Simulation of percolation on massively-parallel computers

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Abstract

A novel approach to parallelize the well-known Hoshen-Kopelman algorithm has been chosen, suitable for simulating huge lattices in high dimensions on massively-parallel computers with distributed memory and message passing. This method consists of domain decomposition of the simulated lattice into strips perpendicular to the hyperplane of investigation that is used in the Hoshen-Kopelman algorithm. Systems of world record sizes, up to $L = 4000256$ in two dimensions, $L = 20224$ in three, and $L = 1036$ in four, gave precise estimates for the Fisher exponent $\tau$, the corrections to scaling $\Delta_1$, and for the critical number density $n_c$.

Percolation is a thoroughly studied model in statistical physics [2]. The algorithm invented by Hoshen and Kopelman in 1976 allows for examining large percolation lattices using Monte Carlo methods [3]. Unfortunately, this algorithm was invented for traditional sequential computers, and implementation on modern parallel computers is far from trivial.

The normal way to parallelize an algorithm which works on regular data structures is domain decomposition. In this case, the investigated lattice is cut into strips, and each processor is assigned one such strip for investigation. As the Hoshen-Kopelman algorithm investigates the lattice hyperplane by hyperplane (line by line in two dimensions; plane by plane in three dimensions), various ways of domain decomposition can be characterized by this hyperplane: for example, strips parallel or perpendicular to that plane.

The easiest way would be to choose parallel strips, as in that case the simulation of each strip can be carried out locally on each processor, only after that communication is necessary (exchanging the borders). Unfortunately, this means that each processor has to store a full hyperplane of $L^{d-1}$ sites for a $L^d$ system. In two dimensions, this no problem at all, but in higher dimensions this limits the size of systems that can be simulated.

When decomposing the system in perpendicular strips, each processor has to store only a part of the hyperplane, and thus larger system sizes can be
simulated. Unfortunately, this advantage comes at a price: Frequent interaction between neighbouring strips is necessary throughout the simulation, thus imposing a burden on runtime and complicating drastically the implementation.

This latter approach was chosen for a masters thesis [1]; a shortened version will be presented here.

1 Parallelizing Hoshen-Kopelman

The main problem when decomposing the lattice into perpendicular strips is to cope with the non-regular communication patterns arising from the Hoshen-Kopelman algorithm.

1.1 Local and global clusters

Clusters that are confined within a strip and are not in touch with interfaces between strips are called local; clusters that extend over several strips are called global.

The Hoshen-Kopelman algorithm describes clusters by labels. In the sequential version, a label can be a root label, describing a real cluster, or a non-root label pointing directly or indirectly to a root label (such labels are generated when during the counting a new cluster seems to emerge, but later is discovered to be part of another cluster).

For the parallel version, it is straightforward to introduce three types of labels: non-root labels, root labels associated with local clusters (local root labels), and root labels associated with parts of global clusters (global root labels).

Associated with local root labels are the number of sites within the corresponding cluster; global root labels carry the number of sites in the cluster within the strip, and additionally pointers to the left and right neighbour labels.

During the simulation, a local label can be changed to global, when it extends to the interfaces of the strip. A global label can be changed to local during the recycling process, when neighbouring labels are discarded.

When two previously different global clusters join at one site, the neighbouring strips have to be informed of that fact, in order to join parts of the corresponding cluster into one. This is called pairing, as pairs of labels are joined. To reduce the number of messages that have to be sent, we gather these and exchange information after the local part.

1.2 Information exchange

After the local part within each strip has been simulated, communication between the processors takes place to find out if clusters extend over the interfaces, and what global labels are interconnected with each other.
1.3 Recycling

An important step for economic memory usage is the frequent recycling of non-root labels, as these carry no information, but are just an artefact of the algorithm that speeds up computation. Additionally, also root labels can be recycled, when they are not present in the current hyperplane of investigation. These methods are known as Nakanishi recycling [10].

In the parallel implementation, we can use the same technique for purely local labels; on the other hand, we have to be careful not to recycle labels that are still referenced by global labels in other strips. We do that by exchanging information about these references; during this process, references to non-root labels can be reclassified. In that way, we can delete all non-root labels, even those pointing to global root labels.

