

# Modelling and Simulation

## Practical Assignment 2: Percolation

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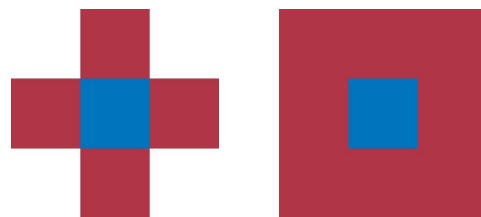
### 1. INTRODUCTION

Kenzel et al. [2] give the following interpretation of the percolation model; it describes the geometry of the randomly generated pores in a porous material through which only certain particles can percolate if the pores form continuous paths. The material is modeled with a square lattice. Although different lattices are possible, we consider only square lattices.

The exact percolation model is described in section 2, this section also presents an implementation of the model in pseudo code. In section 3 we discuss the experiments we have performed with the model and their results.

### 2. METHOD

Algorithm 1 presents our iterative growth process, the method `percolation` expects three arguments `mask`, `probability` and `.`. Given the size parameter `N`, the grid used for the percolation is  $(2N + 1) \times (2N + 1)$ , this causes the grid to have an uneven number of rows and columns. Consequently the grids center is always clearly defined as  $(N + 1, N + 1)$ . The parameter  $p \in [0, 1]$  is the probability that a given site in the cluster becomes occupied. The `mask` is a binary matrix with  $r$  rows and  $c$  columns that determines the used connectivity. Until section 3.4 we only consider four-connected



(a) 4-connectivity (b) 8-connectivity  
**Figure 1:** Connectivity masks for (a) four-connectivity and (b) eight-connectivity. The red squares are considered neighbors of the blue center square.

clusters, for which the mask presented in figure 1a is used.

Initially the only site we have to consider is the center site, which is consequently the only site in the queue at the first iteration. The matrix `probabilities` stores for each site the probability that it may grow, it is generated by sampling an uniform distribution with the range  $[0, 1]$   $(2N + 1)^2$  times.

Each iteration we pop the next `site` from the queue. We grow this point, using the function `grow`. This method considers all neighbors that are connected to `site` as determined by the `mask`. For each of these neighbours we retrieve the value  $z$  from `probabilities`. If  $z \leq p$  we mark the neighbor site as occupied, otherwise it is marked empty. The method `grow` returns the newly occupied neighboring sites, which are then added to the queue, so they can be processed by the `grow` process in a later iteration.

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\*These authors contributed equally to this work.

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**Algorithm 1: percolation**(*mask*, *N*, *p*)

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**input** : *N* size  
          *p* probability  
          *mask*  $r \times c$  binary matrix  
          *seed* for the random generator  
**output** : *grid*  $(2N + 1) \times (2N + 1)$   
          matrix  
  
*center* := (*N* + 1, *N* + 1)  
**push**(*queue*, *center*)  
*grid* := **initGrid**(*N*, *N*)  
*probabilities* := **rand**(*N*, *N*)  
**while** *not isEmpty(queue)* **do**  
    *site* = **pop**(*queue*)  
    *sites* = **grow**(*grid*, *site*, *mask*, *p*,  
                  *probabilities*);  
    **if** *anyOnBorder(sites)* **then**  
        **break**  
    **push**(*queue*, *sites*);

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The growth of the clusters stops when the queue is empty and it thus cannot grow anymore or if it has reached one of the borders of the grid. In the first case the cluster is finite, which means that all neighboring sites of the cluster, according to the connectivity defined by the *mask*, are marked as empty. In algorithm 1 we test for this condition via the guard of the loop; if the queue is empty there are no more neighbors to consider, consequently the cluster must be finite.

A percolating cluster is a cluster that has reached the border of the grid, i.e. if there is an occupied site with row or column number 1 or  $2N + 1$ . We test for this condition with the method **anyOnBorder** which is called before adding newly occupied sites to the queue.

Figure 2 presents three clusters grown with algorithm 1. We can clearly see that the finite

clusters are completely surrounded by a white border, which indicates that these sites are empty and processed. Figure 2c shows a percolating cluster, which has stopped growing due to a site in the lower left corner. Another indication of the percolating nature of the cluster is the fact that there are occupied sites that can still grow, as indicated by their empty, i.e. grey, neighbours.

