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Review

# Percolation in education and application in the 21st century

Joan Adler[a], Shaked Elfenbaum, and Liran Sharir

Technion – IIT, Haifa, Israel

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**Abstract.** Percolation, "so simple you could teach it to your wife" (Chuck Newman, last century) is an ideal system to introduce young students to phase transitions. Two recent projects in the Computational Physics group at the Technion make this easy. One is a set of analog models to be mounted on our walls and enable visitors to switch between samples to see which mixtures of glass and metal objects have a percolating current. The second is a website enabling the creation of stereo samples of two and three dimensional clusters (suited for viewing with Oculus rift) on desktops, tablets and smartphones. Although there have been many physical applications for regular percolation in the past, for Bootstrap Percolation, where only sites with sufficient occupied neighbours remain active, there have not been a surfeit of condensed matter applications. We have found that the creation of diamond membranes for quantum computers can be modeled with a bootstrap process of graphitization in diamond, enabling prediction of optimal processing procedures.

## 1 Introduction

Percolation is a great way to teach Phase Transitions (PT). Amongst his many contributions to PT study, Wolfhard Janke (WJ) has at least 12 papers on percolation. The percolation problem has many variants, but the simplest model for site percolation is a mixture of metal and glass balls in a box. If there is a continuous path of metal from side to side, there would be percolation of electric current when the box is placed in a circuit with a source of electricity. The study of percolation did start not too far from Coventry, (the location of the PT workshop) at Harwell in the early fifties, and was christened by John Hammersley, a probabilist [1,2]. Focus moved to physics for a while, but nowadays percolation seems to be hot again in the probability community. Percolation study is about 60 years young, just like WJ.

It has always been hard to find many real condensed matter percolation applications. Bootstrap percolation (BP) [3] is percolation where some sufficient number of sites have to be occupied in order for current or geometrical order to be transmitted [4]. An application of this model to order in molecular $H_2$ has as a toy model the dilute three-state Potts antiferromagnet on a triangular lattice. A study of the

[a] e-mail: phr76ja@tx.technion.ac.il

latter resulted in Joan Adler(JA)'s only non-series expansion paper with WJ [5]. The final section of this paper will describe an especially cute BP application, relevant to creating diamond membranes for quantum computing [6,7]. New activity in Diffusion Percolation (DP, inverse of BP, initially developed for fluid flow in silted rock systems [8]) is occurring at Tel Aviv University materials right now [9]. In DP vacant sites with some requisite number of neighbours can become occupied. The new DP models are being applied to colloids. In the PT community a variant called negative-weight percolation is under intense study by Melchert, Hartmann and Mezard [10].

## 2 History and variations

Percolation is so simple – you can explain it to your husband!!!! also to grandchildren, etc. The original application concerned carbon granules in a gas mask. The granules had to be large enough so air could flow between them but larger poison molecules could not. Broadbent of the British Coal Utilization Research Association [11] reported on this model to Hammersley at an early Monte Carlo (MC) simulation meeting in Harwell [12]. One of the first MC calculations was made for percolation on the Mercury Ferranti at Harwell by Hammersley in 1955 [1]. The simulations were then used to test an early IBM 7090 at Bell laboratory, in 1960/61, see the historical review by Hammersley in [2] for details.

There are many variations to models for a percolation PT. Many have the same critical exponents, some fall in different universality classes and many of the more interesting ones have "exotic" finite-size scaling behaviour. The most basic distinction is between site and bond percolation. In the former (which is the usual default for simulations), sites are either occupied or vacant. The glass/metal ball mixtures are its exemplar, and it is relevant to many condensed matter models. Bond percolation, where all sites are occupied, but bonds between them may be open or closed, is the default for Renormalization Group (RG) theory or fluid diffusion in soil ($n = 1$ Potts model). The numerical approach to elucidating PT behaviour, series expansions is equally relevant for both. Another feature that distinguishes models is symmetry, which can be isotropic or directional. Directed percolation, where connection is possible only in one direction is in the same universality class as Reggeon Field Theory [13]. This connection was the trigger for a study of corrections-to-scaling in directed percolation series expansions and JA's first project with Vladimir Privman about whom more will be said later. The afore-mentioned BP and analytical and probabilistic results for its finite-size scaling by Schonmann [14] and Van Enter [15] amongst others, are now being researched in endless variations mostly in the probabilility literature.

