighbor[1]).isActive()){
511 bond_neighbor.push_back({BondType::Vertical,     site.row_, site.column_
        });
512 }
513 if(!_lattice.getSite(site_neighbor[2]).isActive()){
514 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
515 }
516
517 return;
518 }
519
520 }
521 // 1 level inside the lattice
522 // not in any the boundary
523 site_neighbor.resize(4);
524 site_neighbor[0] = {site.row_, next_column};
525 site_neighbor[1] = {site.row_, prev_column};
526 site_neighbor[2] = {next_row, site.column_};
527 site_neighbor[3] = {prev_row, site.column_};
528
529 bond_neighbor.reserve(4);
530 if(!_lattice.getSite(site_neighbor[0]).isActive()) {
531 bond_neighbor.push_back({BondType::Horizontal, site.row_, site.column_})
        ;
532 }
533 if(!_lattice.getSite(site_neighbor[1]).isActive()){
534 bond_neighbor.push_back({BondType::Horizontal, site.row_, prev_column});
535 }
536 if(!_lattice.getSite(site_neighbor[2]).isActive()){
537 bond_neighbor.push_back({BondType::Vertical,     site.row_, site.column_
        });
538 }
539 if(!_lattice.getSite(site_neighbor[3]).isActive()) {
540 bond_neighbor.push_back({BondType::Vertical, prev_row, site.column_});
541 }
542
543 }
544
545
546
547 /**
548 *
549 * @param site
```

```
550 * @param edge
551 * @return
552 */
553 bool SitePercolation_ps_v9::check_if_id_matches(Index site, const vector
        <Index> &edge){
554 for(auto s :edge){
555 if(_lattice.getGroupID(site) == _lattice.getGroupID(s)){
556 // no need to put the site here
557 return true;
558 }
559 }
560 return false;
561 }
562
563
564
565 /*******************************************
566 *  Placing sites
567 *
568 *******************************************/
569
570 /**
571 * All site placing method in one place
572 *
573 * @return true if operation is successfull
574 */
575 bool SitePercolation_ps_v9::occupy() {
576 if(_index_sequence_position >= maxSites()){
577 return false;
578 }
579 Index site = selectSite();
580 placeSite_weighted(site);
581 _occuption_probability = occupationProbability(); // for super class
582 return true;
583 }
584
585 /***
586 * Index of the selected site must be provided with the argument
587 *
588 * Wrapping and spanning index arrangement is enabled.
589 * Entropy is calculated smoothly.
590 * Entropy is measured by site and bond both.
591 * @param current_site
592 * @return
```

```
593 */
594 value_type SitePercolation_ps_v9::placeSite_weighted(Index current_site)
        {
595 // randomly choose a site
596 if (_number_of_occupied_sites == maxSites()) {
597 return ULONG_MAX; // unsigned long int maximum value
598 }
599
600 _last_placed_site = current_site;
601 _lattice.activate_site(current_site);
602 ++_number_of_occupied_sites;
603 // find the bonds for this site
604 vector<BondIndex> bonds;
605 vector<Index>     sites;
606 connection_v2(current_site, sites, bonds);
607 _bonds_in_cluster_with_size_two_or_more += bonds.size();
608
609 // find one of hv_bonds in _clusters and add ever other value to that
       place. then erase other position
610 set<value_type> found_index_set;
611 int  base_id = find_cluster_index_for_placing_new_bonds(sites,
       found_index_set);
612
613 subtract_entropy_for_bond(found_index_set, base_id);  // tracking
       entropy change
614 value_type merged_cluster_index = manage_clusters(
615 found_index_set, bonds, current_site, base_id
616 );
617 add_entropy_for_bond(merged_cluster_index); // tracking entropy change
618 // running tracker
619 track_numberOfBondsInLargestCluster(); // tracking number of bonds in
       the largest cluster
620 track_numberOfSitesInLargestCluster();
621 return merged_cluster_index;
622 }
623
624 /***
625 * Index of the selected site must be provided with the argument
626 *
627 * Wrapping and spanning index arrangement is enabled.
628 * Entropy is calculated smoothly.
629 * Entropy is measured by site and bond both.
630 * @param current_site
631 * @return
```

```
632 */
633 value_type SitePercolation_ps_v9::placeSite_weighted(
634 Index current_site,
635 vector<Index>& neighbor_sites,
636 vector<BondIndex>& neighbor_bonds
637 ) {
638 // randomly choose a site
639 if (_number_of_occupied_sites == maxSites()) {
640 return ULONG_MAX; // unsigned long int maximum value
641 }
642 _bonds_in_cluster_with_size_two_or_more += neighbor_bonds.size();
643 _last_placed_site = current_site;
644 _lattice.activate_site(current_site);
645 ++_number_of_occupied_sites;
646 // find one of hv_bonds in _clusters and add ever other value to that
    place. then erase other position
647 set<value_type> found_index_set;
648 int  base_id = find_cluster_index_for_placing_new_bonds(neighbor_sites,
    found_index_set);
649 subtract_entropy_for_bond(found_index_set, base_id);  // tracking
    entropy change
650 value_type merged_cluster_index = manage_clusters(
651 found_index_set, neighbor_bonds, current_site, base_id
652 );
653 add_entropy_for_bond(merged_cluster_index); // tracking entropy change
654 // running tracker
655 track_numberOfBondsInLargestCluster(); // tracking number of bonds in
    the largest cluster
656 track_numberOfSitesInLargestCluster();
657 return merged_cluster_index;
658 }
659
660
661
662 /**
663 *
664 * @return
665 */
666 Index SitePercolation_ps_v9::selectSite(){
667 //    Index current_site = randomized_index_sequence[
    _index_sequence_position]; // old
668 value_type index = randomized_index[_index_sequence_position];
669 Index current_site = index_sequence[index]; // new process
670 ++_index_sequence_position;
```

```
671 return current_site;
672 }
673
674
675 /*************************************************
676 * View methods
677 ************************************/
678
679
680 /**
681 *
682 */
683 void SitePercolation_ps_v9::spanningIndices() const {
684 cout << "Spanning Index : id" << endl;
685 for(Index i: _spanning_sites){
686 cout << "Index " << i << " : id " << _lattice.getGroupID(i) << endl;
687 }
688 }
689
690 void SitePercolation_ps_v9::wrappingIndices() const {
691 cout << "Wrapping Index : id : relative index" << endl;
692 for(auto i: _wrapping_sites){
693 cout << "Index " << i << " : id "
694 << _lattice.getGroupID(i)
695 << " relative index : " << _lattice.getSite(i).relativeIndex() << endl;
696 }
697 }
698
699
700 /*************************************
701 * Spanning Detection
702 ************************************/
703
704
705 /**
706 * success : gives correct result
707 * length        time
708 * 200           7.859000 sec
709 * 500           2 min 18.874000 sec
710 * only check for the cluster id of the recently placed site
711 * @param site : Check spanning for this argument
712 * @return
713 */
714 bool SitePercolation_ps_v9::detectSpanning_v6(const Index& site) {
```

```
715 //    cout << "Entry -> detectSpanning_v4() : line " << __LINE__ << endl
    ;
716 if(_periodicity) {
717 cout << "Cannot detect spanning if _periodicity if ON: line " <<
    __LINE__ << endl;
718 return false;
719 }
720 if(_reached_critical ){
721 return true;  // we have already reached critical point
722 }
723
724 // first check if the site with a cluster id is already a spanning site
725 for(const Index& ss: _spanning_sites){
726 if(_lattice.getSite(ss).get_groupID() == _lattice.getSite(site).
    get_groupID()){
727 //            cout << "Already a spanning site : line " << __LINE__ <<
    endl;
728 return true;
729 }
730 }
731
732 // only check for the newest site placed
733 if(site.row_ == min_index){ // top index
734 if(!check_if_id_matches(site, _top_edge)) {
735 _top_edge.push_back(site);
736 }
737 }
738 else if(site.row_ == max_index){
739 if(!check_if_id_matches(site, _bottom_edge)){
740 _bottom_edge.push_back(site);
741 }
742 }
743
744 // checking column indices for Left-Right boundary
745 if(site.column_ == min_index){ // left edge
746 if(!check_if_id_matches(site, _left_edge)) {
747 _left_edge.push_back(site);
748 }
749 }
750 else if(site.column_ == max_index){
751 if(!check_if_id_matches(site, _right_edge)) {
752 _right_edge.push_back(site);
753 }
754 }
```

