Percollation thresholds on three-dimensional lattices with three nearest neighbors

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Percolation thresholds on three-dimensional lattices with three nearest neighbors

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Abstract. We present a study of site and bond percolation on periodic lattices with three nearest neighbors per site. Essentially all previous studies of percolation in 3D have considered coordination numbers of 4 or higher, but 3-coordinated lattices have attracted recent interest for their unusual symmetries and relevance to self-assembled materials. We have considered four lattices, with different symmetries, different underlying Bravais lattices, and different degrees of longer-range connections. As expected, we find that the site and bond percolation thresholds in all of the 3-connected lattices studied here are significantly higher than in the diamond lattice (a 4-connected lattice). Thresholds for different lattices are similar to within a few per cent, despite the differences between the lattices at scales beyond nearest and next-nearest neighbors. They also confirm an approximate analytical result for the relationship between coordination number and percolation threshold, one that had previously only been compared with simulation results for coordination numbers of 4 or higher.

Keywords: classical phase transitions (theory), percolation problems (theory)

ArXiv ePrint: 1211.6531

\textsuperscript{1} These authors contributed equally.
1. Introduction

Percolation is one of the simplest phase transitions known: sites on a lattice are occupied at random until there is a path that can be traversed from one end of the lattice to the other, traveling only neighbor-to-neighbor on occupied sites[1]. The sites along this path or connected to this path (via neighbor-to-neighbor steps along occupied sites) are called the spanning cluster. In the limit of a large system size (linear dimension $L \gg 1$), the probability of forming a spanning cluster via random occupation of sites goes to unity above a critical occupation probability per site $p_c$ and zero below $p_c$. Percolation models have been used to study a great many phenomena, from porous media to biological systems to propagation of fires and diseases[2].

A well-known trend in percolation on periodic 3D lattices is that $p_c$ increases as the coordination number $z$ (number of nearest neighbors per site) decreases[3]. (See table 5 near the end for examples and more references.) This trend arises from the fact that, when there are fewer neighbors per site, there are fewer ways to navigate around an obstacle. Consequently, more sites have to be occupied to ensure a path spanning from one end of the system to the other. To the best of our knowledge, the lowest coordination number studied for percolation on simple 3D lattices is $z = 4$, the most prominent example being the diamond lattice with $p_c \approx 0.430$ for site percolation[4, 5] and $\approx 0.388$ for bond percolation [6].

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However, \( z = 4 \) is not the lowest possible coordination number. The lowest possible non-trivial coordination number is \( z = 3 \),\(^2\) which has been realized in interesting families of 3D lattices, namely the \((n, 3)\) lattices studied by Wells\[^7\]. The 3 refers to the number of nearest neighbors (bonds) per site, and \( n \) is the smallest number of steps that one would have to take along the lattice sites to return to the same point. In lattice families with multiple members, \((n, 3)\) is followed by a letter, e.g. \((10, 3)\)-a, \((10, 3)\)-b, etc. A total of 30 lattices have been identified in these families, with \( n \) values of 7, 8, 9, 10, and 12.

Recently, the \((10, 3)\)-a lattice has attracted attention because of its unusually high symmetry, possessing a property known as ‘strong isotropy’ \[^9\], shared with only one other 3D lattice (diamond). The \((10, 3)\)-a structure appears in a very wide variety of interesting systems, e.g. block copolymers\[^{10}–{12}\], molecular magnets\[^{13, 14}\], and even butterfly wings\[^{15}\], and it has been proposed as a possible structure for a metastable phase of carbon\[^{16}\]. Moreover, many of the other \((n, 3)\) lattices, in particular \((8, 3)\)-a, have been studied in the context of self-assembly and metal–organic frameworks \[^{17}–{21}\]. Motivated by this recent attention to \((n, 3)\) lattices, as well as the general question of how high the percolation threshold can be for a 3D lattice with \( z = 3 \), we have studied four lattices in this family: \((10, 3)\)-a, its close relatives \((10, 3)\)-b and \((10, 3)\)-c, and \((8, 3)\)-a. These particular lattices are especially easy to study because they can be realized with bonds of uniform length and 120° bond angles, making them easy to construct with ball-and-stick models. These lattices offer a chance to study the interplay between coordination, higher-level connectivity (via \( n \)), and other aspects of lattice geometry (i.e. the differences between, say, \((10, 3)\)-a and \((10, 3)\)-b) for the lowest non-trivial \( z \) value. We are only aware of one study of percolation on lattices in this family, namely the \((10, 3)\)-a lattice\[^{8}\], and that study focused on invasion percolation and trapping, rather than the standard site and bond percolation problems.