## 3 Milestones and early educational websites

But let us return to the beginning. Early series expansions from several researchers in London, predicted the universality between bond and site percolation [16]. A major algorithmic advance was the Hoshen-Kopelman MC algorithm (HK), in 1976 [17] which led to a dramatic increase in the size of lattices that could be studied. Throughout the 1980s RG studies dominated, with extensive study of relevant and irrelevant operators and critical exponents. No survey of percolation history could be complete without a recollection of Stauffer's incessant encouragement of every possible study of any percolation related topic [18], and his famous graphs of percolation papers as a function of year. In this decade interest in the structure of percolation connected clusters also flourished.

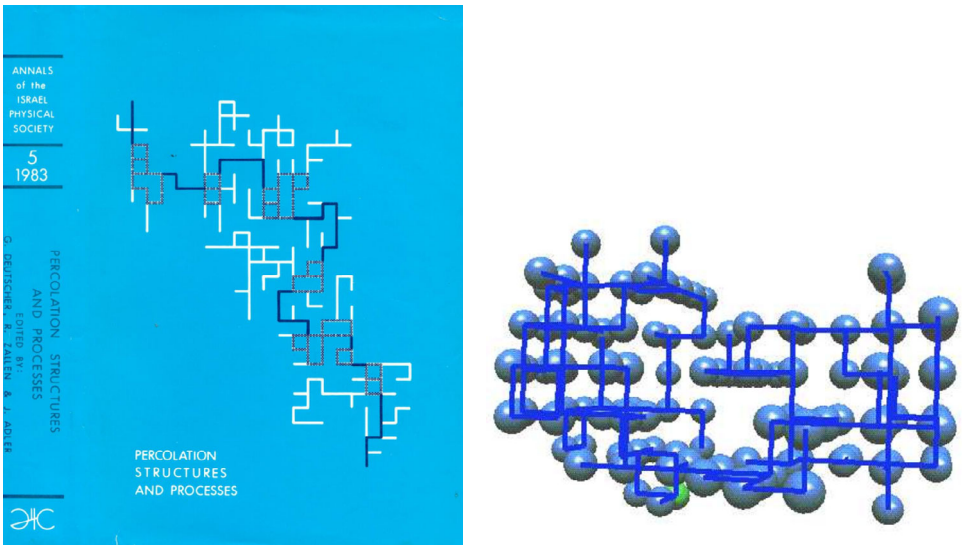


**Fig. 1.** Left: Stanley's blob-link-backbone cluster from 1983 [2]. Right: an image of Nir Yefet's 3D cluster from 1998 [20].

The image at the left of Figure 1 is reproduced from the cover of a book JA co-edited in 1983 [2], and was prepared and suggested for the cover by one of the chapter authors, Gene Stanley. The different types of connections, backbones, loops and dangling bonds were analysed and indicated, and these as well as other structural aspects of a cluster near the critical point discussed. In 1983 we could only manage two-tone color printing.

Percolation is so simple, you can give it to your undergraduates as a project topic. In fact way back in 1974 at UNSW Jaan Oitmaa gave it to me as an undergraduate project, and I have probably given at least a dozen different ones in turn [19]. The 3D image at right is from one of our first percolation websites [20], summarising the project I gave Nir Yefet in 1998 (Mesa and C). On the website the cluster can be rotated. Another project site relevant to the present discussion was a blob-link-backbone one, by Eduardo Warszawski, who reproduced the Stanley image and created dozens more in full color with our AViz [21] visualization code [22].

## 4 Recent developments

The projects described now, resulted from questions asked by Vladimir Privman concerning cluster structure in 3D. To answer these the two images of Figure 1 had to be further developed to elucidate a blob-link-description in 3D. Better 3D images were needed, and an interactive code was found to be desirable. We initially drew some with analglyphic AViz [21], and the procedure for this is given in detail on the AViz website. However, we wanted to move beyond analyglyphic stereo to our own (virtual) reality. Liran Sharir proposed using WebGL, and prepared an interactive website [23] where systems can be prepared and divided into clusters for easy viewing and analysis. They are then drawn in WebGL and can be rotated, analysed and shared. The 2D option provides HK cluster numbers on the images, see Figure 2 at left. The 3D one has distinct colors see Figure 2 at right. The website is accessible from smartphones and tablets, and has an Oculus 3D viewing option.