```
755
756 if(_number_of_occupied_sites < length()){
757 //        cout << "Not enough site to span : line " << __LINE__ << endl;
758 return false;
759 }
760
761
762 vector<Index>::iterator it_top = _top_edge.begin();
763 vector<Index>::iterator it_bot = _bottom_edge.begin();
764 bool found_spanning_site = false;
765 int id = _lattice.getGroupID(site);
766
767 if(_top_edge.size() < _bottom_edge.size()){
768 // if matched found on the smaller edge look for match in the larger
    edge
769 for(; it_top < _top_edge.end(); ++it_top){
770 if(id == _lattice.getGroupID(*it_top)){
771 for(; it_bot < _bottom_edge.end(); ++it_bot){
772 if(id == _lattice.getGroupID(*it_bot)){
773 // match found !
774 if(!check_if_id_matches(*it_top ,_spanning_sites)) {
775 _reached_critical = true;
776 _spanning_sites.push_back(*it_top);
777 }
778 found_spanning_site = true;
779 _bottom_edge.erase(it_bot);
780 }
781 }
782
783 if(found_spanning_site){
784 found_spanning_site = false;
785 _top_edge.erase(it_top);
786 }
787
788 }
789 }
790 }else{
791 for (; it_bot < _bottom_edge.end(); ++it_bot) {
792 if (id == _lattice.getGroupID(*it_bot)) {
793 for (; it_top < _top_edge.end(); ++it_top) {
794 if (id == _lattice.getGroupID(*it_top)) {
795 // match found !
796 if (!check_if_id_matches(*it_top, _spanning_sites)) {
797 _reached_critical = true;
```

```
798 _spanning_sites.push_back(*it_top);
799 }
800 found_spanning_site = true;
801 _top_edge.erase(it_top);
802 }
803 }
804 if(found_spanning_site){
805 found_spanning_site = false;
806 _bottom_edge.erase(it_top);
807 }
808 }
809 }
810
811 }
812
813 found_spanning_site = false;
814 vector<Index>::iterator it_lft = _left_edge.begin();
815 vector<Index>::iterator it_rht = _right_edge.begin();
816
817 if(_left_edge.size() < _right_edge.size()){
818 for(; it_lft < _left_edge.end(); ++it_lft) {
819 if (id == _lattice.getGroupID(*it_lft)) {
820 for (; it_rht < _right_edge.end(); ++it_rht) {
821 if (id == _lattice.getGroupID(*it_rht)) {
822 if (!check_if_id_matches(*it_lft, _spanning_sites)) {
823 _spanning_sites.push_back(*it_lft);
824 _reached_critical = true;
825 }
826 found_spanning_site = true;
827 _right_edge.erase(it_rht);
828 }
829 }
830 if (found_spanning_site) {
831 found_spanning_site = false;
832 _left_edge.erase(it_lft);
833 }
834 }
835 }
836 }else{
837 for (; it_rht < _right_edge.end(); ++it_rht) {
838 if (id == _lattice.getGroupID(*it_rht)) {
839 for(; it_lft < _left_edge.end(); ++it_lft) {
840 if (id == _lattice.getGroupID(*it_lft)) {
841 if (!check_if_id_matches(*it_lft, _spanning_sites)) {
```

```
842 _spanning_sites.push_back(*it_lft);
843 _reached_critical = true;
844 }
845 found_spanning_site = true;
846 _left_edge.erase(it_lft);
847 }
848 }
849 if (found_spanning_site) {
850 found_spanning_site = false;
851 _right_edge.erase(it_rht);
852 }
853 }
854 }
855 }
856
857
858 // now do the matching with left and right for horizontal spanning
859 // meaning new site is added to _spanning_sites so remove them from top
    and bottom edges
860
861
862
863 // filter spanning ids
864
865
866 return !_spanning_sites.empty();
867
868 }
869
870
871
872 /**********************************
873 * Wrapping Detection
874 **********************************/
875 /**
876 * Wrapping is detected here using the last placed site
877 * @return bool. True if wrapping occured.
878 */
879 bool SitePercolation_ps_v9::detectWrapping() {
880 Index site = lastPlacedSite();
881 // only possible if the cluster containing 'site' has sites >= length of
    the lattice
882 if(_number_of_occupied_sites < length()){
883 return false;
```

```
884 }
885
886 if(_reached_critical){
887 return true; // reached critical in previous step
888 }
889 // check if it is already a wrapping site
890 int id = _lattice.getGroupID(site);
891 int tmp_id{};
892 for (auto i: _wrapping_sites){
893 tmp_id = _lattice.getGroupID(i);
894 if(id == tmp_id ){
895 return true;
896 }
897 }
898
899 // get four neighbors of site always. since wrapping is valid if
    periodicity is implied
900 vector<Index> sites = _lattice.get_neighbor_site_indices(site);
901
902 if(sites.size() < 2){ // at least two neighbor of  site is required
903 return false;
904 }else{
905 IndexRelative irel = _lattice.getSite(site).relativeIndex();
906 //        cout << "pivot's " << site << " relative " << irel << endl;
907 IndexRelative b;
908 for (auto a:sites){
909 if(_lattice.getGroupID(a) != _lattice.getGroupID(site)){
910 // different cluster
911 continue;
912 }
913 // belongs to the same cluster
914 b = _lattice.getSite(a).relativeIndex();
915 //            cout << "neibhbor " << a << " relative " << b << endl;
916 if(abs(irel.x_ - b.x_) > 1 || abs(irel.y_ - b.y_) > 1){
917 //                cout << "Wrapping : line " << __LINE__ << endl;
918 _wrapping_sites.push_back(site);
919 _reached_critical = true;
920 return true;
921 }
922 }
923 }
924 // if %_wrapping_indices is not empty but wrapping is not detected for
    the current site (%site)
925 // that means there is wrapping but not for the %site
```

```
926 return !_wrapping_sites.empty();
927 }
928
929 /*****************************************************************
930 * Relabeling
931 *
932 *****************************************************************/
933 /**
934 * Relabels site and also reassign relative index to the relabeled sites
935 *
936 * @param site_a  : last added site index of the base cluster
937 * @param clstr_b : 2nd cluster, which to be merged withe the root
938 */
939 void SitePercolation_ps_v9::relabel_sites_v5(Index site_a, const Cluster
    & clstr_b) {
940 const vector<Index> sites = clstr_b.getSiteIndices();
941 int id_a = _lattice.getGroupID(site_a);
942 int id_b = clstr_b.get_ID();
943 Index b = clstr_b.getRootSite();
944
945 // get four site_b of site_a
946 vector<Index> sites_neighbor_a = _lattice.get_neighbor_site_indices(
    site_a);
947 Index site_b;
948 IndexRelative relative_index_b_after;
949 bool flag{false};
950 // find which site_b has id_a of clstr_b
951 for(auto n: sites_neighbor_a){
952 if(id_b == _lattice.getGroupID(n)){
953 // checking id_a equality is enough. since id_a is the id_a of the
    active site already.
954 relative_index_b_after = getRelativeIndex(site_a, n);
955 site_b = n;
956 flag = true;
957 break;
958 }
959 }
960 if(!flag){
961 cout << "No neibhgor found! : line " << __LINE__ << endl;
962 }
963
964 IndexRelative relative_site_a = _lattice.getSite(site_a).relativeIndex()
    ;
```