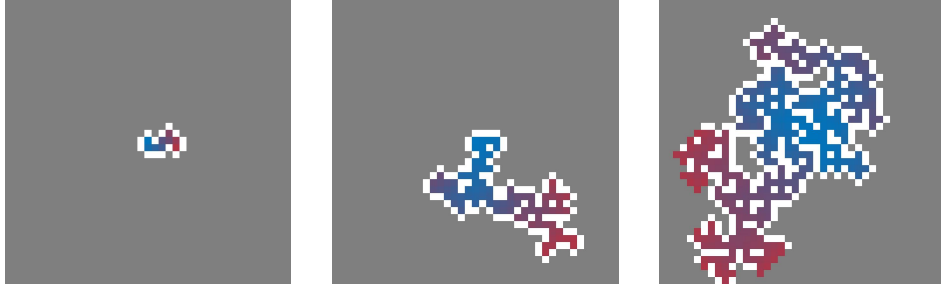
### 3. EXPERIMENTS

This section presents our exploration of the parameter space of the percolation model. In section 3.1 we discuss the influence of the probability parameter *p*. In this section we often use the size of the cluster to explore the influence of different parameters. We have defined the cluster size as the number of sites that are occupied, note that the size of a percolating cluster is not meaningful, since it could have grown much larger if we had not halted it. Therefore we consider the size of percolating clusters to be undefined.

Section 3.2 explores the effect of the size of the system on the generated clusters. In section 3.3 we determine the fractal dimension of a finite cluster. Finally, section 3.4 presents a short analysis of the impact of the used connectivity.

#### 3.1. PROBABILITY

One important property of clusters is their size, and how that size depends on the parameter *p*. As noted before the size of percolating cluster is not meaningful, therefore do not consider percolating clusters in the following discussion. Kenzel et al. [2] describe the relation between the size of a cluster and the parameter *p* as follows: for small values of *p* we get a large number of small clusters. As *p* increases we find positive correlation between *p* and the average cluster size until *p* reaches some threshold value  $p_c$ .



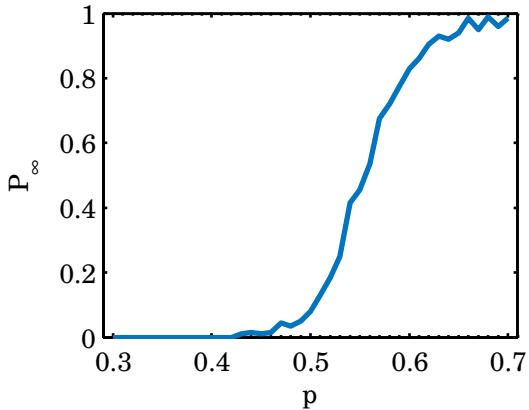
(a)  $N = 20$  and  $p = 0.3$     (b)  $N = 20$  and  $p = 0.5$     (c)  $N = 20$  and  $p = 0.6$

**Figure 2:** Examples of (a) a small finite cluster, (b) a larger finite cluster and (c) a percolating cluster using four-connected neighbours. The colours of the elements in the cluster indicate when that point was added to the cluster, the ‘colder’ the color the earlier in the percolation it was added to the cluster. White cells are empty and gray cells are undetermined.

For  $p > p_c$  we get either a small finite cluster or a percolating cluster. As  $p > p_c$  increases the probability of finding a finite cluster decreases, until we always get a percolating cluster for  $p = 1$ . Note that although in theory this cluster should cover the full grid, this is not necessarily the case in our model, since it stops growing as soon as one border site is occupied.

To find an indication of the value of  $p_c$  with our model we have let it generate a cluster on a  $41 \times 41$  grid for  $p = 0.30, 0.31, \dots, 0.7$ . For each value of  $p$  we grow  $r_{max} = 200$  clusters.

Figure 8 in appendix A.1 presents the mean



**Figure 3:** Ratio of percolating clusters,  $P_\infty$ , as a function of  $p$ . Ratios are calculated over  $r_{max} = 200$  runs on a  $41 \times 41$  grid.

