CLUSTER COUNTING: THE HOSHEN-KOPELMAN ALGORITHM vs. SPANNING TREE APPROACHES

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Two basic approaches to the cluster counting task in the percolation and related models are discussed. The Hoshen-Kopelman multiple labeling technique for cluster statistics is redescribed. Modifications for random and aperiodic lattices are sketched as well as some parallelised versions of the algorithm are mentioned. The graph-theoretical basis for the spanning tree approaches is given by describing the breadth-first search and depth-first search procedures. Examples are given for extracting the elastic and geometric “backbone” of a percolation cluster. An implementation of the “pebble game” algorithm using a depth-first search method is also described.

The algorithmic task of performing cluster statistics (i.e. cluster counting) is almost as old as the computer calculations: one of the pioneers of percolation theory, S. Broadbent, presented a percolation problem at one of the first conferences on Monte Carlo simulations back in 1954. Since then for the physics community the cluster statistics problem has been tightly connected with the percolation theory. Another co-founder of this theory, J. M. Hammersley, argued in the 60-s that the numerical study of percolation models is strongly hindered by the lack of fast enough computers. He predicted that this problem will remain even for the computers of the next century. Only a few years later Hoshen and Kopelman proposed their cluster-labeling algorithm (further quoted as HK76), which made the pessimistic view of J. Hammersley completely irrelevant. Before HK76 it was believed that the computational efforts grow faster than the squared number of “particles” subject to clustering. (Particle here means any geometrical object which could be connected under certain rules with some of its neighbors.) The HK76 algorithm proved that this relationship can be linear. That was the real breakthrough, because very often, especially for percolation models, the number of particles might be well beyond $10^6$: the world largest model percolation system being simulated, has (more than) $10^{14}$ particles. Moreover, the HK76 algorithm solved the serious problem of lack of computer memory for very large percolation systems.

Next we will describe the cluster counting problem itself, then the HK76 algo-
rithm and some modifications will be presented. Afterward the graph-theoretical framework for cluster descriptions will be sketched. The discussion section will be on some comparisons and combined approaches.

1. The cluster counting

Remaining on the ground of physics intuition, let us imagine that we have a large number of objects spread somehow in space. Such objects could be atoms, monomers, polymers, sand grains, ... telephones, computers, computer networks, .. stars, galaxies. For each pair of objects we may determine (following certain rules – often probabilistic) whether they are directly connected (i.e. adjacent, bonded) or not. Indeed some objects might be indirectly connected via chain(s) of direct connections.

Each set of interconnected particles forms a (connectivity) cluster. For each (random) configuration, we will need to extract some statistics for the distribution of the clusters – their size, form, fractal dimension. Then a statistics for an ensemble of configuration could be made.

So, the cluster counting could be thought as the following task:

1. Create a (computer) model structure of the objects for which the spread of connectivity will be studied. In some cases that could be a digitized image of natural objects, e.g. a colony of bacteria.

2. Decide, for each pair of objects, if they are adjacent (bonded) or not.

3. Identify the clusters of connected objects.

4. Make statistics of certain properties of the clusters. Store the statistics for further use.

5. Repeat 1 – 4 (or 2 – 4) enough times in order to have reliable counts for the statistics made within each single realizations; or, follow the evolution of the cluster statistics with time, if the realizations are not independent.

The difficulties are concentrated mainly in item 3 of the list above and the present paper focuses on it. The other items could be also nontrivial as well, and what follows is a short discussion about them.

Item 2 might be a problem (mostly in non-physics applications) if there is no a priori information about which pairs of objects are bonded. Instead there could be some “plausible” assumptions. For example, when the objects are situated in two dimensions one could presume that the bonds should form a mosaic (would not cross each other) and among all possible mosaics one should chose the “less heavy” mosaic. One attaches to each bond (edge of the mosaic) a certain weight (e.g. its length, or the square of the length), and then searches for the mosaic with a minimal weight. It turns out that this search is analogous to the problem of constructing a minimum spanning tree in the framework of graph theory: a further discussion can be found in [5] and references therein.
If the number of objects is very large, the algorithmic bottleneck might be item 1. This problem could be alleviated using techniques similar to those applied in calculation with very large (“monster”) matrices, but this fact does not decrease the virtue of HK76 method to use $d-1$ dimensional cuts of the “sample” – see the next section.

2. The Hoshen-Kopelman Method and its modifications

As many seminal methods, the HK76 algorithm works best for the example, on which it was demonstrated first – the ordinary percolation model on square lattice. Let us describe first the bond percolation model itself.

The “objects”, we have discussed up to now about, are, in the present example, the sites of a square cut (with size $L$) from the infinite square lattice. Each lattice bond might be “open” with probability $p$ ($0 \leq p \leq 1$). As it is known, there is a critical probability $p_c$ such that for $p \geq p_c$ a spanning cluster of open bonds (a cluster which connects the edges of the lattice) appears with probability $S(L,p)$ and $\lim_{L \to \infty} S(L,p) = 1$.