Here, we first discuss the geometries of our lattices in their simplest forms: equal bond lengths and 120° bond angles. We illustrate deformations of the lattices that preserve the topology (connections between nearest neighbors) but enable a mapping onto a cubic lattice, for convenience in enumerating sites in a calculation. (A similar approach has been used in studies of other non-cubic lattices \[^{22}\].) We then summarize key features of the Newman–Ziff algorithm\[^{23}\] used to determine the site and bond percolation thresholds of the lattices, and present the computed percolation thresholds. Finally, we compare with \( p_c \) values for other lattices.

### 2. The lattices under study

#### 2.1. The \((10, 3)\)-a lattice

The \((10, 3)\)-a lattice (shown in figure 1(a)) is a body-centered cubic (bcc) lattice with a four-atom basis. If we work in a coordinate system where the sites of the bcc lattice are at the corners of a cube, one site is at the origin \((0, 0, 0)\), and the edges are of unit length and parallel to the standard \( x \), \( y \), and \( z \) axes, then the three other atoms in the basis

---

\(^2\) In order to have an average coordination number less than 3 (assuming a spatial dimension greater than 1D), one would need at least some sites with \( z = 2 \), but a site with \( z = 2 \) is equivalent to a single bond between two other sites. A physical analogy would be the role of an oxygen atom in a SiO\(_2\) crystal. Therefore, any lattice with average \( z < 3 \) must be equivalent to taking a lattice with \( z \geq 3 \) and placing sites with \( z = 2 \) along some of the bonds.
Figure 1. (a) The (10, 3)-a lattice, with sites numbered. (b), (c) The deformations used to map the lattice onto a cubic grid for computational convenience.

are at \( \mathbf{b}_1 = (0, -\frac{1}{4}, \frac{1}{4}) \), \( \mathbf{b}_2 = (-\frac{1}{4}, \frac{1}{2}, 0) \), and \( \mathbf{b}_3 = (\frac{1}{4}, 0, -\frac{1}{4}) \). These atoms correspond to sites 0 to 3 in the figure (i.e. the atom at the origin and its three nearest neighbors), they sit in the (111) plane, and the bonds to them are separated by 120° angles. The translation vectors are \( \mathbf{a}_1 = (-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \), \( \mathbf{a}_2 = (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}) \), and \( \mathbf{a}_3 = (\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \). Neighbors and next-nearest neighbors of the site at the origin are listed in table 1.

In percolation theory, the geometry of the bonds is less important than the presence of the bonds. A deformation of the lattice and bonds that preserves the connections between sites will not change the percolation threshold of the lattice. In the Newman–Ziff algorithm that we used, all of the relevant information on the lattice is stored in the ‘nn’ array, which contains the labels of the nearest neighbors bonded to each site in the lattice. For convenience in enumerating sites, we have deformed the lattice to fit onto a simple cubic grid, while preserving the bonding structure of the lattice. Our numbering system for sites, and the deformations used to fit them onto a cubic grid, are shown in figures 1(b) and (c).

2.2. The (10, 3)-b lattice

The (10, 3)-b lattice is unusual, because even if we specify unit bond lengths and 120° bond angles we still have an unconstrained structural degree of freedom. Suppose that we define the positions of all of the lattice sites and also the basis. We can then deform the lattice in a manner that uniformly changes the spacing between lattice planes without changing any bond lengths or bond angles. We have chosen to describe this lattice in a form that

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maximizes the symmetry, as this form lends itself to easier visualization with ball-and-
stick models. In this form, the lattice is body-centered tetragonal, with lattice vectors
$a_1 = (\sqrt{3}, 0, 0)$, $a_2 = (0, \sqrt{3}, 0)$, and $a_3 = \left(\frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}, 3\right)$.

The four-atom basis is more complicated. Instead of a central atom with three
neighbors, the basis is a chain of four atoms, located at $b_0 = (0, 0, 0)$, $b_1 = \left(0, \frac{\sqrt{3}}{2}, \frac{1}{2}\right)$,
$b_2 = \left(0, \frac{\sqrt{3}}{2}, \frac{3}{2}\right)$, and $b_3 = \left(-\frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}, 2\right)$. These correspond to sites 0 to 3 in the figure.
Neighbors and next-nearest neighbors of the basis sites are listed in table 2.

