Rigorous confidence intervals for critical probabilities

Oliver Riordan
Department of Pure Mathematics and Mathematical Statistics, Cambridge CB3 0WB, UK.

Mark Walters
Peterhouse, Cambridge, CB2 1RD, UK

We use the method of Balister, Bollobás and Walters to give rigorous 99.9999% confidence intervals for the critical probabilities for site and bond percolation on the 11 Archimedean lattices. In our computer calculations, the emphasis is on simplicity and ease of verification, rather than obtaining the best possible results. Nevertheless, we obtain intervals of width at most 0.0005 in all cases.

I. INTRODUCTION

In this paper we study site and bond percolation on planar lattices, in particular the Archimedean lattices, in which all faces are regular polygons and all vertices are equivalent. The 11 Archimedean lattices are shown in Figure 1, labelled with the notation of Grünbaum and Shephard: each lattice is represented by a sequence listing the numbers of sides of the faces meeting at a vertex, in cyclic order around that vertex.

In site percolation on a graph Λ, each vertex, or site, of Λ is assigned a state, open or closed. In independent site percolation the states of the sites are independent, and each site is open with a certain probability p. The definitions for bond percolation are similar, except that the edges, or bonds, of Λ that are assigned states. We shall write P_p for the corresponding probability measure, suppressing the dependence on Λ and on whether it is site or bond percolation that we consider.

The basic question of percolation theory is 'when is there an infinite open cluster', i.e., an infinite subgraph of Λ all of whose sites (for site percolation) or bonds (for bond percolation) are open. It is not hard to see that there is a certain 'critical probability' p_c, such that for p < p_c there is never (i.e., with probability 0) an infinite open cluster, while for p > p_c there always is. For this and other basic facts about percolation, see Grimmett, or Bollobás and Riordan, for example. When we wish to specify the lattice, and whether it is site or bond percolation that we are considering, then we write P^{c} or P^{b}.

The exact value of p_c is known in rather few cases: in 1980, Kesten proved that p_c(Z^2) = 1/2, where Z^2 is the square lattice. Shortly afterwards, he proved that p_c = 1/2 also holds for site percolation on the triangular lattice T. Later, Wierman used his 'substitution' method to give rigorous proofs of the values p_c(T) = 2 sin(π/18) and p_c(H) = 1 - 2 sin(π/18) for bond percolation on the triangular and hexagonal lattices respectively; these values had been obtained heuristically much earlier by Sykes and Essam. There are two further values that may be easily derived from these: the (3, 6, 3, 6) or Kagomé lattice K is the line graph of the hexagonal lattice, so p_c(K) = p_c(H) = 1 - 2 sin(π/18). Also, the (3, 12^2) or extended Kagomé lattice K^+ is the line graph of the lattice H_2 obtained by subdividing each bond of H exactly once, so

p^{c}_c(K^+) = p^{b}_c(H_2) = \sqrt{p^{b}_c(H)} = (1 - 2 sin(\pi/18))^{1/2}.

These are the only critical probabilities known for Archimedean lattices. Indeed, it may be that the exact values of the other critical probabilities associated to the Archimedean lattices will never be known; they may sim-

FIG. 1: The 11 Archimedean lattices

*Royal Society research fellow
ply be numbers that have no simpler descriptions than their definitions as critical probabilities.

Given the dearth of exact results, it is not surprising that much effort has been put into the estimation of critical probabilities. Almost all results in this area are of one of two types: (1) rigorous upper and/or lower bounds, and (2) heuristic estimates based on computer calculations. There are also a few heuristic derivations of conjectured exact results; we shall return to this briefly in Section V. Examples of (1) are the bounds obtained by Wierman (37, 38, 39) (see also Parviainen and Wierman 25) using his substitution method. Even with considerable work on efficient algorithms and extensive computer calculations, it seems to be hard to obtain narrow intervals between rigorous upper and lower bounds: of the intervals listed in 25, two have width a little under 0.01, but many have width 0.1 or even 0.2.

There are a small number of recent, more accurate, rigorous results, including an interval of width 0.00135 and 0.0046 for site percolation on the (3, 122) and Kagomé lattices obtained by May and Wierman 20.

Turning to (2), there are so many papers on this topic, going back to the 1960s, that it is impossible to attempt even a representative list. Let us mention a couple of examples, however: for p_c(Z^2), Reynolds, Stanley and Klein 20 reported the impressively accurate non-rigorous estimate 0.5931 ± 0.0006 already in 1980. In 1986, Ziff and Sapoval 15 gave the exceedingly accurate estimate of 0.592745(2). In 1990 Yonezawa, Sakamoto and Hori 41 gave estimates for several Archimedean lattices, with error terms a little over 10^{-4}. More recently, many very precise estimates have been given using quite sophisticated methods, for example by Suding and Ziff 32, Newman and Ziff 22, 23 and Parviainen 24. It is very likely that these estimates are extremely accurate; errors of about ±3×10^{-6} are claimed in 32, and even smaller errors in 22, 23, 24. However, these estimates come with no mathematical guarantees, and it is hard to be sure how accurate they really are. Although theoretical error analysis is sometimes given (see Ziff and Newman 44, for example), this is certainly non-rigorous. Even assuming unproved results about the scaling limits of planar percolation models gives only the asymptotic behaviour of these errors; it does not allow us to say anything about the relationship between a finite number of data points and the true value of p_c. Also, there is disagreement about even the asymptotic form of the errors in some cases (see Parviainen 24), and there are several instances where earlier estimates have been contradicted by later ones.