```
965 // with this delta_a and delta_y find the relative index of site_b while
        relative index of site_a is known
966 IndexRelative relative_site_b_before = _lattice.getSite(site_b).
        relativeIndex();
967 int delta_x_ab = relative_index_b_after.x_ - relative_site_b_before.x_;
968 int delta_y_ab = relative_index_b_after.y_ - relative_site_b_before.y_;
969 relabel_sites(sites, id_a, delta_x_ab, delta_y_ab);
970 }
971
972
973
974 void SitePercolation_ps_v9::relabel_sites(const vector<Index> &sites,
        int id_a, int delta_x_ab, int delta_y_ab) {
975 int x, y;
976 Index a;
977 IndexRelative relative_site__a;
978 for (value_type i = 0; i < sites.size(); ++i) {
979 a = sites[i];
980 _lattice.setGroupID(a, id_a);
981 relative_site__a = _lattice.getSite(a).relativeIndex();
982 x = relative_site__a.x_ + delta_x_ab;
983 y = relative_site__a.y_ + delta_y_ab;
984 _lattice.getSite(a).relativeIndex(x, y);
985 }
986 }
987
988
989
990 /*******************************************
991 * Information about current state of Class
992 *******************************************/
993
994 /**
995 * Entropy calculation is performed here. The fastest method possible.
996 * Cluster size is measured by bond.
997 * @return current entropy of the lattice
998 */
999 double SitePercolation_ps_v9::entropy() {
1000 double H{};
1001 double number_of_cluster_with_size_one = maxBonds() -
        _bonds_in_cluster_with_size_two_or_more;
1002 //    cout << " _bonds_in_cluster_with_size_two_or_more " <<
        _bonds_in_cluster_with_size_two_or_more << " : line " << __LINE__ <<
        endl;
```

```
1003 double mu = 1.0/double(maxBonds());
1004 H += number_of_cluster_with_size_one * log(mu) * mu;
1005 H *= -1;
1006 _entropy_current =  _entropy + H;
1007 return _entropy_current;
1008 }
1009
1010
1011
1012 /**
1013 * Only applicable if the number of bonds in the largest cluster is
       calculated when occupying the lattice.
1014 * Significantly efficient than the previous version
       numberOfBondsInTheLargestCluster()
1015 * @return
1016 */
1017 value_type SitePercolation_ps_v9::numberOfBondsInTheLargestCluster_v2()
       {
1018 //     return _clusters[_index_largest_cluster].numberOfBonds();
1019 return _number_of_bonds_in_the_largest_cluster;
1020 }
1021
1022
1023
1024 /**
1025 *
1026 * @return
1027 */
1028 value_type SitePercolation_ps_v9::numberOfSitesInTheLargestCluster() {
1029 value_type  len{}, nob{};
1030 for(auto c: _clusters){
1031 nob = c.numberOfSites();
1032 if (len < nob){
1033 len = nob;
1034 }
1035 }
1036 _number_of_sites_in_the_largest_cluster = len;
1037 return len;
1038 }
1039
1040
1041 /*********************************
1042 * Spanning methods
1043 *********************************/
```

```
1044
1045 /**
1046 *
1047 * @return
1048 */
1049 value_type SitePercolation_ps_v9::numberOfSitesInTheSpanningClusters_v2
     () {
1050
1051 if(! _spanning_sites.empty()){
1052 int id = _lattice.getGroupID(_spanning_sites.front());
1053 if(id >= 0) {
1054 return _clusters[id].numberOfSites();
1055 }
1056 }
1057 return 0;
1058 }
1059
1060
1061 /**
1062 *
1063 * @return
1064 */
1065 value_type SitePercolation_ps_v9::numberOfBondsInTheSpanningClusters_v2
     () {
1066 if(!_spanning_sites.empty()){
1067 //        cout << "number of spanning sites " << _spanning_sites.size()
     << " : line " << __LINE__ << endl;
1068 int id = _lattice.getGroupID(_spanning_sites.front());
1069 if(id >= 0) {
1070 return _clusters[id].numberOfBonds();
1071 }
1072 }
1073 return 0;
1074 }
1075
1076 /**
1077 *
1078 * @return
1079 */
1080 value_type SitePercolation_ps_v9::numberOfSitesInTheWrappingClusters(){
1081 value_type nos{};
1082 int id{};
1083 for(auto i: _wrapping_sites){
1084 id = _lattice.getGroupID(i);
```

```
1085 if(id >= 0) {
1086 nos += _clusters[id].numberOfSites();
1087 }
1088 }
1089 return nos;
1090 }
1091
1092 /**
1093 *
1094 * @return
1095 */
1096 value_type SitePercolation_ps_v9::numberOfBondsInTheWrappingClusters(){
1097 value_type nob{};
1098 int id{};
1099 for(auto i: _wrapping_sites){
1100 id = _lattice.getGroupID(i);
1101 if(id >= 0) {
1102 nob += _clusters[id].numberOfBonds();
1103 }
1104 }
1105 return nob;
1106 }
1107
1108
1109 std::string SitePercolation_ps_v9::getSignature() {
1110 string s = "sq_lattice_site_percolation";
1111 if(_periodicity)
1112 s += "_periodic_";
1113 else
1114 s += "_non_periodic_";
1115 return s;
1116 }
1117
1118 /**
1119 *
1120 * @param filename
1121 * @param only_spanning
1122 */
1123 void SitePercolation_ps_v9::writeVisualLatticeData(const string &
      filename, bool only_spanning) {
1124 std::ofstream fout(filename);
1125 ostringstream header_info;
1126 header_info << "{"
1127 << "\"length\":" << length()
```

```
<< ",\"signature\":\"" << getSignature() << "\""
<< ",\"x\":\"" << lastPlacedSite().column_ << "\""
<< ",\"y\":\"" << lastPlacedSite().row_ << "\""
<< "}" ;

fout << "#" << header_info.str() << endl;
fout << "#<x>,<y>,<color>" << endl;
fout << "# color=0 -means-> unoccupied site" << endl;
int id{-1};
if(!_spanning_sites.empty()){
id = _lattice.getGroupID(_spanning_sites.front());
}
else if(!_wrapping_sites.empty()){
id = _lattice.getGroupID(_wrapping_sites.front());
}

if(only_spanning){
if(id < 0){
cerr << "id < 0 : line " << __LINE__ << endl;
}
vector<Index> sites = _clusters[id].getSiteIndices();
for(auto s: sites){
fout << s.column_ << ',' << s.row_ << ',' << id << endl;
}
}
else {
for (value_type y{}; y != length(); ++y) {
for (value_type x{}; x != length(); ++x) {
id = _lattice.getGroupID({y, x});
if(id != -1) {
fout << x << ',' << y << ',' << id << endl;
}
}
}
}
fout.close();
}
```

The **src/percolation/percolation_site_ballistic_deps_v2.cpp** file

```
#include <cstdlib>
#include <climits>

#include "percolation.h"

```

```
using namespace std;

/**
*
* @param length
*/
SitePercolationBallisticDeposition_v2::
    SitePercolationBallisticDeposition_v2(value_type length, bool
    periodicity)
: SitePercolation_ps_v9(length, periodicity )
{

std::cout << "Constructing SitePercolationBallisticDeposition_v2 object
    : line " << __LINE__ << endl;

initialize_indices();
indices_tmp = indices;
//     randomize_index();
}

/**
*
*/
void SitePercolationBallisticDeposition_v2::reset() {
SitePercolation_ps_v9::reset();
indices_tmp = indices;
}

