Bootstrap Percolation: Visualizations and Applications

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Bootstrap percolation models describe systems as diverse as magnetic materials, fluid flow in rocks and computer storage systems. The models have a common feature of requiring not just a simple connectivity of neighbouring sites, but rather an environment of other suitably occupied sites. Different applications as well as the connection with the mathematical literature on these models is presented. Visualizations that show the compact nature of the clusters are provided.

I Introduction

In Bootstrap Percolation (BP) [1] the lattice is occupied randomly with probability p, and then all sites that do not have at least m neighbours are iteratively removed. For $m = 1$ isolated sites are removed and for $m = 2$ both isolated sites and dangling ends are removed. For $m = 3$ and above the situation becomes interesting and lattice dependent and is currently quite hot amongst probabilists. For sufficiently high m, no occupied sites remain for an infinite lattice, and the interest is in the scaling as a function of system size.

The conference talk on which this manuscript is based came about as follows: Uri Lev asked for a project topic just as Joan Adler was thinking about BP because Scott Kirpatrick's [2] new application to computer memory storage had reminded her that BP was an interesting topic. (Uri Lev's visualizations and website [3] are described in the final section of this paper.) Other recent activity, also motivated from ref [2] has included the study by Kurtsiefer [4], a student of Stauffer. Also, probabilists keep sending Joan Adler preprints that confirm, correct or extend non-rigorous results from 15 years ago. In this framework, Joan Adler suddenly realised that the carbon modelling she spends most of her time on nowadays [5] , which has been identified as percolation for more than 20 years, [6] is actually Bootstrap Percolation. In addition, BP is very Brazilian. Roberto Schonmann who was the first probabilist to do rigorous things with Bootstrap was then based in Sau Paulo. Other Brazilians who have worked on BP include: N. S. Branco and C. J. Silva [7], V. Sidovarius, R. Sanchis and F. Camis. However the main reason to select this topic is that BP accounts for three of Adler's eleven joint papers with Stauffer, and Stauffer made her write a mini-review about BP [1] some time ago.

The name "Bootstrap Percolation" was first mentioned (to our knowledge) in the literature [8] in 1981, but the idea was independently proposed earlier[9]. There are different motivations for the creation of BP models. In the Leath et al and Reiss and Pollak papers mentioned above atoms, were present with probability p, and assumed to participate in a certain ordered state, such as ferromagnetism, only if a requisite number of neighbouring atoms were also present. For some of these early realizations the related high density percolation models (only a single step in the culling process is realized) may be a more suitable description of the materials involved. Adler, Palmer and Meyer, showed in 1987 [10] that environmental effects of a bootstrap type play a crucial role in the orientational ordering process of quadrupoles in solid molecular $(ortho-H_2)_x(para-H_2)_{1-x}$ or $(para-D_2)_x(ortho-D_2)_{1-x}$. The models have connections to rigidity percolation,[11]. Time developments according to the local rules of Bootstrap Percolation can be viewed as cellular automata [12] , and there are also metastable bootstrap models, not considered further here. Models closely related to canonical BP have been proposed as descriptions of fluid flow in porous media. In these cases crack development [13] and/or advance of the fluid front [14] are assumed to be strongly dependent on the local microstructure.

II Applications of Bootstrap Percolation

We show here the importance of the bootstrap principle for several applications. Adler, Palmer and Meyer, [10] showed that environmental effects of a bootstrap type play a crucial role in the orientational ordering process of quadrupoles in solid molecular $(ortho-H_2)_x(para-H_2)_{1-x}$ or $(para-D_2)_x(ortho-D_2)_{1-x}$. Ortho hydrogen and para deuterium are quadrupolar molecules, whereas para hydrogen and or-

tho deuterium are isotropic molecules. The quadrupoles want to hold an orientational ordering called Pa3 whereby they are almost perpendicular, but when diluted by the isotropic molecules they cannot transmit the orientational ordering across the sample. They need sufficient quadrupolar neighbors to remain connected. At $T = 0$ this is a bootstrap variant, with x_c about 0.5, way above p_c for the fcc/hcp lattices. We developed a "toy" model called the 3 PAFT (three state Potts AntiFerromagnet on the Triangular lattice) to model this and got exact bounds on its x_c, by showing that transmission of order of the antiferromagnet groundstates needs a connectivity that is even slightly above the $m = 3$ bootstrap value on the triangular lattice of $p_c = 0.628$. Figures that illustrates these points were given in [10].

The fluid flow applications of Adler and Aharony [13], were made for a model that we called Diffusion Percolation which we showed could be mapped to Boostrap percolation in the infinite time limit. Fluid passed thru an environment of rock with cracks in it, and if sufficient neighbouring sites were vacant, then a site was removed. An animation of a fluid flow model which includes both soft soil and immovable hard rocks was made by Amit Kanigel [15] and can be downloaded and run to illustrate this principle.