As before, we also deform this lattice to represent it on a simple cubic grid. The
numbering system and deformation steps are illustrated in figures 2(b) and (c).

### 2.3. The (10, 3)-c lattice

The (10, 3)-c lattice has a larger basis, requiring six atoms to form a chain. It is
shown in figure 3(a). The underlying lattice is hexagonal in the $(x, y)$ plane, with
lattice points stacked vertically in the $z$ direction. The lattice vectors are $a_1 = (\sqrt{3}, 0, 0)$,
$a_1 = (\sqrt{3}/2, 3/2, 0)$, and $a_3 = (0, 0, 9/2)$. The basis points are at $b_0 = (0, 0, 0)$, $b_1 = (\sqrt{3}/2, 0, 1/2)$,
$b_2 = (\sqrt{3}/2, 0, 3/2)$, $b_3 = (\sqrt{3}/4, 3/4, 2)$, $b_4 = (\sqrt{3}/4, 3/4, 3)$, and $b_5 = (0, 0, 7/2)$. These correspond to sites 0 to 5 in the figure. Neighbors of the basis sites are
listed in table 3.
Table 2. Coordinates of neighbors for the basis sites of the (10, 3)-b lattice. Coordinates are given in terms of the lattice translation vectors \{a_i\} and basis coordinates \{b_i\} discussed in section 2.2.

<table>
<thead>
<tr>
<th>Site coordinates</th>
<th>Neighboring sites’ coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{b}_0 = (0, 0, 0) )</td>
<td>( \mathbf{b}_1 = \left(0, -\sqrt{3}/2, \frac{1}{2}\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_1 + \mathbf{a}_2 = \left(0, 3\sqrt{3}/2, 1\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_3 - \mathbf{a}_3 = (-\sqrt{3}, 0, -1) )</td>
</tr>
<tr>
<td>( \mathbf{b}_1 = \left(0, -\sqrt{3}/2, \frac{1}{2}\right) )</td>
<td>( \mathbf{b}_0 = (0, 0, 0) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_0 - \mathbf{a}_2 = (0, -\sqrt{3}, 0) )</td>
</tr>
<tr>
<td>( \mathbf{b}_2 = \left(0, -\sqrt{3}/2, \frac{1}{2}\right) )</td>
<td>( \mathbf{b}_1 = \left(0, \sqrt{3}/2, \frac{1}{2}\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_3 = \left(-\sqrt{3}/2, \sqrt{3}/2, 2\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_3 - \mathbf{a}_1 = \left(-3\sqrt{3}/4, \sqrt{3}/2, 2\right) )</td>
</tr>
<tr>
<td>( \mathbf{b}_3 = \left(-\sqrt{3}/2, \sqrt{3}/2, 2\right) )</td>
<td>( \mathbf{b}_0 + \mathbf{a}_3 = \left(\sqrt{3}/2, \sqrt{3}/2, 3\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_2 = \left(0, \sqrt{3}/2, \frac{3}{2}\right) )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{b}_2 + \mathbf{a}_1 = \left(\sqrt{3}/2, \sqrt{3}/2, 3\right) )</td>
</tr>
</tbody>
</table>

As before, we also deform this lattice to represent it on a simple cubic grid. The numbering system and deformation steps are illustrated in figures 3(b) and (c).

2.4. The (8, 3)-a lattice

We realized the (8, 3)-a lattice, shown in figure 4(a), in a structure with lattice vectors \( \mathbf{a}_1 = (-5/2, \sqrt{3}/6, 2\sqrt{2}/3) \), \( \mathbf{a}_2 = (5/2, \sqrt{3}/6, 2\sqrt{2}/3) \), and \( \mathbf{a}_3 = (0, 4\sqrt{3}/3, \sqrt{2}/3) \). The lattice’s hexagonal symmetry is not manifestly obvious from inspection of the lattice vectors, but when the larger lattice is viewed, there are barrel-like structures with hexagonal symmetry. This is somewhat analogous to the situation with the fcc lattice, whose primitive unit cell is non-cubic, but which can nonetheless be constructed in an expanded form with a cubic unit cell.