/**
* Called only once when the object is constructed for the first time
*/
void SitePercolationBallisticDeposition_v2::initialize_indices() {
indices = vector<value_type>(maxSites());
for(value_type i{}; i != indices.size(); ++i){
indices[i] = i; // assign index first
}
}



/*****************************************
* Site selection methods
*/

```

```
47 /**
48 *
49 * @param sites
50 * @param bonds
51 * @return
52 */
53 Index SitePercolationBallisticDeposition_v2::select_site(vector<Index> &
       sites, vector<BondIndex> &bonds) {
54 // randomly choose a site
55 value_type r = std::rand() % (indices_tmp.size());
56
57 Index current_site = index_sequence[indices_tmp[r]];
58 cout << "current site " << current_site << endl;
59 // find the bonds for this site
60
61 if (_lattice.getSite(current_site).isActive()){
62 indices_tmp.erase(indices_tmp.begin()+r);
63
64 throw OccupiedNeighbor{"all of the 1nd neighbors are occupied : line " +
       std::to_string(__LINE__)};
65 }
66
67 cout << "choosing " << current_site << " out of the neighbors : line "
       << __LINE__ << endl;
68 sites.clear();
69 bonds.clear();
70 connection_v2(current_site, sites, bonds);
71 return current_site;
72 }
73
74 /**
75 *
76 * @param sites
77 * @param bonds
78 * @return
79 */
80 Index SitePercolationBallisticDeposition_v2::select_site_upto_1nn(
81 vector<Index> &sites, vector<BondIndex> &bonds
82 ) {
83 // randomly choose a site
84 value_type r = _random_generator() % (indices_tmp.size());
85
86 Index current_site = index_sequence[indices_tmp[r]];
87 //     cout << "current site " << current_site << endl;
```

```
88 // find the bonds for this site
89
90 //    connection_v1(current_site, sites, bonds);
91 connection_v2(current_site, sites, bonds);
92
93 if (_lattice.getSite(current_site).isActive()){ // if the current site
       is occupied or active
94 value_type r2 = _random_generator() % (sites.size());
95 current_site = sites[r2]; // select one of the neighbor randomly
96
97 if(_lattice.getSite(current_site).isActive()){
98 // if the neighbor is also occupied cancel current step
99 bool flag = true;
100 //            cout << "if one of the neighbor is inactive. it's engouh
       to go on" << endl;
101 for(auto s : sites){
102 //                cout << s << "->";
103 if(!_lattice.getSite(s).isActive()){
104 // if one of the neighber is unoccupied then
105 flag = false;
106 //                    cout << " inactive" << endl;
107 break;
108 }
109 //                cout << " active"<< endl;
110 }
111 if(flag){
112 // erase the index, since its four neighbors are occupied
113 indices_tmp.erase(indices_tmp.begin()+r);
114 throw OccupiedNeighbor{"all of the 1nd neighbors are occupied : line " +
        std::to_string(__LINE__)};
115 }
116 throw OccupiedNeighbor{"selected 1st neighbor is occupied : line " + std
       ::to_string(__LINE__)};
117 }
118 }
119
120 //    cout << "choosing " << current_site << " out of the neighbors :
       line " << __LINE__ << endl;
121 sites.clear();
122 bonds.clear();
123 connection_v2(current_site, sites, bonds);
124 return current_site;
125 }
126
```

```
127
128
129 /**
130 * Select neighbor upto 2nd nearest neighbor
131 * uses direcion of motion when selecting 2nd nearest neighbor
132 * @param r : index of sites in the randomized array
133 * @param sites
134 * @param bonds
135 * @return
136 */
137 Index SitePercolationBallisticDeposition_v2::select_site_upto_2nn(
138 vector<Index> &sites, vector<BondIndex> &bonds
139 ){
140 value_type r = _random_generator() % (indices_tmp.size());
141
142 Index central_site = index_sequence[indices_tmp[r]];
143 Index selected_site;
144 // find the bonds for this site
145
146
147 connection_v2(central_site, sites, bonds);
148
149 if (_lattice.getSite(central_site).isActive()){
150 bool flag_nn1 = true; // true means all 1st nearest neighbors are
    occupied
151 bool flag_nn2 = true; // true means all 2nd nearest neighbors are
    occupied
152 //        cout << "if one of the neighbor is inactive. it's engouh to go
     on" << endl;
153 for(auto s : sites){
154 //            cout << s << "->";
155 if(!_lattice.getSite(s).isActive()){
156 // if one of the neighber is unoccupied then
157 flag_nn1 = false;
158 //                cout << " inactive" << endl;
159 break;
160 }
161 //            cout << " active"<< endl;
162 }
163
164 value_type r2 = _random_generator() % (sites.size());
165 Index nn1 = sites[r2]; // select one of the neighbor randomly
166 //        cout << "nn1 " << nn1 << " : line " << __LINE__ <<endl;
167 Index nn2;
```

```
168 if(_lattice.getSite(nn1).isActive()){
169 // if the neighbor is also occupied then choose the 2nd nearest neighbor
        in the direction of motion
170 nn2 = get_2nn_in_1nn_direction(central_site, nn1, length());
171 if(!_periodicity){
172 // if periodic boundary condition is not enabled then sites on the
       opposite edges will not contribute
173 vector<Index> tmp_sites;
174 vector<BondIndex> tmp_bonds;
175 // will find all possible neighbors of the selected first nearest
       neighbor
176 connection_v2(nn1, tmp_sites, tmp_bonds);
177 bool valid{false};
178 for(auto s: tmp_sites){
179 if(nn2 == s){
180 //                          cout << "valid 2nd nearest neighbor : line "
       << __LINE__ << endl;
181 valid = true;
182 break;
183 }
184 }
185 if(!valid){
186 throw InvalidNeighbor{"invalid 2nd nearest neighbor : line " + std::
       to_string(__LINE__)};
187 }
188 }
189 //             cout << "nn2 " << nn2 << " : line " << __LINE__ <<endl;
190 // if it is also occupied the skip the step
191 if(_lattice.getSite(nn2).isActive()) {
192 flag_nn2 = true;
193
194 vector<Index> nn2_sites = get_2nn_s_in_1nn_s_direction(central_site,
       sites, length());
195 for(auto x: nn2_sites){
196 if(!_lattice.getSite(x).isActive()){
197 flag_nn2 = false;
198 //                          cout << "inactive";
199 break;
200 }
201 }
202
203 if(flag_nn1 && flag_nn2){
204 // erase the index, since its 1st nearest neighbors are occupied
205 // and 2nd nearest neighbors are also occupied
```

```
206 indices_tmp.erase(indices_tmp.begin()+r);
207 }
208
209 throw OccupiedNeighbor{"2nd neighbor is also occupied : line " + std::
        to_string(__LINE__)};
210 }else{
211 selected_site = nn2;
212 }
213 }else {
214 selected_site = nn1;
215 }
216
217 sites.clear();
218 bonds.clear();
219
220 connection_v2(selected_site, sites, bonds);
221 }else{
222 selected_site = central_site;
223 }
224 return selected_site;
225 }
226
227
228
229 /*******************************************************
230 * SitePercolationBallisticDeposition_v2
231 * select upto 1st nearest neighbor
232 */
233
234 /**
235 *
236 * @return
237 */
238 bool SitePercolationBallisticDeposition_v2::occupy() {
239 // if no site is available then return false
240
241 if(_number_of_occupied_sites == maxSites()){
242 return false;
243 }
244
245 try {
246
247 value_type v = placeSite_1nn_v2();
248 _occuption_probability = occupationProbability(); // for super class
```