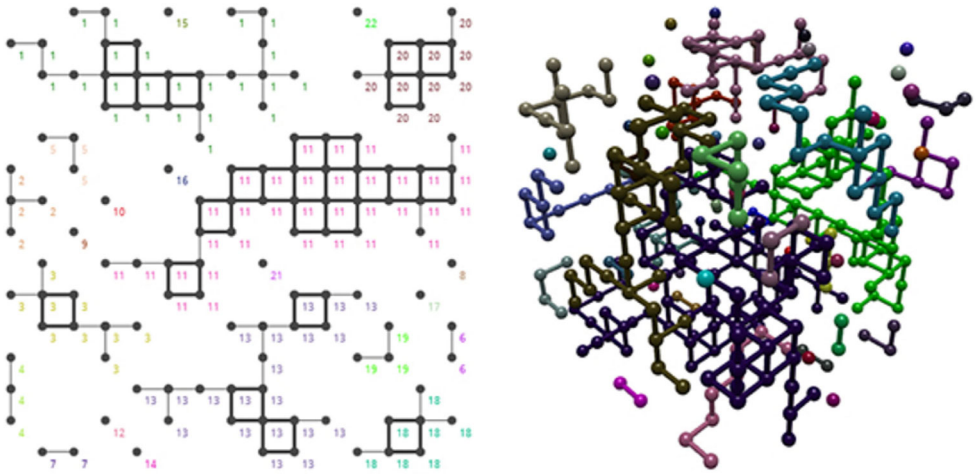

**Fig. 2.** Left: a 2D sample with explicit cluster numbers from [23]. Right: a 3D sample, where each cluster is drawn in a different color [23].

### 4.1 Hebrew material

Since percolation is so easy to explain to your husband and grandchildren, and many grandchildren prefer to learn in hebrew we needed to translate the website into hebrew, for educational use for younger users [24]. (The Technion is heavily involved in Science, Technology, Engineering and Mathematics (STEM) education, especially for our minorities. Two of JA's Computational Physics class students have just finished a hebrew website assigning Wolfgang Christian's physlets to the Israeli High School syllabus. The physlets were translated to hebrew by David Pundak of Ort Braude college.)

Shaked Elfenboim did a great translation job of the WebGL site and also built analog wall displays, with explanations based on the WebGL site. Each display has a power source and switches between boxes with different concentrations of conducting and insulating objects. The wires are hidden behind the boards, with a schematic circuit drawn on the front. The analog displays cover all three dimensions with multiple percolating and non-percolating realizations for 2D and 3D. The full 2D display is shown at left in Figure 3, and one case in detail at right. Likewise in Figure 4 the 3D display is shown, with one box in close-up in 5. Technical issues, especially in 2D, were substantial, as we had to obtain good size match between conducting and insulating objects, and exert sufficient pressure to maintain contact, but not push the sites out of place. The close-ups give some idea of the sample details. The materials used were sourced from craft shops (perspex containers) and the mechanical workshop and lecture demonstration staff of the Technion Physics Department helped in the construction.

## 5 Bootstrap percolation and other recent results

In BP sites that do not have enough neighbours (at least $m$ neighbours are needed) are removed. The culling process is a random cellular automaton. There are interesting critical phenomena and finite size effects, in these models, much studied in the mathematical community [14,15]. Details depend strongly on the lattice structure