We will describe the HK76 algorithm using an analogy with a “brick layering” in which each lattice site is a brick in the wall (the lattice). The “brick layering” (for given $p$ - in this analogy this is the probability to put mortar between two bricks) starts, say, from the lower left brick (vortex) of the wall (the lattice). One adds from left to right vortex after vortex, each time checking if the new vortex is connected with the last one. This “check” consists simply in drawing a (pseudo) random number distributed equally between 0 and 1: if the number is less than $p$ the vortices become bonded.

We start describing the construction of the first row: We assign to the left most vortex a label: “1”. If the next vortex added in the row is connected with the first it accepts the same label (“1”). The label “2” is assigned to the first vortex inside the row for which the connectivity check fail. In general; if the next vortex appears connected to its previous neighbor it accepts the same label — if not, it accepts the next number as a label. So the vortices with the same labels form (one-dimensional) clusters.

Contrary to the masons’ practice, the second row is created by adding bricks in a way so that they contact only one brick from the lower layer. This time the connectivity check should be made with two neighbors: the previous vortex in the same row and the lower vortex.

Here a cluster label conflict may appear: the new vortex bonds with both neighbors, and both may have different labels attached (See Fig. and the similar figure in ...). Indeed, there is a “brute force” method for solving it: attach to the new vortex the smaller of the two numbers (e.g. $n_1 < n_2$); then change all labels $"n_2"$ to labels $"n_1"$ – this is the method that made Hammarsley so pessimistic.

The HK76 approach avoids this need for backward relabeling. Instead of changing the vortex’s labels, a one-dimensional array of “labels-of-labels” ($LL[..]$) is created. The size of this array should be greater than the possible number of different
labels which could be needed. Then the i-th element of this array is “the label” of all labels “i” put on vortices during the “brick layering procedure”. This time a cluster may have vortices with different labels.

The HK76 method needs one more variable: it stores the number of the last used label. When a new vortex (“V”) is added and it is not bonded to its two neighbors this variable increases by one and the vortex label obtains its value (say j). The respective element of the “labels-of-labels” is set to unity ($LL[j] := 1$) – the “current size” of the cluster to which the new vortex belongs. If there is no label conflicts, every new vortex, which is a direct or indirect neighbor to the vortex ”V”, accepts the same label and the content of $LL[j]$ is increased: $LL[j] := LL[j] + 1$.

If a label conflict occurs then the label of the new vortex accepts the smaller number ($n_1$ as above), but this time there is no other change of labels. The values of $LL[n_2]$ and $LL[n_1]$ change instead. If the label conflict occurs for the first time, this change is simply:

$$LL[n_1] := LL[n_1] + LL[n_2]; \quad LL[n_2] := -n_1$$

In that way, the size of the cluster is stored in the array element $LL[n_1]$ and $LL[n_2]$ points to the “root” of the cluster, or, the cluster “owner”. When one examines the third or higher row, the summation above could be done only after checking if the values of $LL[n_1]$ and $LL[n_2]$ are positive. If not, the chain of pointers should be followed:

while $LL[n_i] < 0$ do $n_i := -LL[n_i];$

in order to find the current “root” for that cluster. The details of this procedure could be found elsewhere — e.g. the original paper or the very recent paper of Hoshen et al. If we return to our brick layering, we can see that the considerations for the first two rows could be repeated for the $m$-th and $(m - 1)$-th layers. Without entering into details, the algorithm sketched above allows one to use only two layers during the simulation. After completing the lattice sweep (i.e. ”the brick layering”), the information needed for cluster size statistics is stored in the array of “labels-of-labels” – in its positive elements.

The HK76 algorithm has to be modified in order to allow the identification of a spanning cluster — a cluster which connects two opposite edges of the lattice. This
could be done if label "1" is ascribed to the vortices in the first column and label "2" to the right-most column.

Indeed, properties of clusters other than their size and their spanning could be of interest: e.g. the radius of gyration, the shape anisotropy, certain fractal dimensions and so on; all that for the cluster itself or for subsets of its vortices and/or bonds.

Usually the first thing to be done is to "extract" a certain cluster – that is to find the coordinates of all vortices which belong to it. If the whole structure is kept in memory, this task can just be accomplished by inspection of the $LL[\ldots]$ array. The inspection shows which labels (attached to certain vortices) corresponds to the same cluster, even if there could be multiple labels for one cluster.

In the original HK76 method, the random percolation structure is created “on the fly” – during the “brick layering”, as mentioned above. This portion of the percolation structure which remains behind the “growth zone” is destroyed, so one keeps in the memory only a small fraction ($\propto (d-1)L$, where $d$ is the spatial dimension) of the percolation configuration. After completing the “layering” one gets the whole set of labels which form separate clusters. But the coordinates of the respective vortices are lost at that moment!

A way out is to keep the whole percolation structure in memory, and to lose the memory saving advantage of HK76. Instead, the $(d-1)L$ memory cost might be preserved as follows:\footnote{\textit{\textsuperscript{9}}} After the first “brick layering” for a certain configuration, one memorizes the array $LL[\ldots]$ (say, as $LLold[\ldots]$). Then the procedure is repeated with the same pseudo-random number sequence. During the second sweep, after attaching a label to a new vortex one can determine to which cluster belongs this vortex. This can be done by examination of the $LLold[\ldots]$ array.