```
249
250
251 return v != ULLONG_MAX;
252 }catch (OccupiedNeighbor& on){
253 //         on.what();
254 //         cout << "line : " << __LINE__ << endl;
255 return false;
256 }
257
258 }
259
260
261 /**
262 *
263 * 1. Randomly select a site from all sites
264 * 2. If it is not occupied occupy it.
265 * 3. If it is occupied select one of the 4 neighbor to occupy
266 * 4. If the selected neighbor is also occupied cancel current step
267 * 4. form cluster and track all informations
268 * 5. go to step 1
269 * 6. untill spanning cluster appears or no unoccupied site
270 */
271 value_type SitePercolationBallisticDeposition_v2::placeSite_1nn_v2() {
272
273 vector<BondIndex> bonds;
274 vector<Index>     sites;
275
276 _last_placed_site = select_site_upto_1nn(sites, bonds);
277
278 return placeSite_weighted(_last_placed_site, sites, bonds);
279 }
280
281 /**
282 *
283 * @return
284 */
285 value_type SitePercolationBallisticDeposition_v2::placeSite_2nn_v1() {
286 vector<BondIndex> bonds;
287 vector<Index>     sites;
288
289 try {
290 _last_placed_site = select_site_upto_2nn(sites, bonds);
291 return placeSite_weighted(_last_placed_site, sites, bonds);
292 //    return placeSite_v11(_last_placed_site);
```

```
293 }catch (OccupiedNeighbor& e){
294 //         cout << "Exception !!!!!!!!!!!!!!!!!!" << endl;
295 //         e.what();
296 }catch (InvalidNeighbor& b){
297 //         cout << "Exception !!!!!!!!!!!!!!!!!!" << endl;
298 //         b.what();
299 }
300 return ULONG_MAX;
301 }
```

A.2.8 Utilities

We sometimes need to print an array, std::map, std::vector in the console. Some functions for this task is given here.

The **src/util/printer.h** file

```
1  #ifndef PERCOLATION_PRINTER_H
2  #define PERCOLATION_PRINTER_H
3
4  #include <ostream>
5  #include <unordered_map>
6  #include <set>
7  #include <unordered_set>
8  #include <vector>
9  #include <map>
10 #include <initializer_list>
11
12 template <typename T>
13 std::ostream& operator<<(std::ostream& os, const std::vector<T> & vec){
14 os << '{';
15 for(auto a: vec){
16 os << a << ',';
17 }
18 return os << '}';
19 }
20
21 template <typename T>
22 std::ostream& operator<<(std::ostream& os, const std::set<T> & vec){
23 os << '{';
24 for(auto a: vec){
25 os << a << ',';
26 }
27 return os << '}';
```

```
28 }
29
30 template <typename T>
31 std::ostream& operator<<(std::ostream& os, const std::unordered_set<T> &
       vec){
32 os << '{';
33 for(auto a: vec){
34 os << a << ',';
35 }
36 return os << '}';
37 }
38
39 template <typename K, typename V>
40 std::ostream& operator<<(std::ostream& os, const std::map<K, V> & m){
41 os << '{';
42 for(auto a: m){
43 os << '(' << a.first << "->" << a.second << "),";
44 }
45 return os << '}';
46 };
47
48 template <typename K, typename V>
49 std::ostream& operator<<(std::ostream& os, const std::unordered_map<K, V
      > & m){
50 os << '{';
51 for(auto a: m){
52 os << '(' << a.first << "->" << a.second << "),";
53 }
54 return os << '}';
55 };
56
57 /**
58 *
59 * Prints a horizontal barrier in the console.
60 * @param n              : how many time the middle string is repeated.
61 * @param initial        : string that is printed initially.
62 * @param middles        : middle string.
63 * @param end            : string that is printed at the end.
64 */
65 void print_h_barrier(size_t n, const std::string& initial, const std::
      string& middles, const std::string& end="\n");
66
67 #endif //PERCOLATION_PRINTER_H
```

The **src/util/printer.cpp** file

```
#include "printer.h"
#include <iostream>

using namespace std;

void print_h_barrier(size_t n, const string& initial, const string&
    middles, const string& end){
  cout << initial;
  for(size_t i{}; i < n ; ++i){
    cout << middles;
  }
  cout << end; // end of barrier
}
```

When generating data file we need to name our data file uniquely so that when all of the data files are in one location, no confusion occurs. A good way to do this is to add the time and data stamp at the end of each data file. Although data filename does share a common pattern.

The **src/util/time_tracking.h** file

```
#ifndef PERCOLATION_TIME_TRACKING_H
#define PERCOLATION_TIME_TRACKING_H

#include <string>

std::string getFormattedTime(double t);
std::string currentTime();
std::string getCurrentTime();
#endif //PERCOLATION_TIME_TRACKING_H
```

The **src/util/time_tracking.cpp** file

```
#include "time_tracking.h"
#include <iostream>
#include <sstream>

using namespace std;

/**
*
* @param t -> Time in seconds
* @return
*/
std::string getFormattedTime(double t){
```

```
std::string s;

size_t hr{}, min{};
double sec{}; // hour, min, sec
size_t integer_sec = size_t(t);

if(integer_sec >= 3600)
hr = integer_sec / 3600;
if(integer_sec >= 60)
min = (integer_sec - hr * 3600) / 60;
sec = t -  min * 60 - hr * 3600;

s += to_string(hr);
s += " hr ";
s += to_string(min);
s += " min ";
s += to_string(sec);
s += " sec ";
return s;
}

std::string currentTime() {
time_t t = time(0);   // get birthTime now
struct tm * now = localtime( & t );
stringstream ss;
ss << (now->tm_year + 1900) << '.'
<< (now->tm_mon + 1) << '.'
<<  now->tm_mday << '_'
<< now->tm_hour << '.' << now->tm_min << '.' << now->tm_sec;

return ss.str();
}

/**
formated date
24 hour formated time
*/
string getCurrentTime(){

time_t rawtime;
struct tm * timeinfo;
char buffer [80];

time (&rawtime);
```

```
57 timeinfo = localtime (&rawtime);
58
59 strftime (buffer,80,"%F_%H%M%S",timeinfo);
60 return buffer;
61 }
```

The **src/types.h** file

```
1 #ifndef SITEPERCOLATION_TYPES_H
2 #define SITEPERCOLATION_TYPES_H
3
4 using value_type = unsigned long;
5 using signed_value_type =  long;
6
7 #endif //SITEPERCOLATION_TYPES_H
```

A.2.9 Tests

A template function is required to run for $l0, l1, l2$. The template argument is the class name. The other two argument is the length and ensemble size we need for one file. The three template arguments are

1. SitePercolation_ps_v9
2. SitePercolationBallisticDeposition_L1_v2
3. SitePercolationBallisticDeposition_L1_v2

The **src/test/test_percolation.h** file

```
1 #ifndef SQLATTICEPERCOLATION_TEST_PERCOLATION_H
2 #define SQLATTICEPERCOLATION_TEST_PERCOLATION_H
3
4 #include <iostream>
5 #include <string>
6 #include <chrono>
7 #include "../types.h"
8 #include "../percolation/percolation.h"
9 #include "../util/time_tracking.h"
10
11
12 /**
13 *
14 * @tparam PType : Template type of percolation class
15 * @param argc   : argc from commandline
```