The recent application by Kirkpatrick [2] is of a completely different nature. It relates to the failure of units in a cubic structured collection of computer memories, called a Dense Storage Array. Because it is too expensive to fix individual memory units that fail in such a system, the units are allowed to "fail in place", and it is necessary to ensure that even with a relatively high density of failed units there will still be percolation of data communications.

III Visualizations

Since the Computational Physics Group at the Technion developed animation software (AViz) for atomistic simulations it was interesting to apply this also to Bootstrap Percolation. AViz [16] enables a user to draw and animate atoms (or spins, or pores) that are identified by spatial coordinates and type and then edit the visualizations for color and other highlighting techniques. Visualization can be interactive or post computation and mpeg and other output formats can be created. The technical work on the AViz routines was done by Adham Hashibon and Geri Wagner. They selected the Qt toolkit to prepare the GUI, which is also the basis for the KDE desktop. The objects are drawn in MESA/OpenGL in a similar way to older OpenGL routines prepared in the group, but the interface is a whole lot friendlier, and extends the interactive updating possibilities. The AViz homepage [17] contains examples, sample datafiles and downloadable installation files (including rpm format for Linux Redhat 7 and source tar files for general UNIX) and a manual. Post production visualization from datafiles is also possible; this is the technique that was used to prepare the figures shown below.

Some sample visualizations are given in Figs. 1, 2 and 3, and many more can be viewed in color on the website [3]. Fig. 1 shows the the original freshly occupied lattice as well as the more compact clusters obtained after culling for the case of $m = 2$ on the square lattice. Fig. 2 shows $m = 3$ on the triangular lattice at an initial concentration of $p = 0.66$, above the usual percolation threshold of $p_c = 1/2$ for this lattice. Fig. 3 shows a three dimensional case with initial concentration of $p = 0.66$ after culling. Notice how compact the clusters are in both the latter cases. In addition to animated versions of these figures software to simulate BP and parameters for running the AViz visualizations can be downloaded from the website.

IV Exact Results and Scaling for Large Systems

This is an area of statistical physics where there has not always been total agreement between rigorous results and simulations. In some cases simulation data cannot independently confirm rigorous scaling forms, presumably because the simulations have not yet reached the asymptotic regime. For some applications, especially the geological ones, it is unclear whether the physical interest is in the thermodynamic limit for which the rigorous results are obtained, or rather in the large but finite size regime that is accessible to simulation.

Models with thresholds of $p_c = 1$ where there are no finite clusters and first order transitions, approach the thermodynamic limit in complex logarithmic ways. The first results for the models with $p_c = 1$ were obtained by Straley, [18] rigorised by van Enter [19] and then extended by Aizenman and Lebowitz, [20]. There is also an earlier proof of Frobose and Jackle.

Schonmann [21] was one of the first probabilists to work on this proving, for example, for a d dimensional hypercubic lattice that for $m \geq d + 1$ the threshold is always unity. Aernout van Enter [22] kindly prepared a list of recent rigorous advances, and these include [23] results by R. Cerf and F. Manzo, E. M. N. Cirillo, T. S. Mountford [25] and A. Holroyd [24] from the probability literature. More discussion is given at the website [26] of the conference talk on which this paper is based.

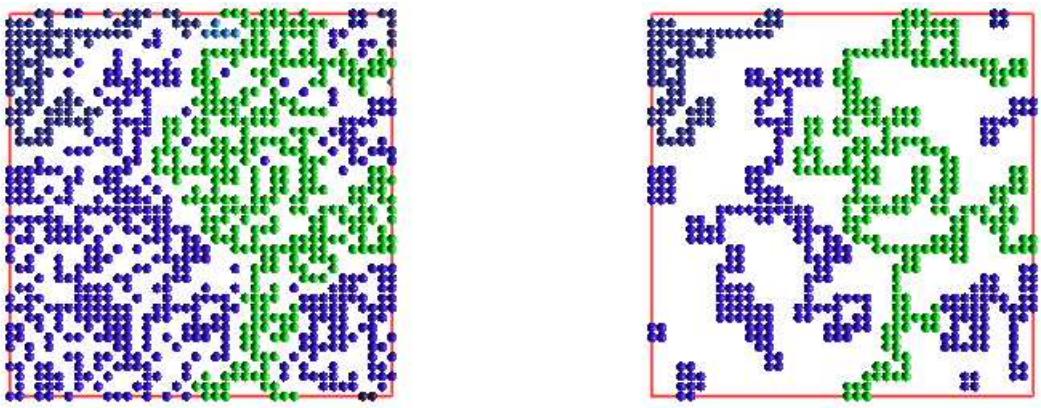

Figure 1. The original freshly occupied lattice shown on the left as well as the more compact clusters obtained after culling, on the right for the case of $m = 2$ on the square lattice, with initial concentration of $p = 0.55$. Although this concentration is below p_c for the infinite lattice this particular realization on the finite lattice does have a cluster (light grey) thats spans top to bottom.