Surprisingly, it is possible to give a result intermediate in nature between a rigorous bound and a heuristic estimate: one can prove that a certain (random) procedure generates a bound that is correct with probability at least 99.9999%, say; in other words, one can rigorously generate confidence intervals for critical probabilities. Such intervals are typically much narrower than the 100% bounds, although nothing like as narrow as the (claimed) uncertainties for heuristic estimates. Results of this kind were first proved by Bollobás and Stacey 7 in the context of oriented percolation, and then by Balister, Bollobás and Walters 8 in the context of (unoriented) continuum percolation. Here we use the method of the latter paper, which applies essentially ‘as is’ to percolation on 2-dimensional lattices, to obtain confidence intervals for the site and bond percolation critical probabilities for all 11 Archimedean lattices. Indeed such an interval for site percolation on the square lattice was given in 8, namely [0.5919, 0.5935] (with a lower confidence of 99.99%). Here, with greater computational effort, we obtain narrower intervals.

II. METHOD

A. The mathematics

The method of Balister, Bollobás and Walters 8 is based on a simple application of the concept of 1-independent percolation (also known as 1-dependent percolation). A bond percolation measure on a graph Λ, i.e., a measure on assignments of states to the bonds of Λ, is 1-independent if, whenever S and T are sets of bonds such that the graph distance from S to T is at least 1, the states of the bonds in S are independent from the states of the bonds in T. In other words, roughly speaking, the states of vertex-disjoint bonds are independent. Such measures arise naturally in percolation theory, in particular in static renormalization arguments (see Section 7.4 of Grimmett 1), and have been considered by many authors. Although the assumption of 1-independence is weaker than independence, it is strong enough to ensure percolation if the individual bonds are open with sufficiently high probability, as shown by the following lemma of Balister, Bollobás and Walters 8.

Lemma 1. Let P be a 1-independent bond percolation measure on Z^2 in which each bond is open with probability at least p_0 = 0.8639. Then the probability that the origin lies in an infinite open cluster is positive.

If the value of p_0 is not important, then a weak form of Lemma 1 (with p_0 replaced by some constant smaller than 1) is more or less immediate from first principles (see Bollobás and Riordan 1, for example). It also follows from the very general results of Liggett, Schonmann and Stacey 18 comparing 1- (or k-) independent measures on general graphs with product measures.

Starting from independent site or bond percolation on a lattice Λ ⊂ R^2, there is a natural way to obtain a 1-independent bond percolation measure P on the square lattice Z^2: given a ‘scale parameter’ s > 0, partition R^2 into disjoint s by s squares S_{uv}, v ∈ Z^2. For each bond e of Z^2 let R_e be the corresponding rectangle, so if e = uv then R_e = S_u ∪ S_v. Let E_e be some event that depends only on the states of the sites or bonds of Λ that lie within R_e, and take the bond e of Z^2 to be open with
respect to \( \tilde{P} \) if and only if \( E_e \) holds. Since the rectangles corresponding to vertex-disjoint bonds of \( \mathbb{Z}^2 \) are disjoint, this defines a 1-independent measure \( \tilde{P} \).

Suppose that the squares \( S_e \) and events \( E_e \) are chosen so that the following condition holds:

whenever there is an infinite path \( v_0v_1v_2\ldots \) such that \( E_e \) holds for each \( e_i = v_iv_{i+1} \), there is an infinite open cluster in the original lattice and then \( p \) is chosen so that

\[
\tilde{P}_p(E_e) \geq 0.8639 \text{ for every bond } e \text{ of } \mathbb{Z}^2.
\]  

(2)

Then Lemma 1 implies that \( p_c \leq p \). Indeed, we have already noted that \( \tilde{P} \) is 1-independent, so from (2) and Lemma 1 there is a positive probability that the origin is in an infinite \( \tilde{P} \)-open cluster. But then (as \( \mathbb{Z}^2 \) is locally finite) there is an infinite \( \tilde{P} \)-open path starting at the origin, so from (1) there is an infinite open cluster in the original percolation with positive probability. Hence \( p \geq p_c \) as required. This type of argument, but in a qualitative form where the value of \( p_0 \) is not important, provides one of the many easy ways of deducing Kesten’s \( p_c^{\ast} (\mathbb{Z}^2) = 1/2 \) result from a suitable ‘sharp-threshold’ result; see Bollobás and Riordan [4, 6].

Here we follow Balister, Bollobás and Walters [8] in our choice for the event \( E_e \). For \( e \in \mathbb{Z}^2 \), let \( \Lambda_e \) denote the subgraph of \( \Lambda \) induced by the sites in \( S_e \). For each bond \( e = uv \) of \( \mathbb{Z}^2 \), let \( \Lambda_e \) by the subgraph of \( \Lambda \) induced by the sites in \( R_e = S_u \cup S_v \). Let \( E_e \) be the event that each of \( \Lambda_u \) and \( \Lambda_v \) contains a unique largest open cluster with these clusters part of the same open cluster in \( \Lambda_e \). Here ‘largest’ simply means containing the most sites. Note that \( E_e \) does depend only on the states of bonds or sites within \( R_e \), so we do obtain a 1-independent measure. Also, it is immediate that (1) is satisfied.