Indeed, modifications of HK76 algorithm for other periodic lattices are more or less straightforward. The case of non periodic lattices needs some discussion and will serve as a bridge to the Graph-Theoretical approaches described in Sec.2.1.

2.1. \textit{A modification for non periodic lattices}

We may return to the brick layering analogy and two dimensional structures. The following consideration could be easily applied to dimensions higher than two.

The space region, where the connecting objects are situated, is divided into sub-cells – so called “imaginary covering mesh”\textsuperscript{10,11} Then the brick layering consist in adding “bricks” with the size of a sub-cell. Each brick may “contain” one or more objects. The number of objects depends on the specific problem: the distribution of the objects’ shape and size, the connectivity rules and so on.

We will refer here to a soft-shell-hard-core disks continuum percolation model (named also \textit{penetrable concentric shell} model\textsuperscript{12}).

One deals with randomly spread disks with equal radii (say, $r = 1$). The disks are “penetrable” up to a distance $\lambda r$ from their center ($\lambda \in [0,1]$). Two disks “are connected” if the distance between their centers is less than $r$ (and greater than $\lambda r$). Indeed the hard core restrictions lead to correlations which can differ depending on
the way the random structure was created.

The limit $\lambda = 0$ leads to the freely overlapping disks model, and the opposite limit ($\lambda = 1$) gives the hard disks model.

The use of space sub-cells and the “bricks” depends on the value of $\lambda$. For $\lambda$ not very small (e.g. $\lambda > 0.1$), one can prescribe that no more than one disk center can lie in a sub-cell. Then the sub-cells should be squares with edge length (slightly) less than $\sqrt{\frac{2}{\lambda}}$. By means of (pseudo) random numbers and an equilibration one determine the disks center coordinates. On each brick could be written the coordinates of a disk’s center (elsewhere the brick is “empty”) if the coordinates are within the respective cell. After adding a new and non-empty brick one checks “in the vicinity” among the already added bricks if there are disk centers at a distance less than $r$. Similar procedure was applied for percolation on aperiodic lattices (quasi-lattices).

The above procedure can not work for $\lambda = 0$ and would be ineffective for very small $\lambda$. An algorithm with more than one disk in a cell was proposed in for the case $\lambda = 0$. Here one faces a “data structure” problem: up to now a representation of data by arrays with fixed size was supposed, but this time one could not determine a priori how many disks there would be in one cell... The quest for a general approach to such kind of problems leads to the notion of linked lists and the graph-theoretical representations which will be discussed later.

### 2.2. The cluster flip dynamics and the parallel algorithms

An important stimulus for developing efficient parallel algorithms for cluster counting became the cluster-flip dynamics for Monte Carlo simulations of spin systems. Such dynamics were proposed first in 1987 (so called Swendsen-Wang dynamics) and after that subjected to numerous modifications.

Some spin variables defined on the lattice sites may form clusters of “equal” (e.g. parallel) spins. Two parallel neighboring spins may belong to one cluster if an additional (probabilistic and temperature dependent) rule is fulfilled. Now “the important property” for a cluster is the spin direction in it, not its size.

For a sequential algorithm one can easily modify the HK76 method to perform cluster-flip dynamics. As usual, the simplest example is the implementation on Ising models. Here clusters with spins ”up” and clusters with spins ”down” might be formed. The vortex labels may then start (say) from three and in the root of the cluster one can put ”-1” for clusters with spins up, and ”-2” for ”down” spins. Now all spins in a cluster may flips their direction just by changing the root from ”-1” to ”-2” and vica versa.

Such kinds of algorithms were proven very effective for large systems at criticality, and many efforts were devoted to developing parallelized codes. Two classes of algorithms could be distinguished: for computers with few but powerful nodes and for massively parallel computers. It appears that massively parallel computers are suitable for small systems and computers with powerful nodes for large systems.

One can map the percolation configuration to the configuration of nodes for a
computer with several thousand (or even hundreds of thousand\textsuperscript{20}) processor nodes — say, one (or several) site(s) per node. The labeling here relays on parallel updating on all nodes. If each node carries one site the labeling can be described as “local diffusion” procedure\textsuperscript{21,20} supposing that all nodes were initialized with different label, on each update step each node checks all its neighbors and chooses the lowest label as its own for the next update step. This is repeated until no more label changes occur, and so, nodes with equal labels form the clusters. Some further discussion for application to spin models can be found in ref.\textsuperscript{19}.

The algorithms for parallel computers with few but powerful nodes attract more attention, at least because each cluster of networked workstations may play the role of parallel computer. In that case the parallelized versions of the HK76 algorithm are of prime interest. It is accepted now that the HK76 algorithm can be successfully parallelized.\textsuperscript{22,23} The idea is to divide the (square) sample into strips: one strip per node. On each strip runs (in parallel with others) a sequential HK76, keeping the labels for the boundary vortices. Then a master node collects the data and recovers the whole configuration.