The (8, 3)-a lattice has a six-atom basis, with unit bond lengths and atoms located at \( \mathbf{b}_0 = (0, 0, 0) \), \( \mathbf{b}_1 = (0, -\sqrt{3}/3, -\sqrt{2}/3) \), \( \mathbf{b}_2 = (1/2, -5\sqrt{3}/6, -\sqrt{2}/3) \), \( \mathbf{b}_3 = (3/2, -5\sqrt{3}/6, -\sqrt{2}/3) \), \( \mathbf{b}_4 = (2, -\sqrt{3}/3, -\sqrt{2}/3) \), and \( \mathbf{b}_5 = (2, 0, 0) \). These correspond to sites 0 to 5 in the figure. Neighbors of the basis sites are listed in table 4.
The steps used to deform the (8, 3)-a lattice so that it fits onto a cubic grid are illustrated in figures 4(b) and (c).

3. Simulations

3.1. Description of the algorithm

We used the Newman–Ziff algorithm to identify the percolation thresholds of finite-sized clusters[23]. In brief, the algorithm works by occupying sites (or bonds) on a lattice of $N$ sites one-at-a-time, in a random order. Relationships between sites are defined in the array $\text{nn}$, which indicates the site numbers for the nearest neighbors of each site. At each step, after a site is occupied we check whether the occupation of the $n$th site produces a cluster that wraps around the entire system. Each cluster is assigned a “pointer” to a root (or parent) site, corresponding to the first site in the cluster, and also a vector that points in the direction of the parent site. (If reaching the parent site requires passing through the boundary of the computational window and going to the other side via a periodic boundary condition, the vector points toward the boundary that would be reached by traveling along the cluster.)

As clusters grow and merge, pointers and vectors are updated to the root of the largest cluster involved in the merger. Wrapping is detected when a newly-occupied site (1) joins two portions of the same cluster and (2) the vectors going from the joined portions of the cluster to the root differ by something other than the displacement vector between the sites. We consider wrapping between parallel faces of the computational volume (i.e. along the $x$, $y$, and $z$ directions) as well as diagonal wrapping. (See the paper doi:10.1088/1742-5468/2013/05/P05014)
Percolation thresholds on three-dimensional lattices with three nearest neighbors

Figure 3. (a) The \((10, 3)\)-c lattice, with sites numbered. (b), (c) The deformations used to map the lattice onto a cubic grid for computational convenience. Only the sites of the unit cell are numbered on this lattice, because of display issues.

Another lattice is then generated, and the process is repeated, until \(N_L\) lattices (\(10^3\) in our work) have been generated. Bond percolation is handled in a completely analogous manner, substituting bonds for sites. Two bonds are considered neighbors if they touch the same site.

This process generates a plot of wrapping probability \(R_L\) versus occupation fraction \(\phi = n/N\), where \(L\) refers to the linear dimension of the lattice. In order to determine \(R_L\) as a function of occupation probability (the usual quantity of interest in percolation theory), it is necessary to convolve \(R_L\) with a binomial distribution,

\[
R_L(p) = \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} R_L(n). \tag{1}
\]

Equation (1) amounts to a weighted sum over all possible realizations of an \(N\)-site lattice with site occupation probability \(p\). The number of realizations that wrap with \(n\) occupied sites enters the sum via \(R_L(n)\). Different occupation numbers \(n\) will have different likelihoods of being realized at the same occupation probability \(p\), i.e. different degeneracies, and this enters the sum via the binomial distributions. Occupation numbers that are not close to \(N \cdot p\) are unlikely, and hence get low weight from the binomial distribution.

doi:10.1088/1742-5468/2013/05/P05014
Table 3. Coordinates of neighbors of the basis sites in the \((10, 3)-c\) lattice. Coordinates are given in terms of the lattice translation vectors \(\{a_i\}\) and basis coordinates \(\{b_i\}\) discussed in section 2.3.