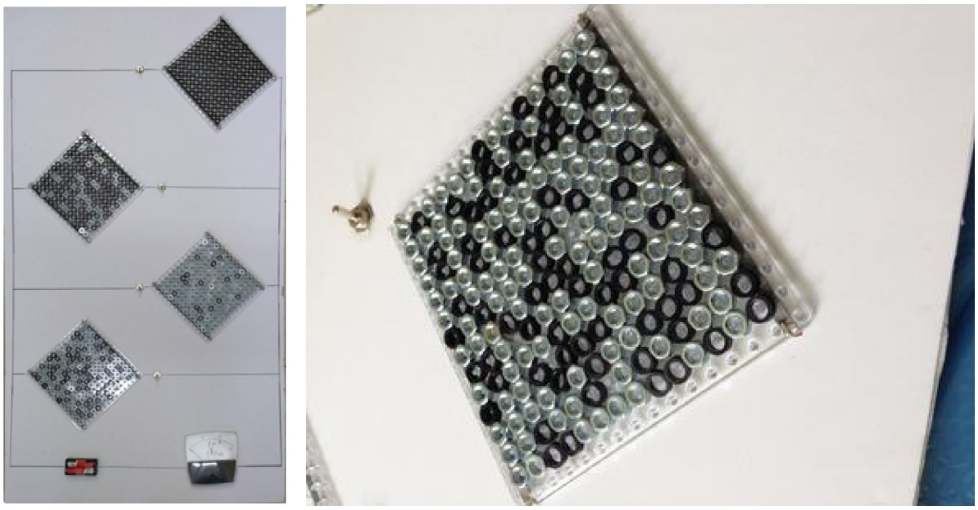

**Fig. 3.** Left: two dimensional display with 4 different concentrations. Right: a closeup of one cell, showing silver (metal conducting) and black (rubber insulating) sites with metal strips at opposite sides.

and on $m$. When $m = 1$ or 2, isolated sites and dangling bonds, respectively, are removed, with critical concentration $p_c$ unchanged. The examples in Figures 6 and 7, show the lowest $m$ values for which there is culling, but the spanning or otherwise nature in an infinite system is unchanged, the clusters merely becoming locally more compact. On the triangular lattice, $m = 3$ simply increases the threshold, as shown in Figure 8, where for an initial theshold of $p = 0.66$ (far above $p_c$ for this lattice) after many culling steps we only have spanning in one direction. On the square lattice $m = 3$ sends the threshold to 1.0, in the infinite system limit, which does not provide a very interesting final still image so is not shown.

We now discuss some condensed matter applications of bootstrap percolation. Since many condensed matter systems have strong quantum mechanical characteristics, adjoining sites usually have complicated interactions, and percolation issues become complicated. The left image of Figure 9 shows a typical concentration/temperature phase diagram for a diluted spin system with Ising symmetry, where the threshold at zero temperature is the percolation threshold. The right image of Figure 9 shows the phase diagram of ordered quadrupolar molecular hydrogen. The zero temperature threshold is near $\mathrm{p} = 0.5$, far above the typical $p_c = 0.3$ of 3D percolation.

For molecular hydrogen, although the molecules are ortho or para due to quantum mechanics the orientational ordering is purely geometic, as shown by hydrogen and deuterium having close thresholds, despite different amounts of "quantumness". In the left panel of Figure 10 a mixed (40 percent diluted), disordered state is shown. As can be see in the right panel of Figure 10 the ordered phase has perpendicular quadrupoles [26] and is known as ($Pa_3$). This immediately leads to suspicions of a bootstrap effect because ordered quadrupoles lose their orientational order if they do not have sufficient neighbouring quadrupoles to retain transmission of perpendicularity. The actual simulations, especially under dilution, with possibilities of a glass phase at moderate disorder, are somewhat complex, and thus a toy "Ising" model for this type of ordering was needed.