3. Graph-Theoretical approaches and spanning trees

In a HK76-like method we start with the assumption that some objects exist in space and a rule is known to determine which pairs of them are directly connected (bonded). This changes a bit when a graph-theoretical framework is used.

It is assumed that a list of (abstract) elements could be composed. Each element has a labeling number and each pair of elements might be “bonded”. The procedure for picking up the elements and finding the bonds between them is a question of technique usually skipped in such consideration. Here follows only a short description of the overall procedure (as one can deduce it form the previous sections):

1. Add a new element (object, vortex..) to the list. Each element could carry some additional information (e.g. spatial coordinates), including some labels eventually subject to further change.

2. Check with all (added to the moment) elements in the list, which of them are connected to the new one.

3. Attach to the new element a sublist which contains the numbers of its neighbors – or (more generally) – supply this element with pointers to its neighbors. Update accordingly the sublists attached to each of the neighbors. (In that way one counts a bond twice, otherwise the graph will become “artificially” directed.)

In that way we obtain a computer presentation of a graph with its vortices (the list elements) and edges (the bonds). (For case of simplicity we consider undirected single edges — with one exception — the pebble game algorithm, which is discussed in Sec.\textsuperscript{2})
A chain of edges (chain of bonds) is called a path. A set of vortices connected with path(s) is a connected component (a cluster) in a particular graph. There are subsets of paths in a cluster, such that the vortices remain connected, but there can not be cyclic routes on such a subset. The name for these subsets of paths is spanning tree. Different spanning trees could be determined for a cluster, but only one might exist at a time.

The well-known forest-fire model\textsuperscript{2} gives an example how a spanning tree can be constructed. (Indeed spanning tree and forest tree came from different terminologies so the similarity is a little misleading: Here a forest tree exists on each vortex, and the bonds between vortices may form a spanning tree.) As a first step a certain tree in “the forest” catches fire. It ignites all its direct neighbors and burns out. At this step connections are drawn between the first tree and all its direct neighbors. At the next step, each burning tree ignites its “green” neighbors and bonds are drawn to the “just ignited” trees from the tree which ignited them. These trees then ignite their neighbors, and so on.

The set of bonds which remains after all forest trees are burnt out is a branched structure which connects all vortices and no cyclic routes exist – a spanning tree for that cluster. Different spanning trees might be constructed depending on the order in which the burning trees are visited on each step.

This method of burning was applied for determining some fractal properties of the critical (the incipient) percolation cluster\textsuperscript{24,25} on square and cubic lattices.

Without the use of graph representations and linked lists algorithms, the above procedure could be quite time consuming:

One has to scan a two- (or three-) dimensional array for the square (or cubic) lattice which contains the studied cluster. The number of scans is equal to the number of steps (the number of burning tree generations) in the above method of “burning”. The number of step ($N_s$) in its turn is proportional to the so called

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{depth-first-search.png}
\caption{An example of numbering of sites by depth-first search.}
\end{figure}
shortest path in a cluster:\(^{25}\)

\[ N_s \propto \ell \propto L^{d_{\text{min}}} \]

where \( L \) is the system size, \( \ell \) is the shortest path, and the fractal dimension of the shortest path is \( d_{\text{min}} \approx 1.13 \) in two dimensions, and \( \approx 1.34 \) in three dimensions.

Another way, based again on fixed-size-array representation, is to perform “walks” through the array-elements, with all drawbacks of the “ant in the labyrinth” algorithms.

Describing the same type of algorithms in a graph theoretical framework will provide the basics for our further considerations:

Let us return to the enumerated list in the beginning of this section. It describes the procedure for the construction of a linked-list data structure. It does not depend explicitly on the underlying periodic or random lattice, neither on the spatial dimensionality. The size of the data structure is proportional to the number of elements irrespective of the spatial extent of its geometric counterpart.

While the case specific issues are concentrated in item 2) in the mentioned list, the general problem for data links management should be solved in the last item. If there is a maximum number of connections (\( C_{\text{max}} \)) for a system (say, with \( N \) elements), a crude solution is to create an array with size \( N \times C_{\text{max}} \) for handling the links. Indeed the better way is to use based on pointers algorithmic constructions as stacks and queues, whose descriptions could be found in any textbook on C or PASCAL (and now FORTRAN90). In the following do not refer to any specific scheme for maintaining data links.

The point is that one can rely on well established procedures for following the links (the connections) between elements. Two of the most important methods for searches on connected subgraphs\(^{26}\) are the depth first search (DFS) and the breadth first search (BFS).

Those methods will be the subject of two examples. First, a DFS function will be applied to cluster size statistics on a percolation model – the same task for which the HK76 method is usually used.

The algorithm could be divided to two steps:

1. Create a linked list with the vortices (and the edges) of the studied percolation structure. Each element should “carry” a Boolean variable “checked” set to ”FALSE”.

2. Pick an element of the list which is ”not checked”. Set to one the variable which will contain the cluster size (\( \text{clust}(i)=1 \)) Perform a DFS procedure which counts the number of direct and indirect neighbors of the picked element, mark them as ”checked”. Store the result. Pick the next ”not checked” element...