Global root labels are recycled using a stepwise reduction of global clusters along the strip: the rightmost strip that carries a part of a global cluster checks if it is still alive; if not, it is recycled and the left neighbour is informed that its right partner has vanished. If the left neighbour has itself no left neighbour, it is converted to a local label.

1.4 Step-by-step description of algorithm

The following list is a semi-formal description of the algorithm. Local and communication part are repeated for each hyperplane the system consists of, recycling is done whenever necessary after the local and communication part, and counting is done after the full system was examined.

1. **Initialization**: Occupy the zeroth plane for busbar, if desired; initialize all data structures; etc.

2. **Local**:
   
   (a) Examine the strip site by site. Do labeling.
   
   (b) When two different global clusters join at one site, generate pairing information for left and right neighbour, but defer communication until after the local part.

3. **Communication**:
   
   (a) Exchange borders of strip with neighbours.
   
   (b) When two clusters of both strips join, convert clusters to global. If they are already global, but not yet connected, generate pairing information.
   
   (c) Exchange pairing information. Pair global labels that belong together. During this, new pairing information can come up.
   
   (d) Check if recycling is necessary due to tight memory conditions.

4. **Recycling** (if necessary):
(a) Reclassify the current hyperplane with root labels.
(b) Delete all non-root labels that point to local root labels.
(c) Reclassify the pointers to left and right of the global root labels by
asking the neighbours for the corresponding root labels.
(d) Delete all remaining non-root labels.
(e) Mark all living local root labels and delete the non-marked ones.
(f) Look for all global root labels that are not present in the current
hyperplane and have no right neighbour; delete them and send the
number of sites to the left neighbour.
(g) When a global label is informed that its right neighbour was deleted,
and it has no left neighbour, convert it to local.

5. Counting:
   (a) Count local clusters.
   (b) Concentrate global clusters.
   (c) Count global clusters.
   (d) Look for a global cluster which has not been concentrated. If it exists,
       we have connectivity. Sum up this cluster explicitly.
   (e) Do output.

2 Results of Monte Carlo Studies

All simulations were done right at the critical threshold \( p_c \) (except those for
Fig. 2) and on square (2d), simple cubic (3d), and simple hypercubic (4d) lat-
tices. The values for \( p_c \) were taken from literature:
\[
\begin{align*}
2d & \quad p_c = 0.5927464 \quad \text{cf. [6]} \\
3d & \quad p_c = 0.311608 \quad \text{cf. [7]} \\
4d & \quad p_c = 0.196889 \quad \text{cf. [8]}
\end{align*}
\]

As boundary conditions, one direction was busbar in two dimensions resp.
open in higher dimensions, one direction was periodic, and for more than two
dimensions all other directions were helical. This mix came quite natural during
implementing the parallel algorithm.

2.1 Cluster size distribution

For the number \( n_s \) of clusters of size \( s \) in our system, we expect a distribution
of kind \( n_s \propto s^{-\tau} \) right at the critical threshold \( p_c \). To make analysis easier, we
look at \( N_s \), the number of clusters with at least \( s \) sites:
\[
N_s = \sum_{s'=s}^{\infty} n_{s'} \sim k_0 s^{-\tau+1}.
\]
In a double-logarithmic plot, we would expect a straight line with slope \(-\tau + 1\). Deviations from the power law would not be visible due to the logarithmic scale, thus we plot \(s^{\tau-1}N_s\) linearly on the y-axis. We can clearly see in Fig. 2.1 the deviation for small \(s\) (due to corrections to scaling, see below) and for large \(s\) (due to boundary conditions).

![Figure 1: Cluster size distribution for \(L = 4000256\) in two dimensions. The dashed line corresponds to the theoretically asymptotic behaviour.](image)

The values found for the proportionality constant \(k_0\) (normalized by number of lattice sites) and the exponent \(\tau\) are:

- 2d \(k_0 = 0.032627(6)\) \(\tau = 187/91\)
- 3d \(k_0 = 0.057423(3)\) \(\tau = 2.190(2)\)
- 4d \(k_0 = 0.0611(4)\) \(\tau = 2.313(2)\)

Below \(p_c\), we expect the size of the largest cluster to be proportional to \(\log(L)\), cf. Fig. 2.1.