To obtain an upper bound on \( p_c \), it remains only to find a pair \( (s,p) \) for which (2) is satisfied. Note that it will suffice to check condition (2) for (usually) one or (occasionally) two bonds \( e \) of \( \mathbb{Z}^2 \): without changing the graph structure, we shall redraw all our lattices \( \Lambda \) so that the vertex set is a subset of \( \mathbb{Z}^2 \), and so that horizontal and vertical translations through some small integer \( C \) act as isomorphisms of \( \Lambda \). For \( u = (a,b) \), \( a,b \in \mathbb{Z} \), we shall take

\[
S_u = \{(x,y) : sa \leq x < s(a+1), sb \leq y < s(b+1)\},
\]

where \( s \) is a ‘scale’ parameter with \( C \) dividing \( s \). Thus all squares \( S_u \) are equivalent with respect to the lattice. Furthermore, for the lattices with an axis of symmetry, our new representation will have the line \( x = y \) as an axis of symmetry. This ensures that all rectangles \( R_e \) are equivalent, so \( \tilde{P}_p(E_e) = \tilde{P}_p(E_f) \) for all \( e, f \). When there is no axis of symmetry, we have to consider one rectangle with each orientation.

So far, we have only discussed upper bounds; this is because we can obtain lower bounds by bounding the critical probability for a related lattice from above. Indeed, given a planar lattice \( \Lambda \), let \( \Lambda^\ast \) be the usual planar dual of \( \Lambda \), with one site for each face of \( \Lambda \), and a bond \( e^\ast \) for each bond \( e \), joining the two sites of \( \Lambda^\ast \) corresponding to the faces in which \( e \) lies. It is ‘well known’ that

\[
\tilde{P}_p^c(\Lambda) + \tilde{P}_p^b(\Lambda^\ast) = 1.
\]  

(3)

Thus, to bound \( p_c(\Lambda) \) from below we may bound \( p_c^b(\Lambda^\ast) \) from above.

Note that while (3) is widely assumed to be true in great generality, it has only been proved under certain symmetry assumptions. Under very general conditions, the upper bound \( p_c^b(\Lambda) + p_c^b(\Lambda^\ast) \leq 1 \) follows immediately from Menshikov’s Theorem [21]. For the lower bound, one shows that it is not possible to have bond percolation in \( \Lambda \) at a parameter \( p \) and also bond percolation in \( \Lambda^\ast \) at parameter \( 1 - p \). For lattices (doubly periodic, locally finite planar graphs) with rotational symmetry of some order \( k \geq 4 \), there is a simple proof of the lower bound due to Zhang; see Lemma 11.12 of Grimmett [9], where this argument is presented for \( \mathbb{Z}^2 \). Recently, Bollobás and Riordan [4, 6] have pointed out that this argument can be easily adapted to lattices with rotational symmetry of any order \( k \geq 2 \). This is important here: all 11 Archimedean lattices have such rotational symmetry, but two, the lattices \((3^2, 4, 3, 4)\) and \((3^3, 4^2)\), do not have rotational symmetry of higher order. Even more recently, Sheffield [29] has given a much more complicated argument that proves (3) for lattices without further symmetry assumptions.

For site percolation, let \( \Lambda^\ast \) be the (in general non-planar) graph obtained from \( \Lambda \) by adding a bond between any two sites in the same face of \( \Lambda \); we shall refer to \( \Lambda^\ast \) as the site dual of \( \Lambda \). One has

\[
p_c^s(\Lambda) + p_c^s(\Lambda^\ast) = 1;
\]

the comments above about symmetry assumptions apply in this case also.

### B. The statistics

For sufficiently small scale parameters \( s \), it is possible to find a \( p \) for which (2) holds by enumerating all possibilities for which sites/bonds in \( R_e \) are open, and so writing \( \tilde{P}_p(R_e) \) as a polynomial in \( p \). Needless to say, this is impractical and gives poor results in practice. The key idea of Balister, Bollobás and Walters [8] is to use a statistical approach, obtaining confidence intervals with precisely calculated error probabilities instead of 100% upper bounds. Indeed, suppose that we have a random procedure \( A \) for generating a pair \((s, A, p_A)\), and that one can prove that, with probability at least 99.9999%, the random pair produced is one for which (2) holds. Then \( (-\infty, p_A) \) is (a random, as always) one-sided 99.9999% confidence interval for \( p_c \) (see below). Such a procedure \( A \) is very easy to define; again, we follow [8], with one small modification (and with different numbers).
Suppose that we have somehow ‘guessed’ values of the scale parameter $s$ and percolation parameter $p$ for which we expect that $P_p(E_c)$ is somewhat larger than 0.8639. We then generate $N = 400$ random simulations of the configuration within $R_n$, and count the number $m$ of them in which $E_c$ holds. If $P_p(E_c) = \pi$, then $m$ has a binomial $\text{Bi}(N, \pi)$ distribution with parameters $N$ and $\pi$. In particular, if $\pi < 0.8639$, then

$$P(m \geq 378) \leq P(\text{Bi}(400, 0.8639) \geq 378) = 1.1489 \cdots \times 10^{-7} < 10^{-6}/6.$$ 

If our simulation does give $m \geq 378$, we can thus assert with very high confidence that $\pi \geq 0.8639$, i.e., that (2) does hold, which, as noted above, implies $p_c \leq p$.