In this way the data structure examination remains independent from its creation. The implementation of DFS for cluster size statistics can be described (in a
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quasi-formal† way) as follows:

line 1  function DFS(vertex.V,i);
line 2  checked.V:=TRUE;clust(i):=clust(i)+1;
line 3  for vertex.W in (neighbors of V): if not checked.W do DFS(vertex.W,i);
line 4  ... the postvisit instructions here ..
line 5  return; (end of the recursive function DFS...)

where "checked.V" a boolean variable included as element of a record (a structure) attached to the list element "V".

The whole program (including the creation of the linked list) would not exceed one page, and, more important, the logic of the program relies only on the five lines here. (Instead of recursive function (a function which can call itself) one can use the stack type of data structure to perform the same graph search.) The algorithmic context for the program instructions is very important in general: the instructions before the line 3 are “previsit” instructions, and these after line 3 – as “postvisit”.

Indeed the label "checked" can hold more than two different values, so the separated clusters may have different labels after completing the cluster statistics. Additional labels could be defined as well; clusters could be moved to other linked lists... One can extract easily the largest cluster and then to apply e.g. a linked-list implementation of the “burning” algorithm mentioned above.

Here follows the second example: the “burning” algorithm will be implemented by means of the breadth first search (BFS) procedure. The task is to find the shortest path between two sites (say, "1" and "2") in a cluster.

1. Create a linked list with the vortices (and the edges) of the studied cluster. Each element should carry two boolean variables: "checked" and "InThe-Queue", both set to "FALSE", and an integer variable("Level") set to 0.

2. Attach labels to two “opposite” vortices (say, "1" for the vertex with the largest y-coordinate and "2" for the vertex with the smallest y).

3. Start from vertex "1" a breadth first search (BFS) for the element with label "2". When the element with label “2” is reached, the BFS could return the length of the shortest path between “1” and “2”, which is proportional to the level of search reached at that moment (see below and ref.25).

In order to describe the BFS function one needs first a description for the queue type data structure. This is a linked list, which works on the principle first-in, first-out, like the flow through a pipe (see Fig.2). It suffices for the proper use of a queue if one is able to add the “last” element(E) of the queue (the respective function will be denoted in the examples as: Inject(queue,E)), to read the first element (Read(queue)), to remove it (Pop(queue)).

The BFS function could be implemented for finding the shortest path in a cluster as follows:

†The notation used here do not follow strictly certain programming language, but hopefully, is clear enough.
function BFS(vertex.V);
    create a queue with the only element V; InTheQueue.V:=TRUE;
    while queue not empty
        V:=Read(queue); Pop(queue);
        checked.V:=TRUE;
        for vertex.W in (neighbors of V)
            if ((not InTheQueue.W) AND (not checked.W)) do
                Level.W:=Level.V + 1;
                InTheQueue.W:=TRUE;
                Inject (queue,W);
            end do;
        end for;
    end while;
end function BFS;

A program flow for this function is illustrated for the graph on Fig.3. The numbers in parenthesis correspond to the variable “Level” attached to that site. The other number corresponds to the order in which the site “enters” the queue.

The solid line boxes below present the queue content before the second execution of the instructions Read(queue) and Pop(queue). The arrows show the changes in the queue content before the third execution of the mentioned instructions.

In order to compare with the “natural” description of the burning method, one should point out that the instruction ”checked:=TRUE” means: the forest-tree ”V” was ignited in the previous step(“Level”) and will ignite its neighbors (which are not yet burning). And, before Inject-ing a burning forest-tree into the queue, one writes down at which step this tree was ignited. A forest-tree for which both labels ”InTheQueue” and ”checked” are set to ”TRUE” is an already-burnt-out one.

After completing the procedure, the integer ”Level” written on each element denotes the shortest path from the respective vortex to the vortex, “where the fire was initiated” – the starting point of the breadth-first search. If the search started from vortex labeled ”1”(see above) the value of ”Level” attached to the vortex labeled ”2” would give the shortest path between these two vortices (supposing all connections have equal length).

Repeating the same procedure from ”2” can give other important characteristics: the vortices which form so called “elastic backbone” — the union of the shortest paths between ”1” and ”2”. Now we suppose that each vortex(the respective list element) carries a second integer label, say, ”BackLevel” (keeping labels ”Level” with its previous values). After completing the second(from ”2” to ”1”) search, the vortices for which:

"Level" + "BackLevel" = TheShortestPathLength

form the “elastic backbone”.

The next step in the determination of the cluster structure could be the extraction of the geometric backbone. (“Almost” synonyms for geometric backbone are:
current carrying part (but see ref.28), or, geometric backbone.)

Just to present another example we will stick to the definition: a vortex belongs to the geometric backbone (in this example) if it lies on a self avoiding walk between ”1” and ”2”. Indeed the geometric backbone includes the elastic one. We will accept that the elastic backbone sites are “black”, the rest of backbone sites are “gray”. All sites are “white” in the beginning. After the end of the search, the sites which remain “white” belong to the “dangling ends” of the percolation structure.