<table>
<thead>
<tr>
<th>Site coordinates (b_i)</th>
<th>Neighboring sites’ coordinates</th>
</tr>
</thead>
<tbody>
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<td>(b_0 = (0, 0, 0))</td>
<td>(b_1 = (\frac{\sqrt{3}}{2}, 0, \frac{1}{2}))</td>
</tr>
<tr>
<td></td>
<td>(b_1 - a_1 = \left(-\frac{\sqrt{3}}{2}, 0, \frac{1}{2}\right))</td>
</tr>
<tr>
<td></td>
<td>(b_5 - a_3 = (0, 0, -1))</td>
</tr>
<tr>
<td>(b_1 = \left(\frac{\sqrt{3}}{2}, 0, \frac{1}{2}\right))</td>
<td>(b_0 = (0, 0, 0))</td>
</tr>
<tr>
<td></td>
<td>(b_2 = \left(\frac{\sqrt{3}}{2}, 0, \frac{3}{2}\right))</td>
</tr>
<tr>
<td></td>
<td>(b_0 + a_1 = \left(\sqrt{3}, 0, 0\right))</td>
</tr>
<tr>
<td>(b_2 = \left(\frac{\sqrt{3}}{2}, 0, \frac{3}{2}\right))</td>
<td>(b_1 = \left(\frac{\sqrt{3}}{2}, 0, \frac{1}{2}\right))</td>
</tr>
<tr>
<td></td>
<td>(b_3 = \left(\frac{\sqrt{3}}{2}, \frac{3}{4}, 2\right))</td>
</tr>
<tr>
<td></td>
<td>(b_3 - a_2 = (0, -\frac{3}{4}, 2))</td>
</tr>
<tr>
<td>(b_3 = \left(\frac{\sqrt{3}}{2}, \frac{3}{4}, 2\right))</td>
<td>(b_2 = \left(\frac{\sqrt{3}}{2}, 0, \frac{3}{2}\right))</td>
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<tr>
<td></td>
<td>(b_4 = \left(\frac{\sqrt{3}}{4}, \frac{3}{4}, 3\right))</td>
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<tr>
<td></td>
<td>(b_2 + a_2 = \left(\sqrt{3}, \frac{3}{2}, \frac{3}{2}\right))</td>
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<tr>
<td>(b_4 = \left(\frac{\sqrt{3}}{4}, \frac{3}{4}, 3\right))</td>
<td>(b_3 = \left(\frac{\sqrt{3}}{2}, \frac{3}{4}, \frac{3}{2}\right))</td>
</tr>
<tr>
<td></td>
<td>(b_5 = (0, 0, \frac{7}{2}))</td>
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<tr>
<td></td>
<td>(b_5 + a_1 + a_2 = \left(3\frac{\sqrt{3}}{2}, \frac{3}{2}, \frac{7}{2}\right))</td>
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<tr>
<td>(b_5 = (0, 0, \frac{7}{2}))</td>
<td>(b_4 = \left(\frac{\sqrt{3}}{4}, \frac{3}{4}, 3\right))</td>
</tr>
<tr>
<td></td>
<td>(b_0 + a_3 = (0, 0, \frac{9}{2}))</td>
</tr>
<tr>
<td></td>
<td>(b_4 - a_1 - a_2 = \left(-5\frac{\sqrt{3}}{4}, -\frac{3}{4}, 3\right))</td>
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</table>

To implement the algorithm we closely followed the code example given in the paper by Newman and Ziff. We implemented the code using Python 2.7 and ran it on multiple machines running Linux (Ubuntu 12.04) with quad core Intel processors. We distributed
Percolation thresholds on three-dimensional lattices with three nearest neighbors

Figure 4. (a) The (8, 3)-a lattice, with sites numbered. (b), (c) The deformations used to map the lattice onto a cubic grid for computational convenience. Only the sites of the unit cell are numbered on this lattice, because of display issues.

the work between each machine using Parallel Python 1.6.3. We checked our code by determining the site and bond percolation thresholds of the 2D square, 2D honeycomb, and 3D simple cubic lattices. Adaptation of the code to the lattices under study only required modification to the function that identifies the nearest neighbors of each site, as well as the vectors from each site to its neighbors. To validate the output for the lattices under study, we generated lattices with small numbers of sites (≈30) and had the code output the list of occupied sites when wrapping occurred. We verified by hand that (1) there was a cluster that wrapped the lattice, and (2) the removal of the most recently occupied site would cause the cluster to not wrap.

Given a plot of the wrapping probability $R_L(p)$ for different lattice sizes $L$, it is possible to obtain an estimate of the percolation threshold $p_c$ by looking for the point where the plot crosses over from low wrapping probability to high (e.g. the steepest point on the plot). An example for the (10, 3)-a lattice is shown in figure 5. For sufficiently large system sizes, this estimate of $p_c$ can be quite accurate. More efficient approaches can obtain high precision and accuracy by comparing $R_L(p)$ plots for several different system sizes $L$. One common way of comparing plots at different sizes is to use the scaling relation $|p_c(L) - p_c| \propto L^{-\omega-\nu}$, where $p_c(L)$ is obtained from the cross-over of an $R_L(p)$ plot and $\omega$ and $\nu$ are universal exponents that depend only on dimension[24].
which the associated uncertainty, is to make plots with $R_p$ as a function of $L$ at constant $p$. $L$ becomes more ‘step-like’ as $p > p_c$. However, a simpler approach, one that enables a very intuitive estimate of $p_c$ and the associated uncertainty, is to make plots with $R_L(p)$ (for fixed $p$) on the vertical axis and $L$ on the horizontal axis. For $p > p_c$, $R_L(p)$ is an increasing function of $L$, and for $p < p_c$, $R_L(p)$ is a decreasing function of $L$. This follows directly from the fact that $R_L(p)$ becomes more ‘step-like’ as $L$ increases. At $p = p_c$, $R_L(p)$ is independent of $L$[25].