This is the heart of the method of Balister, Bollobás and Walters [8] (and also of the related method of Bollobás and Stacey [2]): no matter how we arrive at our ‘guess’ for $s$ and $p$, provided we only perform one ‘final’ simulation, the simple inequality above shows that the probability that we assert an incorrect upper bound for $p_c$ is at most $10^{-6}/6$. Note that we may be unlucky: if $m < 378$, then we can assert only the trivial upper bound 1. In terms of the description above, our random procedure returns the guessed values $(s, p)$ if $m \geq 378$, and the trivial pair $(s, 1)$ otherwise. Note that we have no bound on the probability that we get 1 as an upper bound, but this does not matter for the argument that $(-\infty, p_A]$ is a 99.9999% confidence interval. Of course, to obtain useful results, we want to be reasonably sure that we will have $m \geq 378$, and this is where the careful choice of parameters comes in.

Here we modify the method very slightly: the choice of the number 378 gives us individual error probabilities that are smaller than $10^{-6}/6$. Hence, we can perform up to three different runs with different parameters $s$ and $p$ (which may depend on the results of previous runs), and choose the best bound given by a successful run. It is still true that each run has at most a probability $10^{-6}/6$ of producing an incorrect bound, so the probability that our final bound is incorrect is at most $10^{-6}/2$. Bearing in mind that the same applies to the lower bounds (realised as upper bounds on a dual critical probability), we still obtain 99.9999% confidence intervals.

A small side note: since the lattice $(3^4, 6)$ does not have an axis of symmetry, we ran our method in two directions, horizontally and vertically. This means that we wanted the individual error probability to be smaller than $10^{-6}/12$ which was satisfied by requiring at least 379 successes in this case.

There are two advantages to this method: it turns out to be slightly more efficient (based on heuristic calculations). Bearing in mind that we can stop after one successful run, we can perform three runs each of which has a 90% chance of succeeding, say, more quickly than one run for the same $p$ but a larger $s$ that has 99.9% chance of succeeding. Secondly, if we are not very confident of our guesses, after a failed first run we can choose more conservative parameters for the second and third runs (for example, keeping $p$ fixed but increasing $s$), to be very sure of obtaining reasonable bounds in the end.

C. Random number generation

So far, we have assumed the availability of a suitable source of random numbers. In practice, one usually uses a pseudo-random number generator. This introduces a possible source of error: it could be that there is some pattern in the output of the generator that affects the results of the simulations. To minimize the likelihood of this we used the well known and well trusted MT19937 "Mersenne Twister" generator developed by Matsumoto and Nishimura [19], as updated in 2002. See their website [1] for the source code and related literature.

It would be very easy to modify our program to use other random number generators, or even a hardware generator.

The selection of a random number generator for simulations is often glossed over; here we emphasize this as it is important for our results: the only assumption in our results (that our procedure produces 99.9999% confidence intervals for $p_c$) is that the random numbers used in the simulation may be treated as genuinely random.

D. Choice of parameters

In this subsection we outline the purely heuristic arguments we used to choose suitable parameters for running our final statistical tests. The correctness of the results does not depend on the correctness of these arguments. For this reason we allow ourselves to use consequences of the very widely believed but, except for one lattice, unproved conformal invariance conjecture. This conjecture of Aizenman and Langlands, Pouliot and Saint-Aubin [13] states (among other things) that, for any planar lattice, after a suitable affine transformation, the limiting crossing probabilities for large regions are invariant under conformal mappings, and, more precisely, are given by Cardy’s formula [8]. For more details see Bollobás and Riordan [1], for example. As shown by Smirnov and Werner [31], building on work of Schramm [27] and Lawler, Schramm and Werner [14, 15, 16, 17], this conjecture, if true, enables the values of certain ‘critical exponents’ to be calculated. Note that the conjecture has been proved, by Smirnov [30], only for site percolation on the triangular lattice; for all other lattices it is still open.

Fixing the percolation model under consideration, i.e., fixing the lattice $\Lambda$, and considering either bond or site percolation throughout, let $p_c$ be the appropriate critical probability, and set

$$f(s, p) = P_p(E_c)$$
for one fixed bond $e$ of $\mathbb{Z}^2$, noting that the definition of the squares $S_a$ and hence of the event $E_e$ depends on our scale parameter $s$. It is not hard to convince oneself that $f(s, p_c)$ tends to some constant $0 < a < 1$ as $s \to \infty$, although this does not obviously follow formally from the conformal invariance conjecture.

Turning to the $p$-dependence of $f(s, p)$, it is natural to guess that for fixed $s$, for $p$ not too far from $p_c$, the function $f(s, p)$ will roughly satisfy the differential equation

$$\frac{d}{dp} f(s, p) = C(s) f(s, p)(1 - f(s, p)),$$

where $C(s)$ is a constant depending on $s$ (and on the lattice). For one thing, $f(s, p)$ should decay exponentially, and approach 1 exponentially, as $p$ moves away from $p_c$. Also, by the Margulis-Russo formula, $\frac{d}{dp} f(s, p)$ is exactly the expected number of sites/bonds that are pivotal for the event $E_e$, i.e., such that changing the state of this site/bond from closed to open or vice versa alters whether $E_e$ holds. If a site (say) $v$ is pivotal, then $E_e$ must hold in the configuration with $v$ open, and not hold with $v$ closed, so it is reasonable to guess that for fixed $s$ and a fixed site $v$, the probability that $v$ is pivotal will be roughly proportional to $P(E_e)(1 - P(E_e))$.