### 2.2 Corrections to scaling

For small \(s\), the clusters do not follow the power-law \(n_s \propto s^{-\tau}\); the system is not self-similar under renormalization, as the lattice spacing is an inherent length, very visible for small clusters. Thus our power-law is modified: \(n_s = k_0s^{-\tau}(1 - k_1s^{-\Delta_1})\). We find the exponent \(\Delta_1\) (and the factor \(k_1\)) by plotting \(\log(N_s/(k_0s^{-\tau+1}) - 1)\) against \(\log s\); for carefully adjusted \(k_0\) and \(\tau\), this yields a straight line with slope \(\Delta_1\) and intercept \(k_1\).

We get a straight line only for small and intermediate \(s\). For large \(s\), the finite-size effects increase the \(n_s\) over the expected value and limit the precision,

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*the value for \(\tau\) is supposed to be known exactly*
Figure 2: Average size of the largest cluster versus system size $L$ at $p = 0.5$ in two dimensions. The error bars represent the statistical error. Number of runs done for each $L$: eight for $L < 200k$, four for $200k < L < 1M$, two for $L > 1M$.

cf. Fig. 2.2. Implementing fully periodic boundary conditions could give an improvement in precision.

The values found for the corrections to scaling amplitude and exponent are:

\[
\begin{align*}
2d & \quad k_1 = 0.50(2) \quad \Delta_1 = 0.70(2) \\
3d & \quad k_1 = 0.48(5) \quad \Delta_1 = 0.60(8) \\
4d & \quad k_1 = 0.5(1) \quad \Delta_1 = 0.5(1)
\end{align*}
\]

### 2.3 Number density

The total number of clusters divided by the number of sites in the lattice is called the number density, right at $p_c$ the critical number density. For small systems, we expect finite-size corrections proportional to $1/L$. Statistical fluctuations depend on the total number of sites in the lattice and are proportional to $1/L^d$. Thus finite-size effects can be seen well in higher dimensions.

For two dimensions, we can simulate large $L$ and have no visible finite-size effects. But we can clearly see a dependence on the used random number generator. The classic and simple $\text{ibm = ibm * 16807}$ produces wrong results, whereas others agree well with each other (i. e. $R(103,250)$, $R(471,1586,6988,9689)$, $R(18,36,37,71,89,124)$, even $\text{ibm = ibm * 13**13}$ seems to be acceptable). Thus the number density can serve as a test for bad random numbers, cf. Fig. 2.3.

The values found for the number density are:
Figure 3: Corrections to scaling in two dimensions, for $L = 500k$ (+) and $L = 4M$ (×). The larger system offers higher precision, as the finite-size effects are weaker.

Figure 4: Number densities at $p_c$ for various system sizes $L$ in two dimensions, using different PRNGs: R(103,250) (+), R(471,1586,6988,9689) (×), ibm*16807 (boxes), R(18,36,37,71,89,124) (circles), and ibm*1313 (triangles). The solid line corresponds to the average for the $L = 1M$ runs of the two-tap, four-tap, and six-tap R(…) generators, the dashed lines to the statistical error.
\[ \begin{align*}
2d & \quad n_c = 0.02759791(5) \\
3d & \quad n_c = 0.0524387(3) \\
4d & \quad n_c = 0.0519980(2)
\end{align*} \]

3 Efficiency

When implementing an algorithm on a parallel computer, we want to know how efficient our implementation is, i.e. if not too much time is wasted for communication.

The amount of necessary communication is roughly proportional to the interface between the strips, i.e. \( NL^{d-1} \). This communication is the main difference between the sequential and parallel implementation, and reduces the parallel efficiency.

In two dimensions, a sequential implementation is roughly as fast as the parallel one, which means that the effort for communication is neglectable. In four dimensions, the fraction of runtime needed for communication is significant, but the time for the local part is still larger.

Although the domain decomposition in perpendicular strips requires more communication than other methods, it is still efficient enough for up to four dimensions. For even higher dimensions, this may change.

4 Summary

Parallelizing the Hoshen-Kopelman by dividing the lattice into strips perpendicular to the hyperplane of investigation is a viable approach. Using this method, world record simulations in two, three, and four dimensions have been carried out, beating the old world records.\(^4\)\(^5\) High precision results for the Fisher exponent \( \tau \), the corrections to scaling exponent \( \Delta_1 \), and the number density \( n_c \) have been obtained. The values found are in reasonable agreement with those from other groups.\(^4\)\(^5\)\(^9\)

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