The use of a label “tested/(not tested)” is not enough here, one could use instead a “search number” which is increased after each depth-first search. A site is “not checked”, in the context below, if the “search number” ascribed to it is less than the current search number. If a site is tested during the search it accepts the current search number. (A similar approach has been used in the implementation of the “pebble game algorithm” – see below and ref. 29,30.) The following list presents the main items in an algorithm for backbone extraction based on depth-first search.

- Find the elastic backbone
- Pick a ”black” or ”gray” vortex which has at least one ”white” and ”not checked” neighbor. Start a depth-first search through the ”white” and ”not checked” vortices.
- On each step of the DFS procedure (after the first) check for ”black” or ”gray” neighbors. If one is found, this branch of the search terminates and all sites which will be traversed during the “postvist” instructions, on the way back the origin (the vortex which initiated the search) have to be set gray.
- If the depth first search failed to find a gray or black site; repeat it using as the current search number a very large number (say, greater than the number

Figure 3: An example of numbering of sites by breadth first search. Below is given the queue needed for the second step.
of particles in the system). This is a way one to mark the sites, which do not belong to the backbone, and, hence there is no need to be searched again.

The backbone extraction is completed when no more site eligible for search have remained.

3.1. Which is better?

The sequence of “burning” examples in the previous section was aimed to show how conceptually transparent such algorithms could be if described in a Graph-theoretical framework. One must first adopt the spanning tree concept which might be difficult for the beginner. Other drawbacks exist as well, but we start form the advantages of the graph theoretical approaches based on spanning trees:

First, one can divide the cluster counting and/or cluster description problem to loosely connected parts, each part to be solved separately and (almost) independently from the others. Each part could split in turn in several, well separated subunits. On the higher level one can distinguish i) the task for creating a proper data structure – the linked list of objects, which clustering is studied; and ii) the cluster counting itself.

When the data structure linked list is constructed, subtasks arise as: how to describe the direct connections between elements, the order of elements, what additional information each element should carry: space coordinates, number and type of labels... Sometimes the data structure is created as a result of self-dependent computational problems e.g molecular dynamics simulation or continuous Monte Carlo. Indeed it is important that the input data structure might be subject to extensions, say, adding new labels to each element, or reordering them.

After having the linked list data structure (i.e. having a graph representation), one can explore the generic methods of graph searches and spanning trees. A simple set of primitive searches could be used at that stage: combinations of depth-first search and breath-first search functions can solve in a transparent and effective way many tasks related to the cluster separation and the cluster structure.

The computational complexity of these searches is usually known, so the computational costs could be predictable, and well planned. Usually the efforts rise linearly with the number of elements, the problem is that the proportionality coefficient is usually large. Here start the drawbacks of the linked-lists.

As a rule one must keep in the central memory the whole structure which is in contrast with the HK76 algorithm where only (d-1) dimensional cuts are kept together with the Labels-of-Labels array. Sometimes one must keep the whole structure even with HK76 type of algorithm, but the memory requirements for linked-list approaches might remain higher by factor up to ten, compared with HK76 and other methods based on fixed-size-arrays representation.

The depth of the recursion stack is not infinite, and one should keep in mind its possible overflow for large structures.

Perhaps the most serious problem: one can hardly imagine effective implemen-
tations of parallel codes for a linked list data structure and for recursive searches on it. Instead, one could use the trivial parallelization for statistical problems – to run independent ensemble samplings on the different processing nodes.

The contradiction could be expressed as: a spanning three approach may perform faster for large systems, but needs more memory and can not be parallelized, so, very large systems are inaccessible to it.

Some time combined methods which use both a HK76 scheme and a spanning tree searches might be the best choice. A possible combination could be sketched as follows:

A very large \((L \times L)\) percolation system is studied by a parallel computing system: say, a cluster of \((N + 1)\) workstations – \(N\) nodes and a host. The sample is divided on \(L/N \times L\) strips. It is swepted three times. The first sweep is a parallel version of a HK76 algorithm (e.g. as in ref.\(^{22}\)). A second sweep of the parallel code with the same sequence of random numbers would allow to extract the coordinates of some of the percolation clusters. On the third step clusters these clusters are distributed to the nodes; so each node could perform spanning tree searches on a different cluster. So, in such a combination the Hoshen-Kopelman algorithm would work as a kind of preprocessor for the spanning tree searches.

3.2. A final example: the pebble game in two dimensions

We have considered up to now only simple connectivity clusters and undirected graphs. Here we will present a case where a non-local condition for connection between sites forming a cluster is imposed. It will lead us to search on directed subgraphs.

One considers subclusters to the usual connectivity percolation clusters imagining that each bond represents a rigid bar and each site a (flexible) joint. The task is to recognize the subset(s) of bonds(bars) and sites(joints) which are mutually rigid. It means: if one applies a stress between any two sites which belong to a rigid subset there is no possible movement of the sites without changing the length of some of the bonds in this subset.