Up to a constant factor, $C(s)$ above is just $s^2$ times the probability that a ‘typical’ site (or bond) $v$ is pivotal for $E_e$ at $p = p_c$. Roughly speaking, $v$ is pivotal if and only if, when $v$ is open, two open clusters of (linear) scale $s$ are joined which, if $v$ is closed, are separated by a path of linear scale $s$. Hence, the probability that $v$ is pivotal should scale as $s^{-\alpha_4}$, where $\alpha$ is the ‘multi-chromatic 4-arm exponent’. Roughly speaking, $\alpha_4$ is defined as the scaling exponent of the probability that there are four disjoint paths $P_1, P_2, P_3, P_4$ from $v$ (or from ‘near’ $v$) to points at distance $s$ from $v$, with $P_1$ and $P_3$ open, $P_2$ and $P_4$ closed, with the endpoints of the $P_i$ appearing in cyclic order. Assuming conformal invariance, from [31] we have $\alpha_4 = (4^2 - 1)/12 = 5/4$, so we expect $C(s)$ to scale as $s^{2 - 5/4} = s^{3/4}$.

Putting the above together, it is reasonable to expect the function $f(s, p)$ to have approximately the form

$$\frac{1}{1 + \exp(a - bs^{3/4}(p - p_c))},$$

for some constants $a$ and $b > 0$ that depend on the lattice. Our procedure for choosing the final parameters $(s, p)$ to use is as follows: first, numerically estimate $f(s, p)$ for a fixed small value $s_0$ of $s$ (typically 72) and various values of $p$. Then fit the data with the function above to give a rough estimate of $a$ and $b$. Then calculate values $p_{1/3}, p_{2/3}$ of $p$ at which the formula predicts $f(s_0, p_{1/3}) = 1/3$ and $f(s_0, p_{2/3}) = 2/3$. Next, run more extensive simulations to estimate $f(s_0, p_{1/3})$, and use these two datapoints to calculate better estimates of $a$ and $b$. The reason for this step is that we do not expect [4] to give a very accurate description of the shape of the curve $f(s, p)$ with $s$ fixed and $p$ varying, particularly when $p$ is far from $p_c$, so we wish to extrapolate from consistently chosen points on this curve.

Finally, we aim to choose a (large) $s$ and a $p$ close to $p_c$ such that $f(s, p)$ is approximately 0.957; this is because $P(Bi(400, 0.957) \geq 378)$ is close to 90%, so with these parameters we have a good enough chance of obtaining a valid bound, bearing in mind that we can perform three separate runs. Extrapolating [4] this far does not give very good results; experimentally, when [4] is about 0.945, or a little less, the true value of $f(s, p)$ is large enough. Of course, the larger $s$ is, the closer $p$ can be taken to $p_c$. The exact values of $s$ and $p$ were chosen based on the amount of computer time available, and so that we obtained intervals of width at most 0.0005 in all cases.

### III. Computations and Results

Although our final results are confidence intervals, we are aiming for rigorous confidence intervals, i.e., we must prove that, for each lattice, our procedure has probability at least 99.9999% of producing an interval containing the true value (assuming the random number generator we used is well behaved). The main practical consequence of this is that we must ensure that we evaluate $P_p(E_e)$ for rectangles $R_e$ that fit together exactly in the manner required for the argument in Subsection II.A.

The first step is to transform each lattice so that translations through some small constant $C$ in the $x$- and $y$-directions act as isomorphisms. Such a representation of the lattice $(4, 8^2)$ with $C = 8$ is shown on the left of Figure 2 in this drawing, the vertex set consists of all points $(x, y) \in \mathbb{Z}^2$ with $x + y$ odd (for some of the lattices we use $x + y$ even). The white central portion of the figure shows a square region $S_u$ with scale parameter $s = 8$. It is this drawing of the lattice that we consider when defining $S_u, R_e$ and $E_e$.

Note that $s$ must be a multiple of $C$, so that all squares $S_u$ induce isomorphic subgraphs of the lattice. For the lattices with mirror symmetry (all except for $(3^4, 6)$ and its bond- and site- duals), we choose a representation with the line $x = y$ or $x = -y$ as an axis of symmetry; a rectangle $R_e$ corresponding to a horizontal bond $e$ may be mapped into a rectangle $R_f$ corresponding to a vertical bond by a reflection in either of these lines, so this ensures that all rectangles $R_e$ induce isomorphic subgraphs of $\Lambda$; thus our program need only evaluate $P_p(E_e)$ for one fixed (horizontal) bond of $\mathbb{Z}^2$. For the lattices without such symmetry, we run the same program on two drawings of the lattice, related by reflection in the line $x = y$; the horizontal rectangle considered for the second drawing corresponds to a vertical one in the first.

Most of the representations we use are modifications of those shown in Figure 3 of Suding and Ziff [52], most of which have a horizontal axis of mirror symmetry. Since we want a diagonal axis here, we have rotated may of the representations by 45 degrees, obtaining a graph on
points in $\mathbb{Z}^2$ with $x+y$ even. Our representations for all 11 Archimedean lattices $\Lambda$ and their planar duals $\Lambda^\star$ are shown in the appendix. We have omitted any lattice for which the critical probability is known exactly. (In each case the site dual $\Lambda^\times$ is represented in the same way as $\Lambda$, but with additional bonds added to every face.)

For those lattices represented with vertices in $\mathbb{Z}^2$ with $x+y$ even, it is computationally more efficient to modify the representation to make it more compact, by mapping $(x, y)$ to $([x/2], y)$, say. An example for the lattice $(4, 8^2)$ is shown on the right of Figure 2. Note that an $s/r$ by $s$ rectangle in the compact form corresponds to an $s$ by $s$ square in the original, where $1/r = 1/2$ is the ratio by which we have squashed the lattice when compactifying it. In the program files, this is stored as the field RATIO for each lattice; this squashing is undone in the print Lattice routines.