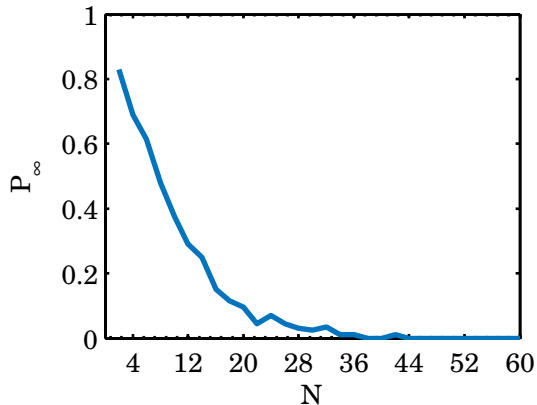
and standard deviation of the size of the finite clusters as a function of  $p$ . In this figure we observe the effect of  $p$  on the mean cluster size described by Kenzel et al. Furthermore, based on these data one would estimate  $p_c$  to be approximately 0.55.

Kenzel et al. also predicted that the number of percolating clusters relative to the number of finite clusters would grow for  $p > p_c$  until  $p = 1$ , where the only possibility would be a percolating cluster. To observe this effect figure 3 shows  $P_\infty$ , which is the ratio of the number of percolating clusters to the number of finite clusters. This graph is based on the same data as figure 8. Based on this graph we would say that  $p_c \approx 0.4$ . This number is lower than the value for  $p_c$  based on figure 8. This is probably caused by the relatively small grid sizes, which causes us to classify some clusters as percolating, that are actually finite.

Stauffer [4] has found  $p_c$  to be approximately 0.5928 for a square lattice. As stated earlier our lower estimation of  $p_c$  is quite likely caused by our small grid.

### 3.2. SYSTEM SIZE

In section 3.1 we postulated that our relatively small grid influenced the found value of  $p_c$ . This section qualitatively discusses the relation between the size of the grid and the cluster. We repeat the experiment discussed in



**Figure 4:** Ratio of percolating clusters to the number of finite clusters,  $P_\infty$ , as a function of  $N$ . Ratios are calculated over  $r_{max} = 200$  runs with  $p = 0.5$ .

section 3.1 but varied  $N = 2, 6, \dots, 60$  instead of  $p$ . Since we are mostly interested in the size of finite clusters we choose  $p = 0.5 < p_c$ . Instead of the size of grid we now measure  $Q$  the ratio of the size of finite clusters to the number of sites in the grid.

Figure 9 in appendix A.2 shows the mean and standard deviation of  $Q$  as a function of  $N$ . In this graph we observe that the average of  $Q$  decreases as  $N$  increases, i.e. the size of the clusters does not grow as hard as the number of sites in the grid.

Figure 4 shows that  $P_\infty$  reaches zero for  $N > 40$ , which indicates that for this value of  $N$  there are no more percolating clusters. This fits with the theory discussed in section 3.1, which states that we get only finite clusters for  $p < p_c$ . We have percolating clusters for  $p = 0.5 < p_c$  since the grid is not large enough to hold the finite clusters.

If the lattice size is infinite we are no longer limited by the size of the lattice, in essence we remove one of our stop conditions. In this situation the theory presented in section 3.1 holds, i.e. as long as  $p < p_c$  we only have finite clusters. As  $p > p_c$  the number of percolating clusters relative to the number of finite clusters

increases until we always get a percolating cluster for  $p = 1$ .

### 3.3. FRACTAL DIMENSION

Falconer [1] describes the fractal dimension as some number  $\rho$  such that

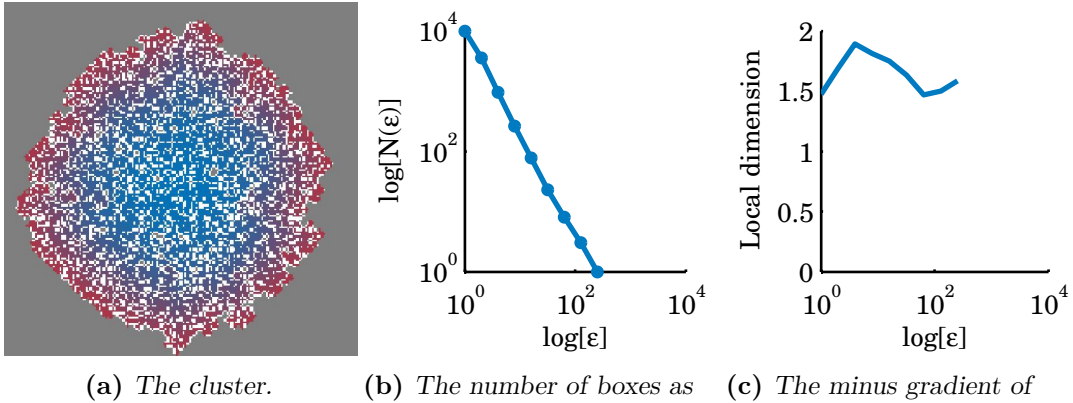
$$(1) \quad M_\varepsilon(\rho) \sim c\varepsilon^{-s}$$