```
16 * @param argv    : argv from commandline
17 */
18 template<class PType>
19 void simulate_site_percolation_T(value_type length, value_type
       ensemble_size) {
20
21 std::cout << "length " << length << " ensemble_size " << ensemble_size
       << std::endl;
22
23 value_type length_squared = length*length;
24 value_type twice_length_squared = 2 * length_squared;
25
26 PType lattice_percolation(length, true);
27
28 std::ostringstream header_info;
29 header_info << "{"
30 << "\"length\":" << length
31 << ",\"ensemble_size\":" << ensemble_size
32 << ",\"signature\":\"" << lattice_percolation.getSignature() << "\""
33 << "}" ;
34
35 std::string tm = getCurrentTime();
36
37 std::string filename_s = lattice_percolation.getSignature() + "
       _cluster_by_site_" + std::to_string(length) + '_' + tm;
38 std::string filename_b = lattice_percolation.getSignature() + "
       _cluster_by_bond_" + std::to_string(length) + '_' + tm;
39 std::string filename_critical = lattice_percolation.getSignature() + "
       _critical_" + std::to_string(length) + '_' + tm;
40 std::string filename_entropy_order_parameter = lattice_percolation.
       getSignature()  + std::to_string(length) + '_' + tm;
41
42 filename_s += ".csv";
43 filename_b += ".csv";
44 filename_critical += ".csv";
45 filename_entropy_order_parameter += ".csv";
46
47
48 std::ofstream fout_s(filename_s);
49 // JSON formated header
50 fout_s << '#' << header_info.str() << std::endl;
51 fout_s << "#each line is an independent realization" << std::endl;
52 fout_s << "#each line contains information about all clusters at
       critical point" << std::endl;
```

```
53 fout_s << "#cluster size is measured by number of sites in it" << std::
       endl;
54
55 std::ofstream fout_b(filename_b);
56 // JSON formated header
57 fout_b << '#' << header_info.str() << std::endl;
58 fout_b << "#each line is an independent realization" << std::endl;
59 fout_b << "#each line contains information about all clusters at
       critical point" << std::endl;
60 fout_b << "#cluster size is measured by number of bonds in it" << std::
       endl;
61
62 std::ofstream fout_critical(filename_critical);
63 fout_critical << '#' << header_info.str() << std::endl;
64 fout_critical << "#data at critical occupation probability or pc" << std
       ::endl;
65 fout_critical << "#<pc>,<sites in wrapping cluster>,<bonds in wrapping
       cluster>" << std::endl;
66
67 // simulation starts here
68 value_type counter{};
69 std::vector<double> entropy(lattice_percolation.maxIterationLimit());
70 std::vector<double> nob_wraping(lattice_percolation.maxIterationLimit())
       ,
71 nob_largest(lattice_percolation.maxIterationLimit());
72
73 for(value_type i{} ; i != ensemble_size ; ++i){
74
75 lattice_percolation.reset();
76
77 bool successful = false;
78 auto t_start = std::chrono::system_clock::now();
79 counter = 0;
80 bool wrapping_written{false};
81 while (true){
82 successful = lattice_percolation.occupy();
83 if(successful) {
84 entropy[counter] += lattice_percolation.entropy();
85 nob_wraping[counter] += lattice_percolation.
       numberOfBondsInTheWrappingClusters();
86 nob_largest[counter] += lattice_percolation.
       numberOfBondsInTheLargestCluster_v2();
87
88 if(!wrapping_written && lattice_percolation.detectWrapping()){
```

```
89 fout_critical << lattice_percolation.occupationProbability() << ","
90 << lattice_percolation.numberOfSitesInTheWrappingClusters() << ","
91 << lattice_percolation.numberOfBondsInTheWrappingClusters()  << std::
       endl;
92
93 std::vector<value_type> site, bond;
94
95 lattice_percolation.get_cluster_info(site, bond);
96
97 for(value_type j{}; j != site.size(); ++j){
98 fout_s << site[j] << ',';
99 }
100 for(value_type j{}; j != bond.size(); ++j){
101 fout_b << bond[j] <<',';
102 }
103
104
105 fout_s << std::endl;
106 fout_b << std::endl;
107 wrapping_written = true;
108 }
109
110
111 ++counter;
112 }
113 if(counter >= lattice_percolation.maxIterationLimit()){ //
       twice_length_squared is the number of bonds
114 break;
115 }
116 }
117
118 auto t_end = std::chrono::system_clock::now();
119 std::cout << "Iteration " << i   << " . Elapsed time " << std::chrono::
       duration<double>(t_end - t_start).count() << " sec" << std::endl;
120
121 }
122
123 fout_b.close();
124 fout_s.close();
125 fout_critical.close();
126
127
128
129 std::ofstream fout(filename_entropy_order_parameter);
```

```
130 fout << '#' << header_info.str() << std::endl;
131 fout << "#<p>,<H(p,L)>,<P1(p,L)>,<P2(p,L)>" << std::endl;
132 fout << "#p = occupation probability" << std::endl;
133 fout << "#H(p,L) = Entropy = sum( - u_i * log(u_i))" << std::endl;
134 fout << "#P1(p,L) = Order parameter = (number of bonds in largest
    cluster) / (total number of bonds)" << std::endl;
135 fout << "#P2(p,L) = Order parameter = (number of bonds in spanning or
    wrapping cluster) / (total number of bonds)" << std::endl;
136 fout << "#C(p,L) = Specific heat = -T dH/dT" << std::endl;
137 fout << "#X(p,L) = Susceptibility = dP/dp" << std::endl;
138 fout << "#u_i = (number of bonds in the i-th cluster) / (total number of
     bonds)" << std::endl;
139 for(size_t i{}; i < lattice_percolation.maxIterationLimit(); ++i){
140 fout << (i+1) / double(lattice_percolation.maxIterationLimit()) << ",";
141 fout << entropy[i] / double(ensemble_size) << ",";
142 fout << nob_largest[i] / double(ensemble_size /* lattice_percolation.
    maxBonds()*/) << ",";
143 fout << nob_wraping[i] / double(ensemble_size /* lattice_percolation.
    maxBonds()*/) ;
144 fout << std::endl;
145 }
146 fout.close();
147 }
148
149 #endif //SQLATTICEPERCOLATION_TEST_PERCOLATION_H
```

A.2.10 Main

The main function receives 3 additional command line argument. First one is an integer $l \in \{0,1,2\}$ which determine the range of interaction. Second one is the length of the lattice. And third one is the size of the ensemble. For example, 12005000 will run the program for $l = 1$, $L = 200$ for ensemble size of 5000.

The *run_in_main(int, char**)* function is the one where the *simulate_site_percolation_T<>(size_t, size_t)* executes for different classes.

The **src/main.cpp** file

```
1 #include <iostream>
2 #include <fstream>
3 #include <ctime>
4 #include <chrono>
5 #include <thread>
6 #include <mutex>
```

```
7
8  #include "lattice/lattice.h"
9  #include "percolation/percolation.h"
10 #include "util/time_tracking.h"
11 #include "util/printer.h"
12
13 #include "tests/test_percolation.h"
14
15
16 using namespace std;
17
18
19 /****
20 *  All the function that is run in main
21 * @param argc
22 * @param argv
23 */
24 void run_in_main(int argc, char** argv){
25
26 int l = atoi(argv[1]);
27 value_type length = atoi(argv[2]);
28 value_type ensemble_size = atoi(argv[3]);
29
30 if(l==1) {
31 cout << "Simulating site percolation for l=1" << endl;
32 simulate_site_percolation_T<SitePercolationBallisticDeposition_L1_v2>(
       length, ensemble_size); // 2018.11.03
33 }
34 else if(l==2) {
35 cout << "Simulating site percolation for l=2" << endl;
36 simulate_site_percolation_T<SitePercolationBallisticDeposition_L2_v2>(
       length, ensemble_size); // 2018.11.03
37 }else{
38 cout << "Simulating site percolation for l=0" << endl;
39 simulate_site_percolation_T<SitePercolation_ps_v9>(length, ensemble_size
       );
40 }
41 }
42
43
44
45
46 /**********************************
47 *  The main function
```