The program perc.c, available from our website [2] reads in the lattice, assigns states to the sites or bonds randomly, and then finds the largest open clusters in the left- and right- halves $\Lambda_u$ and $\Lambda_v$ of $\Lambda_v$, the subgraph of $\Lambda$ induced by the sites in $R_v$. (In fact, to avoid using too much memory, these two processes are done concurrently, see below for details.) Finally, it tests whether these open clusters are joined in $\Lambda_v$. The open clusters are found using a simple incremental algorithm that scans $S_u$ from the left and $S_v$ from the right. The method used to find the largest open cluster is (a simplified form of) that of Balister, Bollobás and Walters [3], and works as follows. We divide the square $S_u$ into strips which are narrow but are sufficiently wide that no edge jumps an entire strip (i.e., all the edges meeting the strip are entirely contained in the union of the strip and its two neighbouring strips).

We find the component structure of the open subgraph restricted to the two left most strips. Then we look at the next strip and find the new component structure formed. At each stage we have an equivalence relation on the vertices in a strip where two vertices are equivalent if they are in the same open cluster in the part of $S_u$ to the left of the current strip. We also keep track of the size of each of these clusters, and the size of the largest open cluster we have seen so far. When we get to the right hand edge of the square $S_u$ we know exactly which vertices (if any) in that strip are part of the largest open cluster of $\Lambda_u$.

We repeat the process on $S_v$ but working from right to left. Finally we add the edges between the right most strip of $S_u$ and the left most of $S_v$ and see whether the largest open clusters in each are joined.

The important thing to note about this algorithm is that the storage required is proportional to the side length of $S_u$, i.e. to $s$, not to the area of $S_u$.

IV. RESULTS

For our percolation bounds see Table 1. For full results, including numbers of successes, please see our website [2]. Note that in the 400 simulations associated with each bound (or with each attempt to obtain a bound) we have always seeded the random number generator with 400 consecutive seeds starting from 12345678. This means that the exact results of our simulations should be reproducible as a way of checking the program. Also, it shows that we have not performed many different runs and finally chosen seeds that work!

The computations were performed running in the background on around 70 (mostly fairly old) computers in the Department of Pure Mathematics and Mathematical Statistics, University of Cambridge, over a period of around 2 weeks. This was made much easier by the fact that the department uses Linux rather than Windows! We are grateful to the computer officer, Andrew Aitchison, for technical assistance.

V. CONCLUSIONS

We have shown that it is practical to use the method of Balister, Bollobás and Walters [3] to obtain narrow confidence intervals for the critical probabilities for site and bond percolation on Archimedean lattices. Unlike the (presumably) much more precise estimates obtained by other methods, these intervals come with mathematically guaranteed error bounds. The intervals are much narrower than those that can be 100% proved, and the error probabilities are very small; the running time does not increase much with a large decrease in the desired error probability, so a probability that is in practice zero (here 1 in a million for each lattice) may be achieved.

We have tried to keep the computations relatively simple; there is no point in using an algorithm that is proved correct if it is not possible to verify the computer program used. At the cost of more complicated programming, better results could be obtained in two ways. Firstly, the current program could be made to cache better and hence run faster by scanning the rectangle $R_v$ in a more complicated manner: this $2s$ by $s$ rectangle could be broken down into $k$ by $k$ squares small enough that the boundary of one square fits into the processors primary cache,
and these squares could then be processed column by column. The overall storage requirement is approximately the same (one entire column must be stored), but the frequency of cache misses is reduced by a factor of about $k$.

A more significant improvement could be obtained by considering a different event $E_c$. Let $E_b$ be the event that there is an open path crossing $R_c$ from left to right, and that there is an open path crossing the left-hand end square of $R_c$ from top to bottom. As noted by Bollobás and Riordan [8], for example, this event still has the property (1). (Essentially this observation was used by Balister, Bollobás and Walters [8] in obtaining a lower bound on the critical parameter for a certain continuum percolation model.) Also, the scaling behaviour of $P_p(E_b)$ near $p_c$ should be the same as for the event considered here. The gain is that whether or not $E_b$ holds in a given configuration can be tested faster, using an interface following algorithm of the type used by Ziff and Cummings [43] in 1984, for example. Assuming conformal invariance, the expected length of the interface is $s^{a_3-3} = s^{4/3}$, where $a_3 = (3^2 - 1)/12$ is the multi-chromatic 3-arm exponent for $SLE_6$. Note, however, that to use this algorithm in practice without running into memory/caching problems, one needs to generate the state of each site/bond from a pseudo-random function, rather than a pseudo-random number generator.

All the exactly known critical probabilities associated to Archimedean lattices are roots of (simple) polynomial equations with integer coefficients. While it is easy to construct other lattices whose critical probabilities may be found in this form (see Ziff [42], for example), it may well be that there are no such expressions for the remaining Archimedean lattices, although some have been conjectured. In particular, Wu [40] conjectured that for bond percolation on the Kagomé lattice, $p_c^b = 0.524429$, a root of the equation $p^6-6p^5+12p^4-6p^3-3p^2+1 = 0$. Tsallis [35] conjectured the values $p_c^b = 0.522372$ and $p_c^b = 0.739830$ for bond percolation on the Kagomé and (3,122) lattices, respectively. Tsallis’s conjectures have been effectively ruled out some time ago by experimental estimates (see [41], for example); they are rather far from the current best estimates of 0.5244053 and 0.74042195. They have not yet been rigorously disproved, although the latest results of May and Wierman [20] come close. For both lattices, our results provide a rigorous ‘99.9999% disproof’ of Tsallis’s values - they lie outside our rigorous 99.9999% confidence intervals.