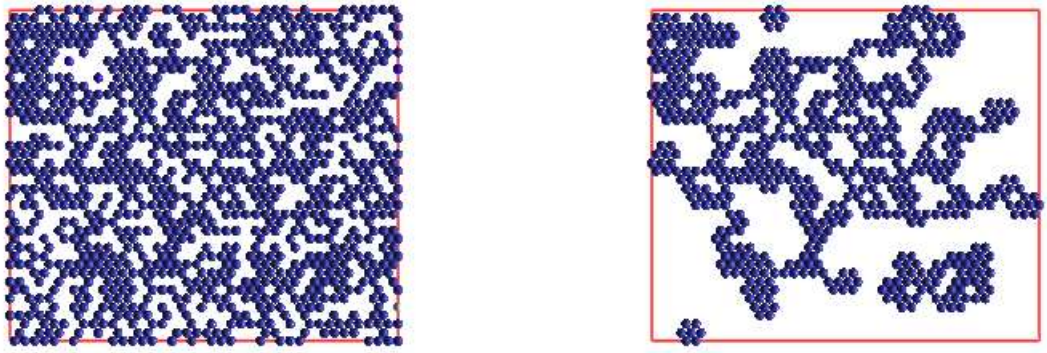

Figure 2. The initial freshly occupied lattice shown on the left for $m = 3$ on the triangular lattice at an initial concentration of $p = 0.66$, above the usual percolation threshold of $p_c = 1/2$ for this lattice. For initial occupation there is indeed an infinite cluster, but after culling there is a more compact cluster that does not percolate, as shown on the right.

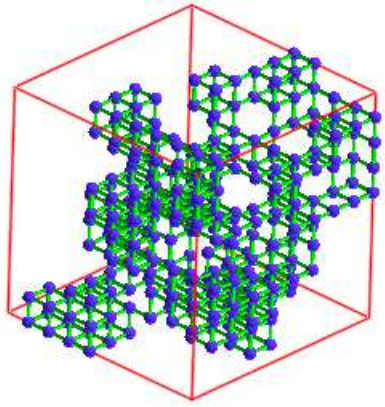

Figure 3. A three dimensional case, for $m = 3$, culled from an initial occupation of 0.66.

V Discussion

Bootstrap percolation has been an interesting system, because of the unusual scaling behaviour, interaction with mathematicians and ongoing surprises. As van Enter pointed out, "Larry Gray [27] discusses Bootstrap Percolation in his extremely critical review of Wolfram's new book, giving it as an example of a model–not mentioned in the book– which should warn you that simulations without mathematical understanding can easily mislead you." This is a very reasonable viewpoint (of course, not everyone may agree with it) and leads to the final result to be discussed here.

Returning to Dietrich Stauffer's own contributions to the topic his student, Kurtsiefer [4] has recently explored three-dimensional cubic Bootstrap models and did not find optimal agreement for one exact scaling form at $N = L^3$ sites with $L = 4544$. Stauffer [28] returned to the $m = 3$ square lattice with L above $L = 10^5$ sites, estimating that perhaps simulations would meet the Holroyd scaling result at $L = 10^{20}$ or 10^{60}, many orders of magnitude above the number of atoms in real materials. By assuming corrections to scaling proportional to a small power of $\log L$, he fitted (encouraged by M. Sahimi) his data to $(1-p_c(L)) \cdot \ln(L) = 0.548311 - 0.45/(\ln L)^{0.2}$ to force agreement with Holroyd's prediction 0.548311; see Fig. 4. Other asymptotic

predictions could also be fitted to the same data.

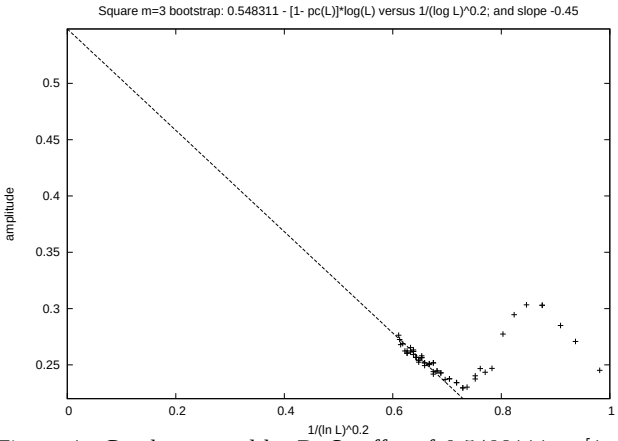

Figure 4. Graph prepared by D. Stauffer of $0.5483111 - [1 - p_c(L)] \cdot \log L$ versus $1/(\log L)^{0.2}$ and the slope of -0.45 for comparison.

If as physicists or material scientists we wish to study real materials then does one take the infinite system limit or stop at a few orders of magnitude above Avogadro's number For the fluid flow applications there may be tens of thousands of cracks, but possibly not an infinite number. Kirkpatricks's [2] dense storage arrays consist of thousands of units and so it is finite results rather than the thermodynamic linit that is of interest for this realistic application of BP.

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