Table 4. Coordinates of neighbors for the basis sites in the (8, 3)-a lattice. Coordinates are given in terms of the lattice translation vectors $\{a_i\}$ and basis coordinates $\{b_i\}$ discussed in section 2.4.

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<td>$b_3 + a_3 = (\frac{3}{2}, -\frac{\sqrt{3}}{2}, 0)$</td>
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</tbody>
</table>

However, a simpler approach, one that enables a very intuitive estimate of $p_c$ and the associated uncertainty, is to make plots with $R_L(p)$ (for fixed $p$) on the vertical axis and $L$ on the horizontal axis. For $p > p_c$, $R_L(p)$ is an increasing function of $L$, and for $p < p_c$, $R_L(p)$ is a decreasing function of $L$. This follows directly from the fact that $R_L(p)$ becomes more ‘step-like’ as $L$ increases. At $p = p_c$, $R_L(p)$ is independent of $L$[25]. The value of $p_c$ can thus be estimated simply by looking at the different plots of $R_L$ versus $L$ (at constant $p$) and identifying the flattest one. When the plot of $R_L$ oscillated somewhat as a function of $L$ (due to randomness in the simulations), we identified the value of $p$ for which $R_L$ oscillated without a pronounced upward or downward trend.
3.2. The uncertainty in the percolation threshold

There is an easy way to determine the uncertainty in \( p_c \) based only on the simulation output, and without any assumptions about critical exponents. In a plot of wrapping probability \( R_L \) versus occupation probability \( p \), the percolation transition is identified by looking for a value of \( p \) at which the wrapping probability is approximately stationary as the system size changes. However, the wrapping probabilities are determined from finite samples in Monte Carlo simulations, and this gives rise to statistical fluctuations in \( R_L \) for all \( p \) values. A vertical fluctuation \( \delta R_L \) shifts the curve along the horizontal \( p \) axis by an amount \( \delta R_L/(dR_L/dp) \), where \( dR_L/dp \) is the slope of the \( R_L \) versus \( p \) curve.

In order to get the uncertainty in \( R_L(p) \), let us first consider \( R_L \) as a function of occupation number \( n \) rather than occupation probability \( p \). We generate \( N_L \) lattices with \( n \) occupied sites, and use the Newman–Ziff algorithm to determine the number \( N_L R_L(n) \) that wrap. If we were to carry out this process repeatedly, we would find that the number of lattices that wrap obeys a binomial distribution with mean \( N_L R_L(n) \) and variance \( N_L R_L(n)(1 - R_L(n)) \), and so the fraction \( R_L(n) \) that wrap has mean \( R_L(n) \) and variance \( R_L(n)(1 - R_L(n))/N_L \).

When we go from \( R_L(n) \) to \( R_L(p) \), the convolution with a binomial distribution means that \( R_L(p) \) is a weighted sum of different \( R_L(n) \) values. We cannot treat these \( R_L \) values as independent random variables, since \( R_L(n + 1) \) is generated by occupying one more site (or bond) in each of the lattices used to determine \( R_L(n) \). Near \( p_c \), \( R_L(n) \neq Np_c \) is approximately a linear function of \( n - Np_c \),

\[
R_L(n) \approx R_L(Np_c) + c \cdot (n - Np_c) + \eta(n),
\]

where \( c \) is an unknown constant and \( \eta \) is a noise term.

This expression for \( R_L(n) \) is convolved with a binomial probability distribution that is approximately Gaussian for large \( N \) (and hence even about \( p_c \)). The normalization of the probability distribution means that the convolution with the first term gives \( R_L(Np_c) \). The symmetry of the peak of the distribution means that the convolutions with the second and third terms vanish. We thus conclude that \( R_L(p = p_c) \approx R_L(n = Np_c) \), and so we will
Figure 6. Plots of wrapping probability $R_L$ versus lattice size $L$ for different occupation probabilities $p$, for site percolation on a cubic lattice. The flattest curve is taken to be the one with $p = p_c$.