```
48 *
49 ************************************/
50 int main(int argc, char** argv) {
51
52 cout << "Running started at : " << currentTime() << endl;
53 cout << "Compiled on         : " << __DATE__ << "\t at " << __TIME__ <<
       endl;
54 std::cout << "Percolation in a Square Lattice" << std::endl;
55 auto t_start = std::chrono::system_clock::now();
56
57 time_t seed = time(NULL);
58 srand(seed);     // seeding
59
60 run_in_main(argc, argv);
61
62 auto t_end= std::chrono::system_clock::now();
63 std::chrono::duration<double> drtion = t_end - t_start;
64 std::time_t end_time = std::chrono::system_clock::to_time_t(t_end);
65 cout << "Program finished at " << std::ctime(&end_time) << endl;
66 std::cout << "Time elapsed "   << getFormattedTime(drtion.count()) <<
       std::endl;
67 return 0;
68 }
```

A.2.11 CMakeLists

All the header and source files are listed here and how the compiler should link them is generated by running cmake. https://cmake.org/cmake-tutorial/

The **CMakeLists.txt** file

```
1 cmake_minimum_required(VERSION 3.0)
2 project(SqLatticePercolation)
3
4 set(CMAKE_CXX_STANDARD 11)
5
6 #set (CMAKE_C_COMPILER                /usr/bin/gcc)
7 #set (CMAKE_CXX_COMPILER              /home/shahnoor/software/pgi/linux86
      -64-llvm/2018/bin/pgc++)
8 #set (CMAKE_MAKE_PROGRAM              /usr/bin/make)
9 SET( CMAKE_CXX_FLAGS  "-pthread -fopenmp")
10 #SET( CMAKE_EXE_LINKER_FLAGS  "${CMAKE_EXE_LINKER_FLAGS} ${
      GCC_COVERAGE_LINK_FLAGS}" )
11
```

```
12 set(SOURCE_FILES
13 src/main.cpp
14 src/types.h
15 src/exception/exceptions.h
16 src/index/index.cpp
17 src/index/index.h
18 src/lattice/bond.cpp
19 src/lattice/bond.h
20 src/lattice/bond_type.h
21 src/lattice/lattice.cpp
22 src/lattice/lattice.h
23 src/lattice/site.cpp
24 src/lattice/site.h
25 src/percolation/cluster.cpp
26 src/percolation/cluster.h
27 src/percolation/percolation.cpp
28 src/percolation/percolation.h
29 src/percolation/percolation_site_ballistic_deps_v2.cpp
30 src/util/printer.h
31 src/util/time_tracking.cpp
32 src/util/time_tracking.h
33 src/util/printer.cpp
34 src/percolation/percolation_site_v9.cpp
35 src/tests/test_percolation.h)
36
37 add_executable(SqLatticePercolation ${SOURCE_FILES})
```

A.2.12 complete code

Complete code for RSBD model on square lattice is available at https://github.com/sha314/SqLattice_RSBD or use the git link to clone the repository https://github.com/sha314/SqLattice_RSBD.git

Detailed version of the same program with other extensions are available at https://github.com/sha314/SqLatticePercolation or the git link https://github.com/sha314/SqLatticePercolation.git

Appendix B

Convolution

Say we want to measure an observable Q, for example, for a specific occupied number of sites(bonds) in site(bond) percolation. But doing this we ignore the fact that we would have chose to fix a probability p first and starting occupying the lattice sequentially then after we have had visited all the sites we would not have $p = n/(L^2)$ for site or $p = n/(2L^2)$ for bond percolation each time. Therefore it would lead to some error. We can solve this dilemma by the following process. The trick [56, 50] is to measure Q for fixed numbers of occupied sites (or bonds) n in the range of interest. Let us refer to the ensemble of states of a percolation system with exactly n occupied sites or bonds as a "microcanonical percolation ensemble," the number n playing the role of the energy in thermal statistical mechanics. The more normal case in which only the occupation probability p is fixed is then the "canonical ensemble" for the problem. (If one imagines the occupied sites or bonds as representing particles instead, then the two ensembles would be "canonical" and "grand canonical," respectively. Taking site percolation as an example, the probability of there being exactly n occupied sites on the lattice for a canonical percolation ensemble is given by the binomial distribution

$$B(N,n,p) = \binom{N}{n} p^n (1-p)^{N-n} \tag{B.1}$$

The same expression applies for bond percolation, but with N replaced by M , the total number of bonds. Thus, if we can measure our observable within the microcanonical ensemble for all values of n, giving a set of measurements Q_n, then the value in the canonical ensemble will be given by

$$Q(p) = \sum_{n=0}^{N} B(N,n,p) Q_n = \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} Q_n \tag{B.2}$$

Thus we need only measure Q_n for all values of n. [77].

B.1 Algorithm

But using this formula to calculate $Q(p)$ is quite expensive since the number of sites(bonds) can be quite large direct evaluation of the binomial coefficients using factorials is not possible. We use alternative way to measure $Q(p)$, which is basically does the same thing but in an efficient way.

Instead, therefore, we recommend the following method of evaluation. The binomial distribution, Eq. (1), has its largest value for given N and p when $n = n_{max} = pN$. We arbitrarily set this value to 1. Now we calculate $B(N,n,p)$ iteratively for all other n from

$$B(N,n,p) = \begin{cases} B(N,n-1,p)\frac{N-n+1}{n}\frac{p}{1-p} \text{ if } n > n_{max} \\ B(N,n+1,p)\frac{n+1}{N-n}\frac{1-p}{p} \text{ if } n < n_{max} \end{cases}$$

Then we calculate the normalization coefficient $C = \sum_n B(N,n,p)$ and divide all the $B(N,n,p)$ by it, to correctly normalize the distribution [76, 77].

B.2 Code

In order to use convolution the following function can be used. It is very efficient and uses OpenMP for parallel run, meaning, all the cores of the processors performs the same task in a divide-and-conquer manner. This function takes an array as input and returns the convoluted version as output.

```
vector<double> convolution(vector<double>& data_in) {
size_t N = data_in.size();

std::vector<double> _forward_factor(N);
std::vector<double> _backward_factor(N);

for (size_t i=0; i < N; ++i)
{
_forward_factor[i]  = (double) (N - i + 1) / i;
_backward_factor[i] = (double) (i + 1) / (N - i);
}

vector<double> data_out(N);

```

```
15  long step = N / 1000;
16  #pragma omp parallel for schedule(dynamic)
17  for (long j=0; j <N; ++j) // start from j=1
18  {
19  double prob     = (double) j / N;
20  double factor   = 0;
21  double binom    = 0;
22  double prev     = 0;
23  double bn_tot   = 1; // normalization factor
24  double sum      = data_in[j];
25
26  // forward iteraion part
27  factor = prob / (1-prob);
28  prev   = 1;
29
30  for (long i=j+1; i<N; ++i)
31  {
32  binom     = prev * _forward_factor[i] * factor;
33  bn_tot += binom;
34  sum      += data_in[i] * binom;
35  prev      = binom;
36  }
37
38  // backward iteration part
39  factor = (1-prob)/prob;
40  prev   = 1;
41
42  for (long i=j-1; i>=0; --i)
43  {
44  binom     = prev * _backward_factor[i] * factor;
45  bn_tot += binom;
46  sum      += data_in[i] * binom;
47  prev      = binom;
48  }
49
50  // normalizing data
51  data_out[j] = sum / bn_tot;
52  cout << bn_tot << endl;
53
54  }
55
56  return data_out;
57  }
58
```

Complete code for convolution is available at https://github.com/sha314/Convolution.

The program linked above works using command line arguments. And the uses is as follows