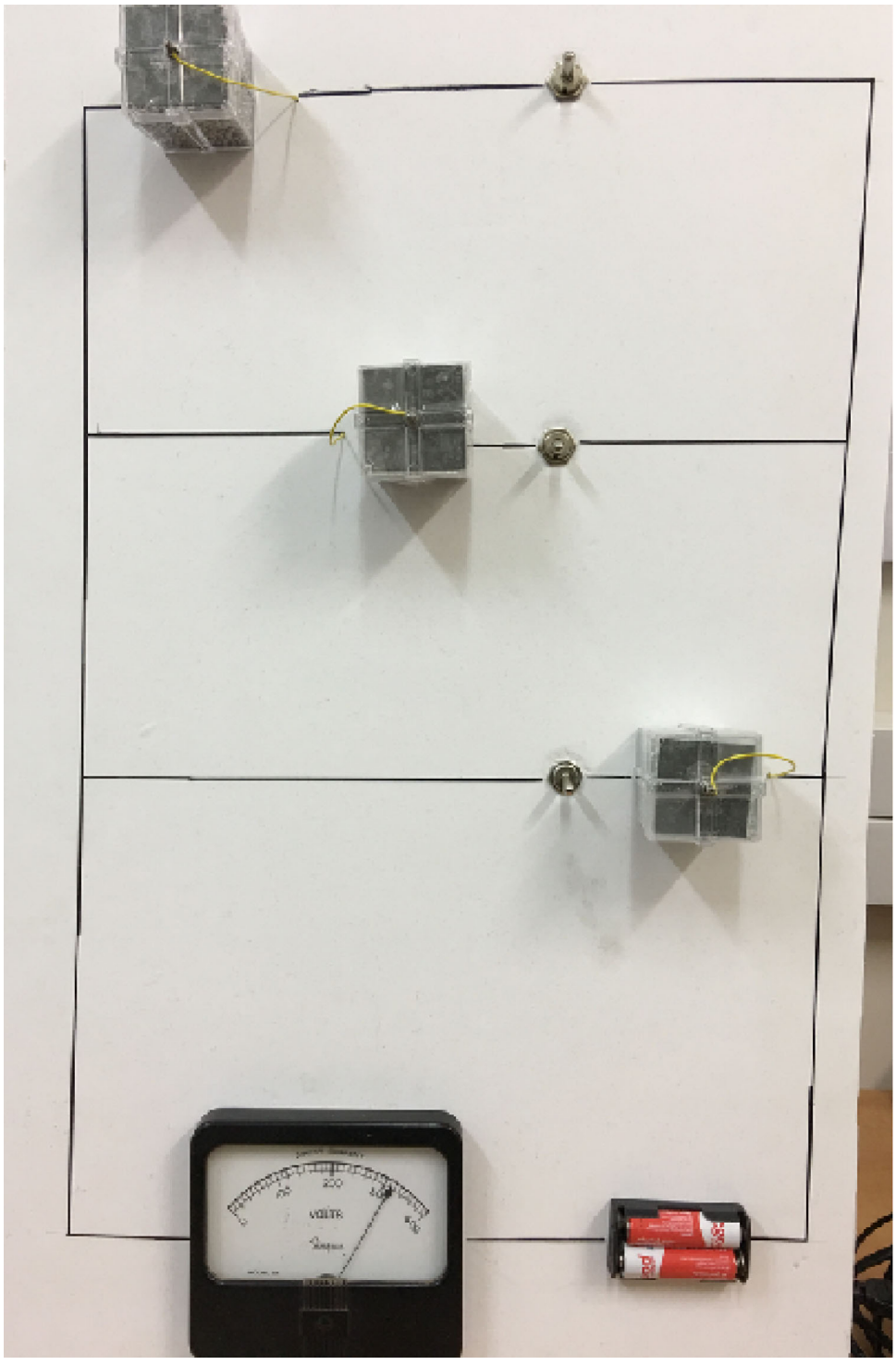


**Fig. 4.** Three-dimensional display with three different concentrations, with the switch set to bring the box full of metal balls into the circuit. Note the ammeter current reading.

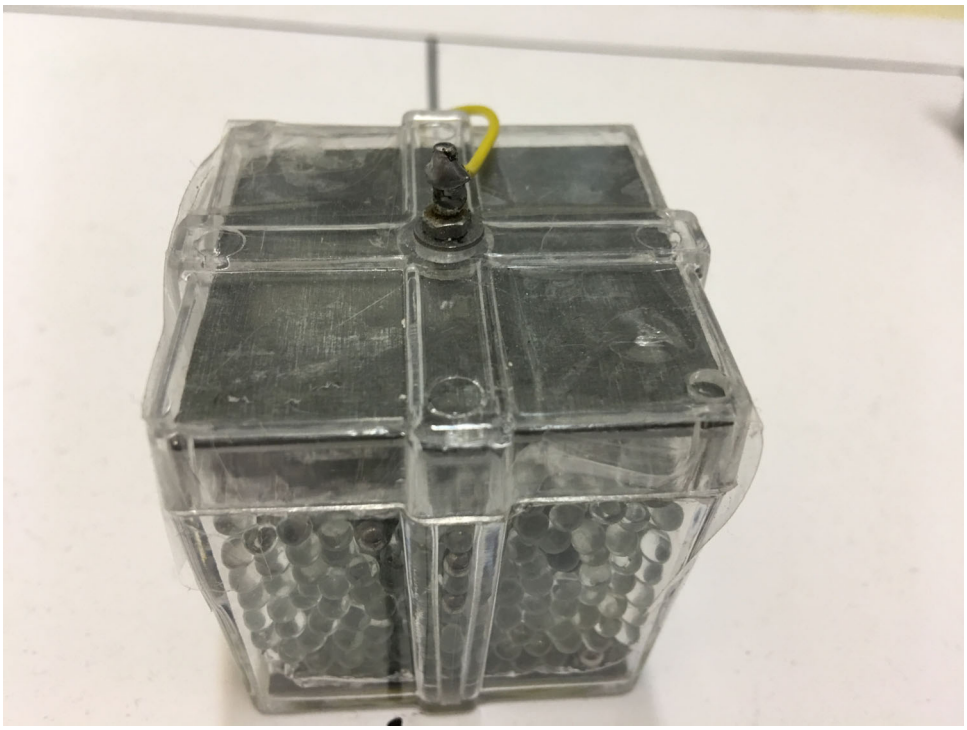

**Fig. 5.** Closeup of the central box, containing a mix of metal balls and glass beads (chemical filters), as well as top and bottom metal plates.