We have neglected the variance of the weighted sum of the noise terms $\eta(n)$ in equation (2), but that variance is small because $\eta(n)$ exhibits correlations for nearby $n$ values. The fact that $R_L(n)$ is an increasing function of $n$ means that downward fluctuations of $R_L(n)$ are limited in magnitude by the fluctuations of $R_L(n - 1)$. The fact that $R_L \leq 1$ reduces the probability of successive upward fluctuations.

In equation (3), we use the slope of the steepest $R_L$ versus $p$ curve. If the steepest curve were perfectly vertical, fluctuations of the other curves would be completely irrelevant, and the point of intersection would remain on that curve at the value of $p$ where it rises. Consequently, the finite slope of the steepest curve is the limiting factor in our determination of $p_c$.

As a check on our method, in figure 6 we show $R_L$ as a function of $L$ for site percolation on the simple cubic lattice. We identify $p_c$ by fitting straight lines to plots of $R_L$ versus log $L$ and looking for the smallest slope. The mean value of $R_L$ is used to compute the uncertainty if the plot fluctuates noticeably. The literature value is $p_c = 0.3116080$, with an uncertainty of 4 in the last decimal place[26]. Our value is $p_c = 0.311593$, with an uncertainty of 72 in the last 2 decimal places. This is fully consistent with the literature value.

4. Results

Figures 7–10 show $R_L$ versus $L$ (for different $p$ values), for site and bond percolation on the lattices under study. The number of unit cells in a realization of each lattice is $L^3$, so that the number of lattice sites ($N$ in our uncertainty formulas) is $4L^3$ (for the (10, 3)-a and (10, 3)-b lattices) or $6L^3$ (for (8, 3)-a and (10, 3)-c). The number of bonds (also $N$ in the uncertainty formulas) is $6L^3$ (for (10, 3)-a and (10, 3)-b) or $9L^3$ (for (8, 3)-a and (10,
Percolation thresholds on three-dimensional lattices with three nearest neighbors

Figure 7. Wrapping probability $R_L$ versus $L$ for (a) site and (b) bond percolation on (10, 3)-a lattices, for different occupation probabilities $p$. (Selected $p$ values are shown to the right of the plots.) The percolation threshold $p_c$ is the value of $p$ that gives the flattest overall trend. The uncertainty is determined via (3).

Figure 8. Wrapping probability $R_L$ versus $L$ for (a) site and (b) bond percolation on (10, 3)-b lattices, for different occupation probabilities $p$. (Selected $p$ values are shown to the right of the plots.) The percolation threshold $p_c$ is the value of $p$ that gives the flattest overall trend. The uncertainty is determined via (3).

3)-c). In all plots, the site occupation probability $p$ was incremented in steps of 1/number of sites or bonds for the smallest $L$ value.

5. Discussion

The percolation thresholds identified for the 3-coordinated lattices considered here are higher than typical values for three-dimensional lattices that have been studied previously. This point is illustrated in table 5, which shows percolation thresholds for a variety of common three-dimensional lattices, organized by their coordination number $z$. It is clear from the table that $p_c$ increases as $z$ decreases. This makes intuitive sense: with lower coordination numbers, it is easier to destroy a spanning cluster by removing a few sites or bonds at key points, while in lattices with higher coordination numbers there are more paths that can be navigated to circumvent a missing site or bond. Interestingly, among the 3-connected lattices the site and bond percolation thresholds are correlated with $r > 0.999$, doi:10.1088/1742-5468/2013/05/P05014 14
Figure 9. Wrapping probability $R_L$ versus $L$ for (a) site and (b) bond percolation on (10, 3)-c lattices, for different occupation probabilities $p$. (Selected $p$ values are shown to the right of the plots.) The percolation threshold $p_c$ is the value of $p$ that gives the flattest overall trend. The uncertainty is determined via (3).