where  $c$  and  $s$  are constants and  $M_\varepsilon(\rho)$  are measurements at different scales  $\varepsilon$  for  $\varepsilon \rightarrow 0$ . Falconer then shows that the fractal dimension can be estimated “as minus the gradient of a log-log graph plotted over a suitable range of  $\varepsilon$ ” [1].

One way to get the measurements  $M_\varepsilon$  is to use box-counting. When one uses this algorithm the different scales mentioned in Falconer’s definition are the sizes of the boxes.

We have used the function `box-count` by Moisy [3] to determine the fractal dimension of one percolation cluster. This implementation of the box-counting algorithm uses box sizes that are a power of two, consequently  $\varepsilon = 1, 2, 4, \dots, 2^q$  where  $q$  is the smallest integer such that  $q \leq (2N + 1)$ .

Figure 5a shows the cluster of which we have determined the fractal dimension using box-counting. It was generated with  $N = 80$ ,  $p = 0.7$ . Figure 5b presents the number of boxes as a function of the size of the boxes, figure 5c presents the minus of the gradient of figure 5b. From this graph we can infer the box-counting dimension by finding the local dimension for which the gradient is approximately stable. Using this method we find the fractal dimension to be 1.879, which neatly approximates the dimension 1.896 mentioned by Stauffer [4]. The small difference between these numbers can be explained by the relatively small size of our cluster and the fact that we present the fractal dimension of only cluster instead of the average over multiple clusters.



**Figure 5:** (a) The cluster ( $N = 80, p = 0.7$ ) used to compute the box-counting dimension. (b) The number of boxes used to cover that cluster as a function of the box size. (c) The gradient of the function plotted in (b).

### 3.4. CONNECTIVITY

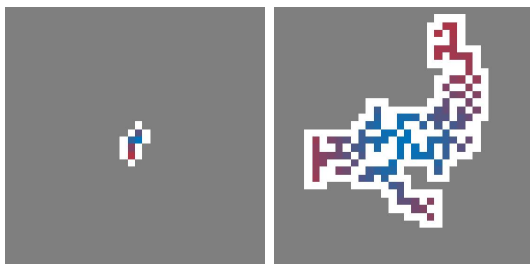
We consider two different connectivities, namely four- and eight-connectivity, which are illustrated in figure 1. In this section we discuss the influence of the 8-connectivity on the size of the cluster.

Figure 6 shows two clusters which have been grown using the same probabilities but different connectivities. We see that in this case the 8-connected cluster is much larger than the 4-connected cluster. Although a different seed for the algorithms may result in different clusters in general one would expect the 8-connected cluster to grow larger than the 4-

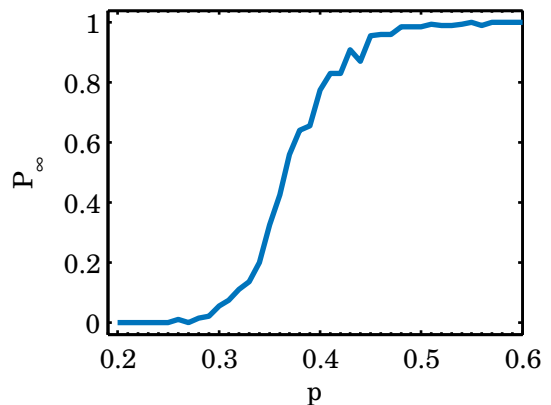
connected version. Since the expected number of sites that are occupied in each grow step when 8-connectivity is used is twice as high as the expected number of occupied sites with 4-connectivity.

The results of performing the same experiment as discussed in section 3.1 with the eight-connectivity mask, are presented in figure 10 in appendix A.3 and figure 7. We have changed the range of  $p$  to  $p = 0.2, 0.21, \dots, 0.6$ , since even for  $p = 0.3$   $P_\infty$  was close to zero.