```
Usage:
convolution [-f <STRING>] [-a <INT>,<INT>,...[:[<STRING>,<STRING>,...]]]
perform convolution based on provided options.
Options                    Description
-a,                        columns that we want in the output file withou
No default value.
-b,                        columns that we want in the output file with p
No default value.
-c,                        If provided the header and comment from the in
without modification to the output file. Header is the first line of the
input file.
-d                         Delimeter to use. Default value is ' '.
-f                         name of the input file that we want to convolu
-i                         Info to write as comment in the output file
-o                         name of the output file. If not provided the s
appended to the input file.
-p, --precision            Floating point precision when writing in the d
-s                         Number of rows to skip from the input file. De
-t                         to test the performance of the convolution pro
--threads                Explicitly specify number of thread to use. Defaul
allowed by the system.
-h, --help                 display this help and exit
-v, --version              output version information and exit
-w                         If provided input b data will be written to th
The INT argument is an integer.
The STRING argument is a string of characters.
A line that begins with '#' is considered a commented line.
Exit status:
0  if OK,
1  if minor problems (e.g., cannot access subdirectory),
2  if serious trouble (e.g., cannot access command-line argument).
```

Appendix C

Finding Exponents

C.1 Algorithm

C.1.1 Specific Heat and Susceptibility

exponent for scaling the y-values

To find the best exponent for scaling the y-values of specific heat and susceptibility the following approach is pretty helpful.

Finding approximate value of the exponent

1. get the x and y values of the convoluted data for all lengths (L)
2. get the maximum value or the peak value of y as $y_{max} = max(y)$ for each length
3. now plot $\log(y_{max})$ vs $\log(L)$
4. slope of this graph is the approximate value of the exponent

Finding the best exponent

Now that we know the approximate value of the exponent, ex_{approx}, we can find the best exponent in the following way

1. take a list of all the exponent in the range $E = [ex_{approx} - \varepsilon, ex_{approx} + \varepsilon]$ where ε is a small number (usually ~ 0.05)
2. for each value of the exponent in the range above do the following
   (a) get the x and y values of the convoluted data for all lengths (L)
   (b) scale the y value with the exponent and call it $y' = y * L^{-ex}$

(c) get the maximum value or the peak value of y' as $y'_{max} = max(y')$ for each length

(d) if the y'_{max} values for different exponents does not lie in the order of 10 then scale $y'_{max} = y'_{max}/max(y'_{max})$ to normalize y'_{max}. By order of 10 I mean that if the order y'_{max} for ex_i is 10^-1 and for ex_j is 10^-2 then when comparing between std_{ex_i} and std_{ex_j} we will get the std_{ex_j} is lower always. Thus just because the standard deviation is lower we cannot say it is the best exponent if the order of y'_{max} is different.

(e) find the standard deviation of all the y'_{max}'s and call it std_{ex} where the subscript denotes the current selected exponent

3. out of a number of selected exponent find the one with the minimum standard deviation and the exponent corresponding to this deviation is the best exponent denoted as ex^*. Symbolically

$$ex^* = argmin_{ex \in E}\ std_{ex} \tag{C.1}$$

exponent for scaling the x-values

Usually the exponent that scales the x-values is called $1/\nu$. The critical point is denoted as x_c To find an estimate from the data that looks like the graph of specific heat or susceptibility, the following algorithm is very helpful

1. get the x and y values of the convoluted data for all lengths (L)
2. get the x value at a specific height, h, and call it x_h
3. plot a graph of $\log(|x_h - x_c|)$ vs $\log(L)$ where $||$ denotes the absolute value.
4. slope of this graph is the estimate for the exponent $1/\nu$

Now to find the exponent that best collapses the data is the main goal. To do this the following algorithm can be followed.
Finding the standard deviation of the points at height h after scaling x-values with an approximate value of the exponent $(1/nu)_approx$ that is obtained from the graph of $\log(|x_h - x_c|)$ vs $\log(L)$.

1. write a function that takes h, x_{scaler}, y_{scaler}, lr as argument where, h is the height at which we will be taking x-values, x_{scaler} is the exponent that scales the x-values, y_{scaler} is the exponent that scales the y-values and lr is the argument that tells if the left or right side of the critical point should be taken under consideration. call this function *find_x_deviation*

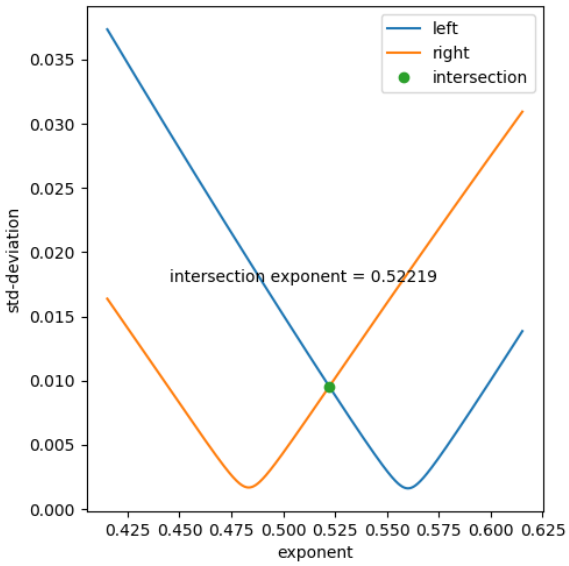

Fig. C.1 Best collapsing on either right or left
??

2. take $x' = (x - x_c)L^{x_{scaler}}$ and $y' = yL^{-y_{scaler}}$. Note that there is a minus sign used for scaling y values because the $y$max increases as L increases in our present case which is observed when finding y_{scaler} previously.

3. at height h we draw a horizontal straight line and the intersection of this line with the curve gives corresponding x value at h. For each length L we obtain the x value and denote it with x_L.

4. after that we find the standard deviation of all x_L's that we have found and this function returns the standard deviation

5. if lr is 0 then the left points of the critical point is considered and if lr is 1 then the right points of the critical point is considered for getting x_L's.

Note that at a specific height there are two points on on the left of the critical point and another is on the right. So if we find the exponent that best collapses the points on the left, it might not best collapse the points on the right **??**. To resolve this problem we take following approach

1. take a range $ex = [(1/nu)_{approx} - \varepsilon, (1/nu)_{approx} + \varepsilon]$, where ε is usually ~ 0.05.

2. for each value in this range find the standard deviation for left and right points of the critical point and call it d_{left} and d_{right} respectively

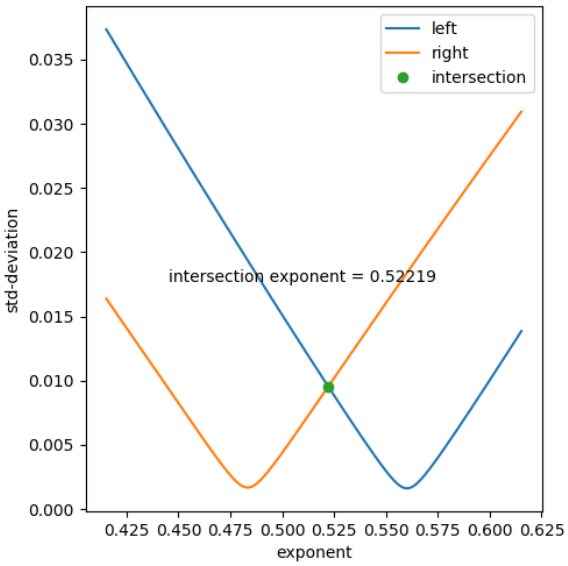

Fig. C.2 Minimizing exponent for scaling x-values

3. plot d_{left} vs ex and d_{right} vs ex on the same graph
4. the minima of line corresponding to d_{left} vs ex graph gives the exponent that collapses left points of the critical point at best.
5. the minima of line corresponding to d_{right} vs ex graph gives the exponent that collapses right points of the critical point at best.
6. the intersection of the graph is the value where both left and right points of the critical point fits better.

The figure C.2 gives the visual of the above process.