Figure 10. Wrapping probability $R_L$ versus $L$ for (a) site and (b) bond percolation on (8, 3)-a lattices, for different occupation probabilities $p$. (Selected $p$ values are shown to the right of the plots.) Although there is some oscillation, the percolation threshold $p_c$ is the value of $p$ that gives the flattest overall trend. Because the graph for bonds exhibited greater oscillation than some, more $L$ values were used. The uncertainty is determined via (3).

but there is no correlation between the percolation threshold and the number of atoms in the unit cell: the largest unit cells ((10, 3)-c and (8, 3)-a) correspond to the smallest and largest percolation thresholds respectively.

The information shown in table 5 can be compared with an analytical expression\cite{3} for the approximate dependence of $p_c$ on spatial dimension $d$ and coordination number $z$,

$$p_c = p_0 \left( (d - 1)(z - 1) \right)^{-a} d^b,$$

(4)

where $a = 0.6160$ for sites and 0.9346 for bonds, $b = 0$ for sites and $b = a$ for bonds, and $p_0 = 1.2868$ for sites and 0.7541 for bonds. This comparison is made in figure 11. For ease of presentation we only show the (10, 3)-a lattice on these plots, but the percolation thresholds of the other 3-connected lattices differ by only about 1%. Crucially,
Figure 11. A log–log plot of computationally-determined site (a) and bond (b) percolation thresholds versus \((z - 1)\) for different 3D lattices, and a comparison plot of the formula of Galam and Mauger[3]. The computationally-determined values for (10, 3)-a are from figure 7. The computationally-determined values for the other lattices are from the references in table 5. Data points represent computational values, and the line represents the formula of Galam and Mauger.

Table 5. Site and bond percolation thresholds for important three-dimensional lattices with different coordination numbers \(z\). Uncertainties are given in parentheses, and refer to the last one or two digits, depending on the number of digits in the uncertainty. Bibliographic references are given in brackets [ ].

<table>
<thead>
<tr>
<th>Lattice</th>
<th>(z)</th>
<th>(p_c) (site)</th>
<th>(p_c) (bond)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(8, 3)-a</td>
<td>3</td>
<td>0.578 029(43)</td>
<td>0.555 785(28)</td>
</tr>
<tr>
<td>(10, 3)-a</td>
<td>3</td>
<td>0.571 404(40)</td>
<td>0.551 060(37)</td>
</tr>
<tr>
<td>(10, 3)-b</td>
<td>3</td>
<td>0.565 442(40)</td>
<td>0.546 694(33)</td>
</tr>
<tr>
<td>(10, 3)-c</td>
<td>3</td>
<td>0.559 603(39)</td>
<td>0.542 422(34)</td>
</tr>
<tr>
<td>Diamond</td>
<td>4</td>
<td>0.430 1(4) [5]</td>
<td>0.389 3(2) [5]</td>
</tr>
<tr>
<td>Simple cubic</td>
<td>6</td>
<td>0.311 6080(4) [26]</td>
<td>0.248 8126(5) [27]</td>
</tr>
<tr>
<td>bcc</td>
<td>8</td>
<td>0.245 9615(10) [26]</td>
<td>0.180 2875(10) [27]</td>
</tr>
<tr>
<td>fcc</td>
<td>12</td>
<td>0.199 2365(10) [27]</td>
<td>0.120 1635(10) [26]</td>
</tr>
<tr>
<td>hcp</td>
<td>12</td>
<td>0.199 2555(10) [22]</td>
<td>0.120 1640(10) [22]</td>
</tr>
</tbody>
</table>

The percolation thresholds of the 3-connected lattices are all very close to the theoretical plot.

We have not explored the entire family of 3-connected nets studied by Wells. Thus, it is an open question as to whether there are simple three-dimensional periodic lattices with higher percolation thresholds than those found here. We qualify the previous sentence with the word ‘simple’ because it is intuitively obvious that one could trivially increase the percolation threshold of a crystalline structure by inserting chains of 2-connected sites between sites with higher coordination numbers. The interesting question is whether one can construct crystals with higher \(p_c\) without making use of 2-connected sites between higher-coordinated sites. The agreement with analytical predictions for \(p_c\) suggests little prospect for higher \(p_c\) values in non-trivial lattices, but this prediction needs confirmation in simulations.

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In conclusion, we have used Monte Carlo simulations to determine the percolation thresholds of several interesting lattices that have not, to the best of our knowledge, been studied previously. We find that these lattices have substantially higher percolation thresholds than other three-dimensional lattices, due to their low coordination numbers. The results for both site and bond percolation thresholds are very close to theoretical predictions for thresholds on 3D lattices with $z=3$.

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References

Percolation thresholds on three-dimensional lattices with three nearest neighbors