It should be noted that for some values of  $p$ , especially larger values there are no mean



**Figure 6:** The results of growing a cluster with the same grid of probabilities with (a) four-connectivity and (b) eight-connectivity. Note that although the clusters are generated on a grid with  $N = 80$ , we have plotted them on a grid with  $N = 16$ .



**Figure 7:** Ratio of percolating clusters,  $P_\infty$ , as a function of  $p = 0.2, 0.21, \dots, 0.6$  when eight-connectivity is used. Ratios are calculated over  $r_{max} = 200$  runs on a  $41 \times 41$  grid.

cluster sizes, since no finite clusters were found. This indicates that one is much more likely to encounter a percolating cluster with eight-connectivity than with four-connectivity for the same value of  $p$ . Which fits with our earlier observation that the expected number of newly occupied sites with eight-connectivity is twice as high when compared with a four-connected cluster.

That for higher values of  $p$  a percolating cluster is more likely than a finite cluster is confirmed by figure 7, where we find that only for very low values of  $p$   $P_\infty$  is zero, and that  $P_\infty$  quickly approaches 1.

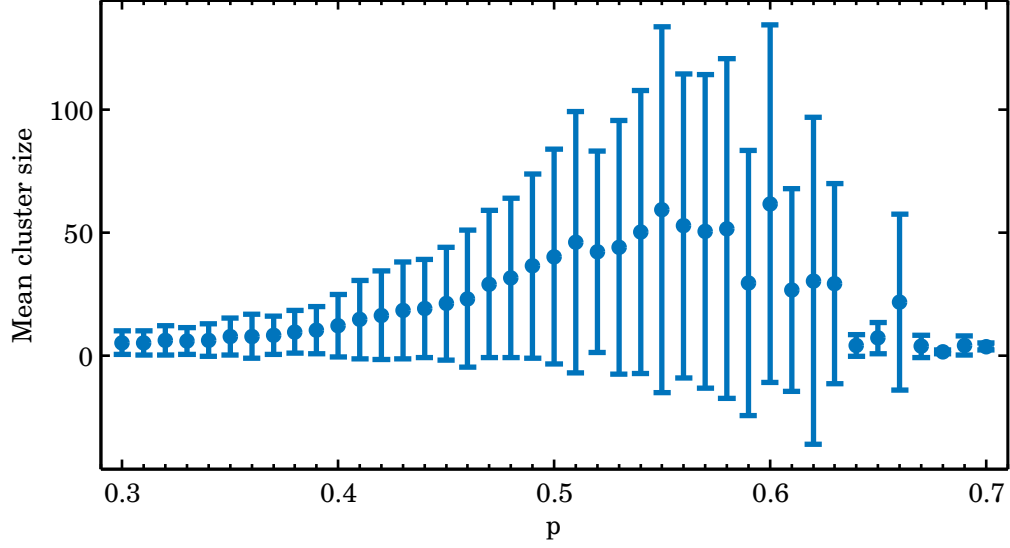
These findings suggest that  $p_c$  is much lower when eight-connectivity is used. Based on this, admittedly small experiment, one would guess  $p_c$  to be approximately 0.2 when eight-connectivity is used. More research is needed to find the actual value of  $p_c$  for eight-connected clusters.

## REFERENCES

- [1] Kenneth Falconer. *Fractal geometry: mathematical foundations and applications*. John Wiley & Sons, 2004.
- [2] Wolfgang Kenzel et al. *Physics by computer*. Springer-Verlag New York, Inc., 1997.
- [3] F. Moisy. *Computing a fractal dimension with Matlab: 1D, 2D and 3D Box-counting*. 2008. URL: <http://www.fast.u-psud.fr/~moisy/ml/boxcount/html/demo.html>.
- [4] Dietrich Stauffer. *Introduction to percolation theory*. Taylor & Francis, 1985. Chap. 2, pp. 15–58.