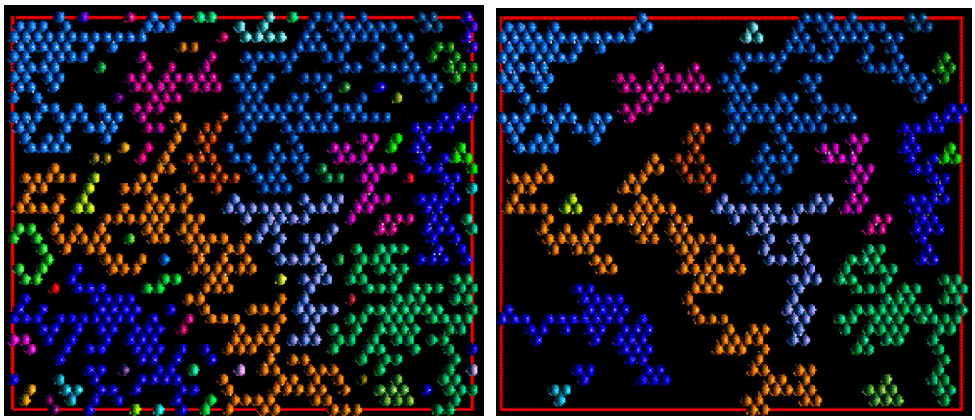

**Fig. 6.** Bootstrap percolation for the $m = 3$ case on a triangular lattice with an initial occupancy of $p = 0.51$. Left: initial occupancy. Right: final state after culling.

The 2D analog, of the solid hydrogen model is the 3 state Potts antiferromagnet on the triangular lattice (3PAFT) which also exhibits this effect. It has an interesting weak first order phase transition in its pure form. A graphical explanation the bootstrapped raising of the percolation threshold, is illustrated in Figure 11, from [4]. We observe the need for double or multiple paths of connectivity to transmit ordered groundstates.

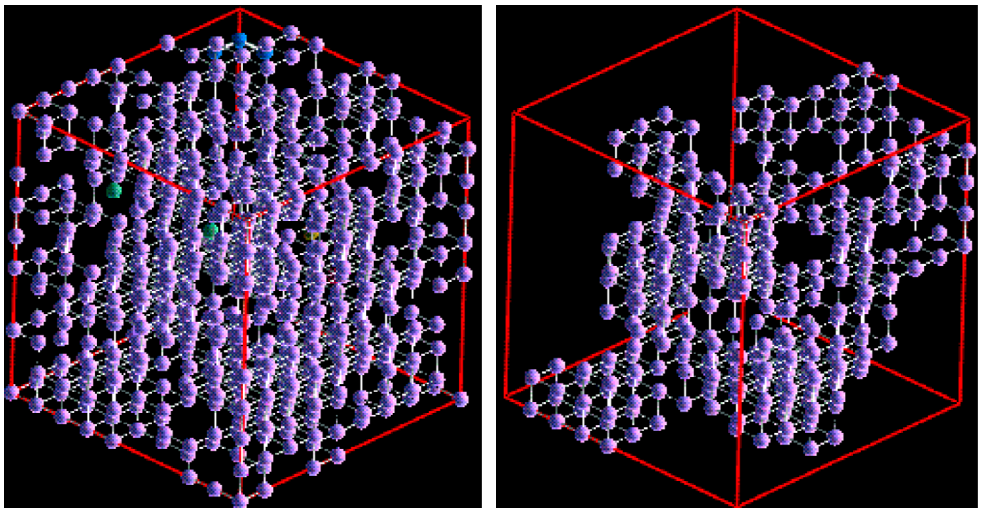

**Fig. 7.** Bootstrap percolation for the $m = 3$ case on a simple cubic lattice with an initial occupancy of $p = 0.66$. Left: initial occupancy, note the very few sites not connected to the infinite cluster in the initial state. Right: final state after culling.