Wu’s conjectured value for $p_c^b(K)$ seems to be much closer to the truth; it is well within the confidence interval we obtain. Nevertheless, it is still believed to be false; see Ziff and Suding [40], for example. More recently, Seulliard and Ziff [28] have predicted certain values for $p_c^b$ for the Kagomé and (3,122) lattices, using a heuristic version of the star-triangle transformation. Although they leave open the ‘possibility’ that one of these values might be exact, there seems no reason (to us, or, apparently, to them) to really believe this: the method is (as they admit) non-rigorous, and the value obtained in the same way for the Kagomé lattice (given earlier by Hori and Kitahara without derivation) is outside the error bounds of existing experimental results.

| Lattice          | Site   | Width     | Bond   | Width     |
|------------------|--------|-----------|--------|-----------|
| Square           | 0.5925,0.5930 | 5 × 10⁻⁴ | 0.5    | 0         |
| Triangular       | 0.6968,0.6973 | 5 × 10⁻⁴ | 1 sin(π/18) | 0         |
| Hexagonal        | 0.52415,0.52465 | 5 × 10⁻⁴ | 0.7402,0.7407 | 5 × 10⁻⁴ |
| (3,12²)          | 0.5246,0.525 | 5 × 10⁻⁴ | 0.4194,0.4199 | 5 × 10⁻⁴ |
| (3²,4,6)         | 0.5505,0.5505 | 5 × 10⁻⁴ | 0.4139,0.4144 | 5 × 10⁻⁴ |
| (3²,4,3,4)       | 0.75925,0.75975 | 5 × 10⁻⁴ | 0.4341,0.4345 | 4 × 10⁻⁴ |
| (4,6,12)         | 0.7476,0.7480 | 4 × 10⁻⁴ | 0.6935,0.6940 | 5 × 10⁻⁴ |
| (4,8²)           | 0.7295,0.7300 | 5 × 10⁻⁴ | 0.6766,0.6770 | 4 × 10⁻⁴ |

TABLE I: Rigorous 99.9999% confidence intervals for critical probabilities for site and bond percolation

VI. APPENDIX

Figure 6 shows the representations of the Archimedean lattices $\Lambda$ that we used; the representations of the planar duals $\Lambda^*$ are shown in Figure 3. The representations of the site duals $\Lambda^*$ that we used are based on those of the original lattices $\Lambda$, with extra edges. The planar duals $\Lambda^*$ of lattices for which the critical probability for bond percolation is known exactly are omitted.

Let us make some remarks about specific lattices. We wanted our lattices to have an axis of symmetry at 45 degrees to the horizontal through a corner of each fundamental region $S_{\Lambda^*}$; in all the pictures except (3,12²) this is the line down and to the right. In the bond dual of the (4,6,12) lattice the picture looks asymmetric but that is only due to our squashing to make it fit the square lattice. In other words if we reflect the graph about a line at
45 degrees to the horizontal we get an isomorphic graph.

One lattice, (3\(^4\), 6), does not have an axis of symmetry, so we ran the program horizontally and vertically on this lattice. Both representations are shown and it is easy to see that one is the reflection of the other about a line 45 degrees to the horizontal.

For efficiency we tried to avoid having holes (vertices of the lattice not involved in the graph) in our representations: it was not practical to avoid this for the Kagomé and (3, 12\(^2\)) lattices (and their site duals) and the bond dual of (4, 6, 12).
Kagomé \((3, 6, 3, 6)\) \((3^4, 6)\) Horizontal \((3^4, 6)\) Vertical

\((3, 12^2)\) \((3^3, 4^2)\) \((3^2, 4, 3, 4)\)

\((4, 8^2)\) \((3, 4, 6, 4)\) \((4, 6, 12)\)

FIG. 4: The bond duals of 9 of the Archimedean lattices.

[1] \url{http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html}

[2] \url{http://www.dpmms.cam.ac.uk/~walters/lattice_bounds/}

[3] P. Balister, B. Bollobás, and M. Walters, *Continuum percolation with steps in the square or the disc*, Random Structures Algorithms 26 (2005), 392–403.

[4] B. Bollobás and O. Riordan, *Percolation*, Cambridge University Press, 2006.

[5] , *Percolation on dual lattices with \(k\)-fold symmetry*, Preprint available from http://arxiv.org/math.PR/0606149, 2006.

[6] , *A short proof of the Harris–Kesten Theorem*, Bull. London Math. Soc. 38 (2006), 470–484.

[7] B. Bollobás and A. Stacey, *Approximate upper bounds for the critical probability of oriented percolation in two dimensions based on rapidly mixing Markov chains*, J. Appl. Probab. 34 (1997), 859–867.

[8] J. L. Cardy, *Critical percolation in finite geometries*, J. Phys. A 25 (1992), L201–L206.

[9] G. Grimmett, *Percolation*, second ed., Springer, xiv+444 pp, 1999.

[10] B. Grünbaum and G. C. Shephard, *Tilings and patterns*, W. H. Freeman, xii+700 pp, 1987.