The task could be solved in a very elegant way by using an analogy taken from the classical mechanics of point masses. As known the total number of degrees of freedom\((F)\) for a system of \(N\) point masses in \(d\) dimensions is simply \(F = d.N – C\), where \(C\) is the total number of independent restrictive conditions. In our case each point mass is a site (a joint) and each constraint is imposed by adding a bond(rigid bar), between given two sites. So, a rigid (sub)cluster corresponds to a rigid body in the sense of classical mechanics: such cluster should have three degrees of freedom only (in 2d): they correspond to two translations and one rotation of the whole set of point masses.

The task is reduced to answering the question: which constraints are independent? The way of getting this answer could be described again by a build-up analogy: this time instead bricks each time new bar is added and a decision is taken if this bar impose a new constraint or it is redundant for the percolative rigidity.
Now a “pebble game” can be introduced: we start with the sites of an unconstrained lattice (point mass system). To each site (point mass) are attached two free pebbles which correspond to the two degrees of freedom of the point mass. The “pebble game” starts with adding the first bar (present bond) between two (neighboring) sites. Then one of the sites is chosen at random and one of “its” free pebbles is moved to “cover” the bar: it becomes “anchored” to the closer end of the bar. In this way a direction is defined: say, pointing outward from the anchor end. The site on the anchor and still has two pebbles but one of them is “anchored” and the other is “free”. So the system of two joints and a rigid bar connecting them has now three degrees of freedom, and represent a directed subgraph with two sites and a directed bond between them. Adding each new bond one has to check if there are two free pebbles on each of the sites “under connection”. If one of the sites has less than two free pebbles then the respective site belongs to a directed subgraph and one or both of its pebbles are anchored to (a) previously added bond(s).

Now one has to mention that in directed subgraph one can change the direction (preserving the attachment of two “initial” degrees of freedom to each site) of a bond if there is at least one free pebble on the site to which the bond is pointing. Then the free pebble can be anchored to the opposite end freeing the previous anchor. This changes the direction of the bond and moves a free pebble from one site to its neighboring site. Using such elementary steps one can shuffle the free pebbles along Cretan paths in the subgraph.

The aim of the “pebble game” is always to ensure four free pebbles for the two sites to which a new bar is added. Three pebbles could be always ensured. If the search for the forth failed this mean that the new constraint is not independent. The prove for this could be find elsewhere we will start the description of pebble game implementation based on depth-first search in the directed subgraphs.

It is supposed that all the sites in the lattice are (consecutively) numbered, and each line in the input file consists of two numbers – the numbers of sites which share a bond. A proper linked-list structure for the lattice sites should be designed as well. Here, the neighbors sublists attached to each site should be enlarged with a label for each “out-coming” bond: in case a pebble is attached to it or not. The number of bonds with pebbles for this site can be found after inspecting these labels. Now the free pebbles on a site are just $2 - \text{TheNumberofBondsWithPebbles}$. The following description could show what a proper structure should be.

1. Read a bond. Add each of the two sites into the linked list, if not already added. If one (or both) of them are already in the list, rearrange the neighbors list for this (these) site(s).

2. Try (by a DFS function – see below) to free two pebbles on both sides of the bond (all together 4 pebbles)

   (a) Check how many free pebbles belong to the two sites. If this number is 4 attach one of them to the new bond.
if not:

* Pick one of the bonded sites (say, $n_1$):
  
  • if not found 2 free pebbles on it do DFS($n_1$);

* Pick the second end site ($n_2$) and repeat the same (... DFS($n_2$)...).

(b) Repeat from item 2; until 4 pebbles are found, or until the search originated from both sites failed

(c) If the search failed to free 4 pebbles, the new bond is redundant (in view of rigidity).

3. Repeat starting from 1, reading new bonds ...

The application of the depth-first search algorithm in the “pebble game” requires one argument – the site for the next visit. The DFS($s$) function itself returns a boolean value: free pebble found or not (DFS($s$) = TRUE or FALSE). The function traverses this time a directed graph. The “out” direction starts from the bond end where a pebble is attached.

The previsit instructions here consist in:

Check if there is at least one free pebble on the visited site,

if yes then:
  DFS:= TRUE; exit from this instance of the recursive function...

If a free pebble is not wound during the previsit, then a new site for the next search have to be chosen:

**Peek** a neighbor of $s$, say, $os$. If site $os$ has not been visited this search ($\text{tag}(os) < \text{search tag}$) and the bond is directed outward ($s \rightarrow os$) then call recursively the same function (DFS) with argument $os$. This call could be realized as an assignment:

$$\text{FoundFreePebble}:=\text{DFS}(os);$$

If $\text{FoundFreePebble}$ is TRUE; during the postvisit instructions an exchange is made: The pebble which belong to $s$ and was attached (“anchored” 29,30 to the bond $s \rightarrow os$ now becomes free and the previously free pebble of $os$ is attached to the traversed bond from the $os$ side, this way changing its direction: $s < \rightarrow os$. This is repeated recursively until the free pebble reaches the site where the search was originated.

This completes the description of a depth-first search implementation for counting of redundant constraints in a rigidity percolation model. The whole example program (about 60 lines of text) could be obtained upon request from the author.