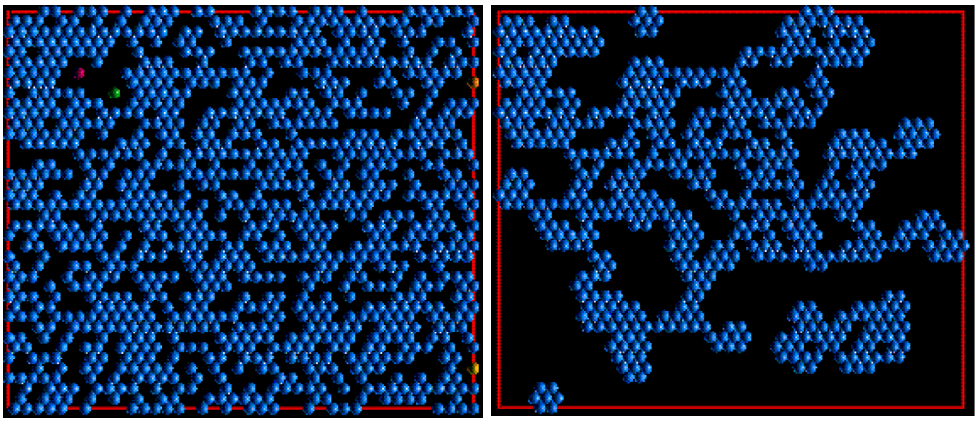

**Fig. 8.** Bootstrap percolation for the $m = 3$ case on a triangular lattice with an initial occupancy of $p = 0.66$. Left: initial occupancy, note the very few sites not connected to the infinite cluster in the initial state. Right: final state after culling.

Studying the diluted 3PAFT has the additional complication of the pure model's very weak first order transition. In fact, until simulations indicated clearly that there is a ordered state, the prevailing wisdom was that it does not have a transition at all, because Rodney Baxter proved rigorously that it cannot have a second order transition. I had to call in WJ to help understand the pure model's transition. We found [5] a weak first order transition. The dilute version analysis and crossover is still open, not to speak of searching for a glassy phase here or in the dilute quadrupole model.

Another application of BP has recently been found in a totally different system, videlicit diamond films for use in quantum computers. These are prepared by irradiating several layers in the diamond to turn them into graphite that could be etched away. This has been observed in experiments and modeled with molecular dynamics.

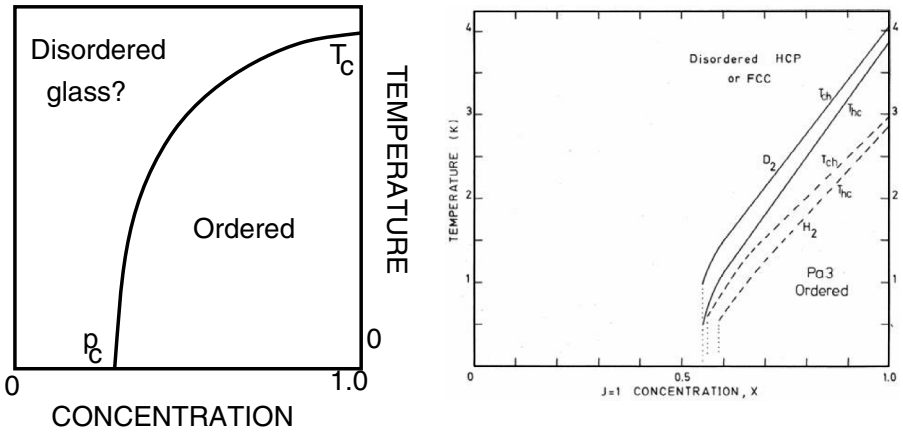


**Fig. 9.** Left: temperature/dilution phase diagram of an Ising spin symmetry model. Right: experimental phase diagram of $Pa_3$ ordered moledular hydrogen, from [27].

