Percolation on A Square Lattice

What is Percolation Theory?

The theory of percolation deals with number and properties of clusters within a square lattice. A square lattice is simply a square of points, in which some of the points are connected to each other. Percolation theory is the study of these interconnected points (clusters) and the size and distribution of the clusters.

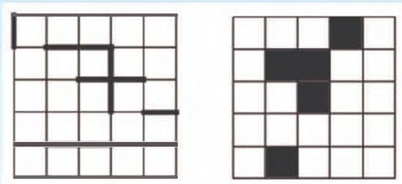


Fig 1, Simple examples of Bond and Site Percolation

Percolation theory is used to simulate a number of real life situations, such as the spread of forest fires, oil fields and fractals, and chemical reactions.

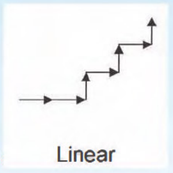
For example you could simulate a forest fire, starting from a fixed point (the initial fire) that grows exponentially from that point. The fire would grow from a point in the lattice, setting fire to another point next to it, then to another point next to that - forming a chain of fire that could spread across the whole forest (a chain of points across the whole lattice - i.e. a critical cluster).

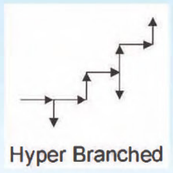
Why Do This Project?

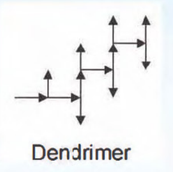
Percolation theory is used extensively in the theory of chemical reactions (at the molecular level). When molecules of different chemicals are mixed together they react to form chains (or clusters) of molecules. These molecules can be of varying length and width (a large cluster size and distribution) and can be branched a number of times. The molecules produced have different physical and chemical properties, and are used for different applications.

There are three main types of molecules (clusters) produced:

- Dendrimers - Have maximum branching.
- Hyper branched - Have some branching.
- Linear - Has no branching, is just a straight chain of molecules.







Dendrimers have special properties that make them good for use in things like one-coat paint or drug delivery. These molecules are very expensive to manufacture. This project should help to simulate the creation of such molecules and help assist in further research and development in this area.

Evaluating The Project

Using the program some analytical feedback for the user should be produced, which will be both relevant and useful in the understanding and further research of percolation theory, e.g. radius of gyration, molecular weight distribution. The data should then be used to compare the clusters produced with sample data from actual chemical reactions.

The data produced should have similar characteristics (i.e. similar branching levels and cluster sizes) to the actual chemical reaction. If the results are very similar, and if the results produced replicate the results of actual dendrimers then the product has produced what it set out to.

The product would be finished if it would replicate the actual results of a chemical reaction and would prove that the theory of percolation can be used to model certain chemical reactions. The longer the length of the clusters gained, then the better the chances of produced molecule. If the product produces a critical cluster (a long molecule that spans the whole lattice) then it could prove to be a useful tool for simulating several physical applications.

Aims, Objectives & The Product

Throughout the development of the project there should be a number of produced deliverables.

- The aims in this project are to look into the simulation and modelling of percolation theory for analytical purposes. The system modelled will be a 2D square lattice, clusters are formed by randomly making bonds between neighbouring sites.
- The generation of a program that will simulate the random growth of clusters within a square lattice. This program would need to have a suitable graphical interface to enable users to easily view and understand the result set generated.
- The simulation will produce analysis of the lattice's clusters and enable a user to apply percolation theory to this sort of system.
- It may be possible to produce some kind of 3-dimensional representation of the lattice so that a user can view various parts of lattice in a way that is a more realistic representation of the theory.

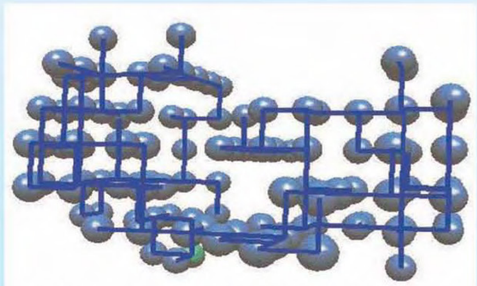


Fig 2, Example of a 3D representation of a cluster.

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REFERENCES

Fig 1. (2004) [Online image]. Available from: <http://mathworld.wolfram.com/PercolationTheory.html> /p1img2258.gif, [Accessed 8 December 2004].

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