[11] H. Kesten, *The critical probability of bond percolation on the square lattice equals \( \frac{1}{2} \)*, Comm. Math. Phys. 74 (1980), 41–59.

[12] , *Percolation theory for mathematicians*, Birkhäuser, iv+423 pp, 1982.

[13] R. Langlands, P. Pouliot, and Y. Saint-Aubin, *Conformal
invariance in two-dimensional percolation, Bull. Amer. Math. Soc. 30 (1994), 1–61.

[14] G. F. Lawler, O. Schramm, and W. Werner, Values of Brownian intersection exponents. I. Half-plane exponents, Acta Math. 187 (2001), 237–273.

[15] ———, Values of Brownian intersection exponents. II. Plane exponents, Acta Math. 187 (2001), 275–308.

[16] ———, One-arm exponent for critical 2D percolation, Electron. J. Probab. 7 (2002), no. 2, 13 pp. (electronic).

[17] ———, Values of Brownian intersection exponents. III. Two-sided exponents, Ann. Inst. H. Poincaré Probab. Statist. 38 (2002), 109–123.

[18] T. M. Liggett, R. H. Schonmann, and A. M. Stacey, Domination by product measures, Ann. Probab. 25 (1997), 71–95.

[19] M. Matsumoto and T. Nishimura, Mersenne twister: A 623-dimensionally equidistributed uniform pseudorandom number generator, ACM Trans. on Modeling and Computer Simulation 8 (1998), 3–30.

[20] W. D. May and J. C. Wierman, The application of non-crossing partitions to improving percolation threshold bounds, Combin. Probab and Comput (to appear).

[21] M. V. Menshikov, Coincidence of critical points in percolation problems, Dokl. Akad. Nauk SSSR 288 (1986), 1308–1311.

[22] M. E. J. Newman and R. M. Ziff, Efficient Monte Carlo algorithm and high-precision results for percolation, Phys. Rev. Lett. 85 (2000), 4104–4107.

[23] ———, Fast Monte Carlo algorithm for site or bond percolation, Phys. Rev. E 64 (2001), 016706, 16.

[24] R. Parviainen, Estimation of bond percolation thresholds on the Archemedian lattices, Preprint available from http://www.ms.unimelb.edu.au/~robertp/, 2005.

[25] R. Parviainen and J. C. Wierman, Ordering bond percolation critical probabilities, 2002.

[26] P. J. Reynolds, H. E. Stanley, and W. Klein, Phys. Rev. B 20 (1980), 1223.

[27] O. Schramm, Scaling limits of loop-erased random walks and uniform spanning trees, Israel J. Math. 118 (2000), 221–288.

[28] C. R. Scullard and R. M. Ziff, Predictions of bond percolation thresholds..., Phys. Rev. E 73 (2006), 045102.

[29] Scott Sheffield, Random surfaces, ASTERISQUE 304 (2003).

[30] S. Smirnov, Critical percolation in the plane: conformal invariance, Cardy’s formula, scaling limits, C. R. Acad. Sci. Paris Sér. I Math. 333 (2001), 239–244.

[31] S. Smirnov and W. Werner, Critical exponents for two-dimensional percolation, Math. Res. Lett. 8 (2001), 729–744.

[32] P. N. Suding and R. M. Ziff, Site percolation thresholds for archimedean lattices, Phys. Rev. E 60 (1999), 275–283.

[33] M. F. Sykes and J. W. Essam, Some exact critical percolation probabilities for site and bond problems in two dimensions, Phys. Rev. Lett. 10 (1963), 3–4.

[34] ———, Exact critical percolation probabilities for site and bond problems in two dimensions, J. Mathematical Phys. 5 (1964), 1117–1127.

[35] C. Tsallis, J. Phys. C: Solid State Phys. 15 (1982), L757.

[36] J. C. Wierman, Bond percolation on honeycomb and triangular lattices, Adv. in Appl. Probab. 13 (1981), 298–313.

[37] ———, Bond percolation critical probability bounds for the Kagomé lattice by a substitution method, Disorder in Physical Systems: A Volume in Honour of John Hammerley (G. R. Grimmett and D. J. A. Welsh, eds.), Oxford University Press, 1999, pp. 349–360.

[38] ———, Bond percolation critical probability bounds for three Archimedean lattices, Random Structures Algorithms 20 (2002), 507–518.

[39] ———, Upper and lower bounds for the Kagomé lattice bond percolation critical probability, Combin. Probab. Comput. 12 (2003), 95–111.

[40] F. Y. Wu, J. Phys. C: Solid State Phys. 12 (1979), L645.

[41] F. Yonezawa, S. Sakamoto, and M. Hori, Percolation in 2 dimensional lattices 1. a technique for the estimation of thresholds, Phys. Rev. B 40 (1989), 636–650.

[42] R. M. Ziff, Generalized cell-dual-cell transformation and exact thresholds for percolation, Phys. Rev. E 73 (2006), 016134.

[43] R. M. Ziff, P. T. Cummings, and G. Stell, J. Phys. A: Math. Gen. 17 (1984), 3009.

[44] R. M. Ziff and M. E. J. Newman, Convergence of threshold estimates for two-dimensional percolation, Phys. Rev. E 66 (2002), 016129, 10.

[45] R. M. Ziff and B. Sapoval, J. Phys. A: Math. Gen. 19 (1986), 1169.

[46] R. M. Ziff and P. N. Suding, J. Phys. A: Math. Gen. 30 (1997), 5351.