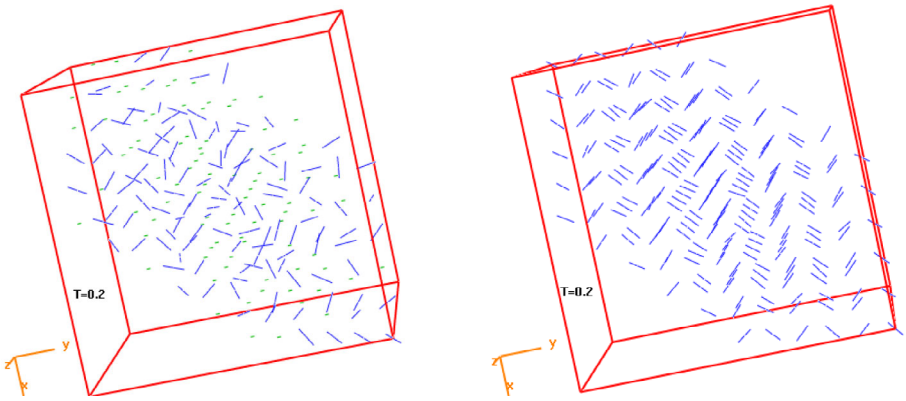


**Fig. 10.** Left: a sample of a model with 40 percent non-quadrupolar and 60 percent quadrupolar hydrogen molecules. Right: a sample of a model of $Pa_3$ ordered molecular hydrogen, both from [26].

The graphite is etchable because while carbon in the diamond structure has 4 neighbours, graphite has only 3 and is formed because irradiation weakens bonds [6,7]. When one of the 4 diamond bonds is sufficiently weakened, the threefold coordinated graphitic allotrope results. Since atoms with less than 2 close diamond neighbours are removed in the etching it can be modeled by a sequential, bootstrapping process and in Figure 12 images are presented. The final sample yields parallel (relatively) flat diamond surfaces, suitable for use in a quantum computer.

## 6 Conclusions

Percolation remains an active field, with both new applications and additional variations, many of which are also application motivated. The simple concepts entice students into the study of phase transitions, and the applications enhance understanding of complex growth and diffusion processes.

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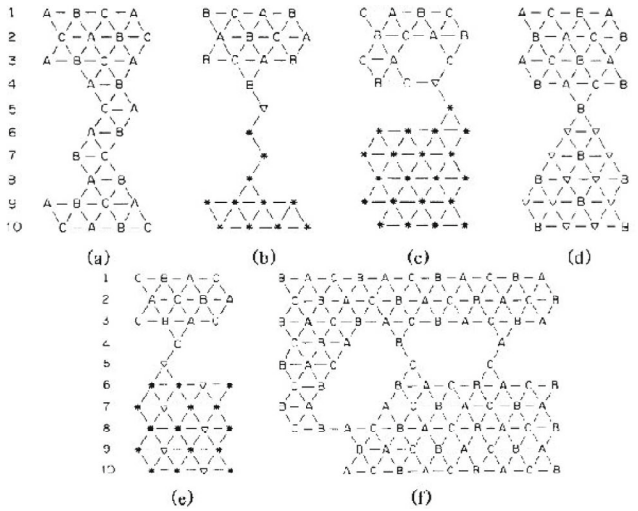


**Fig. 11.** Different diluted realizations of the 3PAFT, showing how transmission of order breaks down under site dilution, from [4]. The figure illustrates the propogation of order in a diluted 3PAFT at $T = 0$, with the three possible Potts states represented by R(ed) B(lue) and G(reen) and a site that is limited to two possibilities by an empty inverted triangle. Sites that are not determined relative to the top row are shown as asterisks.

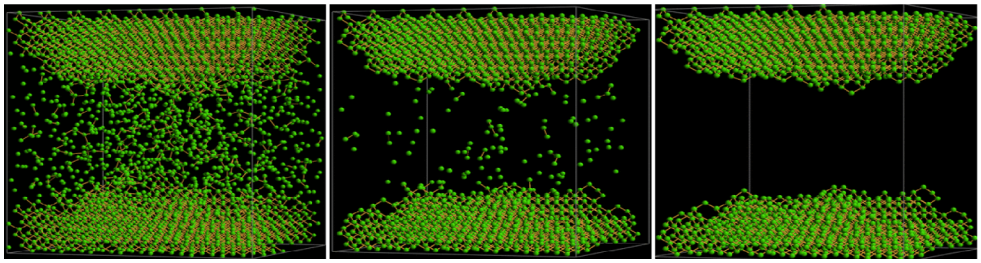

**Fig. 12.** Left: initial configuration of the diamond after irradiation from [6]. Center: after 4 rounds of culling carbon atoms with less than two close diamond neighbours. Right: final state, after 11 rounds, from [7], and its associated website.

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