The program could be modified for counting of the rigid clusters if one keeps in mind that a site may belong to more than one rigid cluster 29,30 and that two sites belong to one cluster if they share a bond or if a new (long range bond) added between them appears redundant. The bad news is that the performance scaling of this program is $\approx N^{\varpi}$ with $N$ the number of sites and $\varpi \approx 1.8 - 2$. One can
improve the algorithm performance scaling to $\tau \approx 1.1 - 1.2$ by “artificially” changing the connections between sites: either by “triangularization”\(^{32}\) or by introducing of supersites (“rigid bodies” – with three degrees of freedom each — see ref. \(^{33,34}\)). So, the plain use of spanning tree searches is not a guarantee to develop a fast algorithm.

In conclusion I would stress again that in my opinion it is very important one to be aware of the general properties of these two approaches to the cluster counting problem. I hope that this work might show what should be expected from a program for cluster counting and what kind of improvements or modifications could be looked for. So, for every particular case one can choose the more suitable approach, or to look for a combination between them. Generally said the Hoshen-Kopelman algorithm is more suitable for very large systems (say, above $10^7$ or $10^8$ “particles”) and is easy for parallelisation. The spanning tree approaches can solve easier more sophisticated tasks (e.g. for percolation backbone extraction, or for identifying rigidity percolation clusters) on systems with moderate size.

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References

1. J.M. Hammersley, p.47 in: Percolation structures and processes (eds: G. Deutscher, R.Zallen, J.Adler), Adam Hilger, Bristol 1983.
2. D. Stauffer, A. Aharony, Introduction to percolation theory, Taylor & Francis, London, 1992; second printing 1994.
3. S.R. Broadbent, J.M.Hammersly, Proc. Camb. Phil. Soc. 53 (1957) 629.
4. J.Hoshen, R. Kopleman, Phys. Rev. B 14 (1976) 3438.
5. C. d’Iribarne, G.Rasigni, M. Rasigni, Phys. Lett. A 209 (1995) 95.
6. W.H. Press, S.A. Teukolsky, Computers in Physics 6 (1992) 400.
7. E.R. Davidson, Computers in Physics 7(5) (1993) 519
8. J. Hoshen, M. W. Berry, K. S. Minster, Phys. Rev E 56 (1997) 1455.
9. F.Babalievski, Phys. Rev. E 51(6B) (1995) 6230.
10. E.T. Gawlinski, H.-E. Stanley, J. Phys. A 14 (1981) L291.
11. J. Kertesz, T. Vicsek, Z. Phys. B 45 (1982) 345.
12. S.B. Lee, S. Torquato, Phys. Rev. A 41 5338.
13. F. Babalievski, O. Peshev, Comput. Phys. Commun. 60 (1990) 27.
14. R.H. Swendsen, J.-S. Wang, Phys. Rev. Lett. 58 (1987) 86.
15. U. Wolf, Phys. Rev. Lett. 62 (1989) 361.
16. U.J. Wiese, H.P. Ying, H.P. Ying, Phys. Lett. A 168, (1992) 143.
17. H.G. Evertz, G. Laka, M. Marcu, Phys. Rev. Lett. 70 (1993) 875.
18. C. Dress, W. Krauth, J. Phys. A 29 (1995) L597; LANL e-print: cond-mat/9612183
19. F.Babalievski, Comput. Phys. Commun. 67 (1992) 453.
20. P.D. Hortensius, H.W. Card, L.D. McLeod, J. Comput. Phys. 84 (1989) 76.
21. R.C. Brower, P. Tamayo, B. York, J. Stat. Phys. 63 (1991) 73.
22. R. Hackl, H.-G. Matitus, J.M. Singer, T.H. Husslein, I. Morgenstern, Int. J. of Mod. Phys. C 4 (1993) 1117.
23. J. Kertesz, D. Stauffer, Int. J. Mod. Phys. C 3 (1992) 1275.
24. H.J. Herrmann, D.C. Hong, H.-E. Stanley, J. Phys. A 17 (1984) L261.
25. H. J. Herrmann, H.-E. Stanley, J. Phys. A 21 (1988) L829.
26. R.E. Tarjan, SIAM CBMS-NSF Regional Conf. series in appl. math. 44; R.E. Tarjan, SIAM J. Comput., 1 (1972) 146.
27. W. Lipski, *Kombinatoryka dla Programistow*, Widwanictwa Naukowo-techniczne, Warsaw 1982; (Rusian Transl: Mir, Moskow 1988; ISBN 5-03-000979-5).
28. S. Roux, A. Hansen, J. Phys. A, 20 (1987) L1281.
29. D. J. Jacobs, M. F. Thorpe, Phys. Rev. Lett. 75 (1995) 4051.
30. D. J. Jacobs, M. F. Thorpe, Phys. Rev. E 53 (1996) 3682.
31. B. Hendrickson, SIAM J. Comput., 21 (1992) 65.
32. D. J. Jacobs, 1995 — unpublished, see ref. 24 in the Jacobs and Thorpe paper.
33. C. Moukarzel, P. M. Duxbury, Phys. Rev. Lett. 75 (1995) 4055.
34. C. Moukarzel, J. Phys A 29 (1996) 8079.