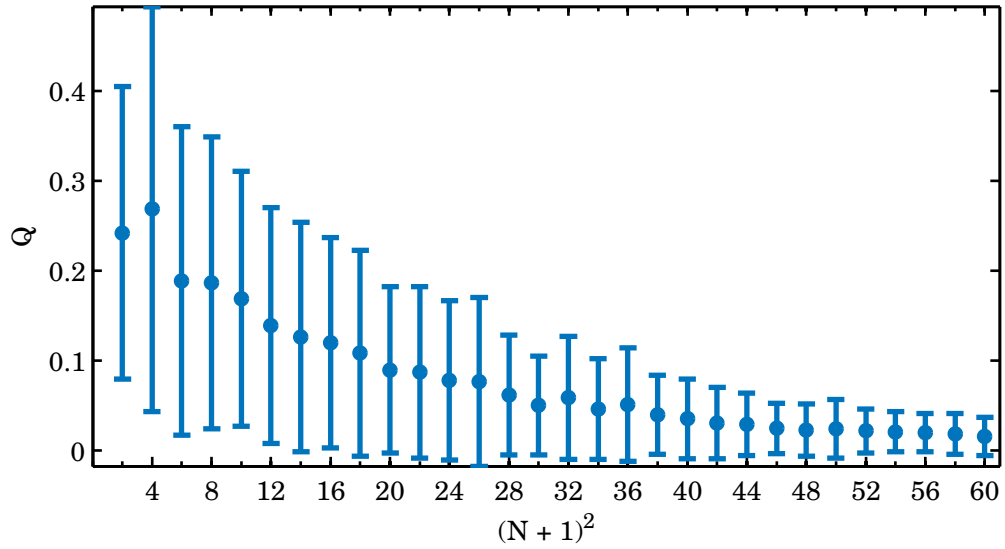
## A. RESULTS

### A.1. PROBABILITY



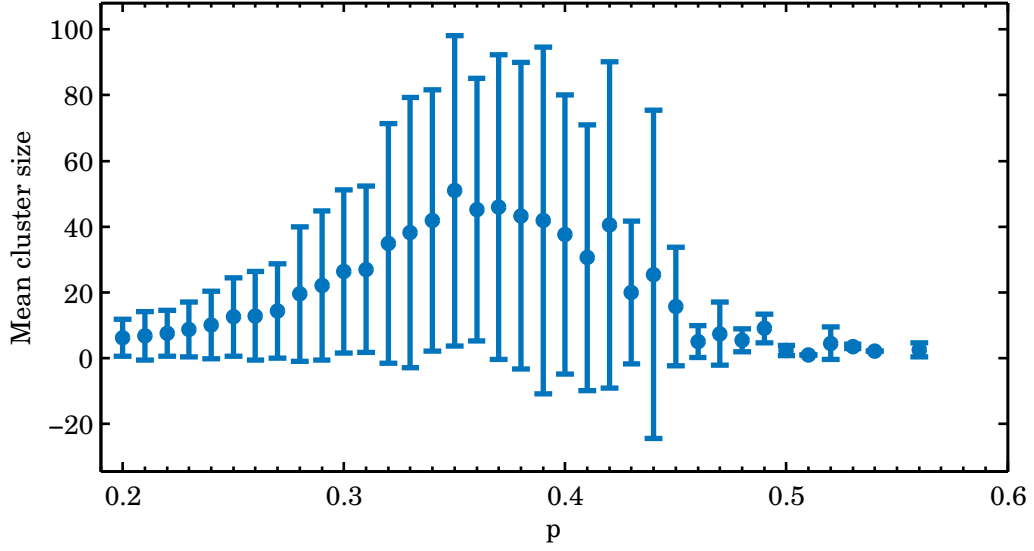
**Figure 8:** Mean cluster sizes, represented as points, and standard deviations, indicated by the vertical error bars, as a function of  $p$ , with a step size of 0.1. The mean and standard deviation were calculated over 200 runs on a  $41 \times 41$  grid.

### A.2. SYSTEM SIZE



**Figure 9:** The mean, represented as points, and standard deviations, indicated by the error bars, of the ratio of the cluster size to number of sites in the grid, i.e.  $(N+1)^2$ . The mean and standard deviation were calculated over 200 runs with  $p = 0.5$ .

### A.3. CONNECTIVITY



**Figure 10:** Mean cluster sizes, represented as points, and standard deviations, indicated by the vertical error bars, as a function of  $p = 0.2, 0.21, \dots, 0.6$  when eight-connectivity is used. The mean and standard deviation were calculated over 200 runs on a  $41 \times 41$  grid.