PERFORMANCE OF RANDOM LATTICE ALGORITHMS

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We have implemented different algorithms for generating Poissonian and vectorizable random lattices. The random lattices fulfil the Voronoi/Delaunay construction. We measure the performance of our algorithms for the two types of random lattices and find that the average computation time is proportional to the number of points on the lattice.

Keywords: Delaunay Random Lattices; Voronoi Tessellations; Algorithms; Dynamic Pointer Structures;

1. Introduction

There is a large range of applications for random lattices spanning from materials science, modelling of the large-scale structure of the universe, kinetic growth models, sand piles to quantum field theory. A random lattice is a way of discretizing a system without introducing any kind of anisotropy. It can, however, also be used to describe cellular structures, such as grain mosaics, biological tissues and foams. So it is important to have efficient algorithms for generating random lattices, and, furthermore, algorithms which allow the random lattice to be dynamically maintained throughout a simulation.

An extensively used type of random lattice is the Delaunay random lattice, which is a triangulation of space based on a given set of \( N \) points. The Voronoi tessellation is dual to this lattice and gives a division of space into cells. It is described as follows: For each point one determines the region of space which is closer to this point than to any other point. This procedure called the Voronoi tessellation of space will divide the space into convex cells. There exist other ways of dividing space into cells, such as the Laguerre partition and, recently, a generalized Voronoi construction was used in order to model soap froths.

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In the present paper we discuss static and dynamic algorithms for generating Delaunay random lattices determined according to the Voronoi tessellation of space. We will restrict the discussion of the Voronoi construction to two dimensions; it can be generalized to any dimension. We determine the computation time for our algorithms, and will denote this by $T(N)$ for a random lattice with $N$ points. Results for both the Poissonian random lattice (PRL) and the vectorizable random lattice (VRL) will be given. The PRL is obtained when the points are put at independently and randomly chosen positions all over the entire lattice and then connected according to the Voronoi construction. This implies that the PRL random lattice is completely free of anisotropies.

The VRL lattice is a modified form of the PRL random lattice. Now the space is divided into square cells and each cell contains exactly one point. The position of a point inside a cell is chosen randomly. The motivation for introducing the VRL random lattice was to have a vectorizable program when solving an equation on the lattice, e.g., the Laplace equation describing the numerical growth of Diffusion-Limited Aggregation (DLA) clusters. Furthermore, the VRL lattices possess for all practical purposes no anisotropies and since a vectorized code can increase computation time significantly VRL lattices are very useful.

First, in Sec. 2, the Voronoi and Delaunay constructions are described in more detail. In Sec. 3 we discuss our different algorithms. Section 4 contains a discussion of the performances and finally we conclude.

2. Voronoi Tessellations and Delaunay Random Lattices

The Voronoi construction or tessellation for a given set of points is defined as follows: For all points determine the associated cell consisting of the region of space nearer to this point than to any other point. Whenever two cells share an edge they are considered as neighbours. By drawing a link between the two points associated to (located in) the cells one obtains the triangulation of space that is called the Delaunay lattice. The Delaunay random lattice is dual to the Voronoi tessellation in the sense that points correspond to cells, links to edges and triangles to the vertices of the Voronoi tessellation.

The triangulation (tessellation) of the plane with $N_P$ points (cells), $N_L$ links (edges) and $N_T$ triangles (vertices) are constrained by the Euler relation

$$N_P - N_L + N_T = \chi$$

where $\chi$ is the Euler characteristic, which equals 2 for a graph on a surface with the topology of a sphere and 0 for a torus. Furthermore, $3N_T = 2N_L$ holds for a triangulation (a triangle has three sides/links and $3N_T$ then counts each link twice).

An equivalent way to obtain the Delaunay random lattice is the following: Construct for all sets of three points the circle defined by these points. If there are no other points inside this circle the three points will define a Delaunay triangle and are connected by three links. The centers of these circumscribing circles will be the vertices of the Voronoi tessellation.
3. Algorithms

Three different algorithms for generating two-dimensional Delaunay random lattices and the associated Voronoi tessellations are presented. The programs were written in the C programming language and run on workstations.

First we describe an algorithm for the VRL case, and, secondly, the PRL random lattice. Thirdly, a dynamic algorithm for generating both the VRL and PRL lattices is described. We call this algorithm dynamic because it allows one to change a random lattice slightly and then obtain the new random lattice by only carrying out local rearrangements of the links. Examples of VRL and PRL random lattices are shown in Fig. 3.

3.1. Vectorizable random lattices

In the case of the vectorizable random lattice the region where the points are distributed is first divided into square cells as shown in Fig. 1(a). Each cell is of unit area. Then exactly one point is put into each cell with the position inside the cell being random and uniformly distributed.

Each point only can be connected to points in the 36-cell neighbourhood as shown in Fig. 1(a). In Fig. 1(b) the probabilities for the center point to be connected to another point in this neighbourhood are shown (cf. Ref. 3). So if a point belongs to a triangle the other two points are contained in two of the cells of this neighbourhood. Therefore, to find a triangle one only has to search for neighbouring points in this restricted area. An upper limit for the distance two neighbouring points can have is \( \sqrt{4^2 + 2^2} = \sqrt{20} \approx 4.472 \) as can be seen from Fig. 1(a).

3.1.1. VRL algorithm

After putting the random points the algorithm determines an initial triangle (cf. Fig. 1(a)). One point \( A \) is chosen. For each pair of points in the neighbourhood of \( A \) it is checked if the circle defined by these three points contains any other point of the neighbourhood. The first triplet of points found for which this circle does not contain any other point is connected with three links. These links are given a counter clockwise orientation, as shown by the arrows in Fig. 1(a).

When the lattice is completed each link is either connected to two triangles or it is a border link, i.e., it is part of the border which limits the entire lattice. Each link is assigned a flag \( \text{front} \) which has the value 0 if the two triangles connected with this link have been found or if the link is a border link. If only one triangle has
been found \textit{front} has the value 1. We call such a link a \textit{front link}, due to the fact that this is the front of the search algorithm. So after finding the initial triangle its three links $AB$, $BC$ and $CA$ are front links. The following steps are now carried out:

For each front link $AB$ check if a point $P$ in the neighbourhood of $A$ can be found such that the circumscribing circle of the triangle $APB$ does not contain any other point (cf. Fig. 1(a)). This is then a Delaunay triangle. First it is checked if the point $P$ is on the right or the left side of the link $AB$, i.e., if the determinant of the matrix with the column vectors $AB$ and $AP$ is negative or positive.\footnote{If $P$ is on the left side, $APB$ cannot be a new triangle of the random lattice because in this case it has already been found.} Then the next point in the neighbourhood has to be checked. If no point $P$ completing $AB$ to a Delaunay triangle can be found the link $AB$ is a border link and its \textit{front} flag is assigned the value 0. The program continues by treating the next front link. If a point $P$ with this property is found there are three new links $AP$, $PB$ and $BA$. One of them $BA$ is identical with the just checked front link $AB$, it only has a different orientation. The \textit{front} flag of $AB$ is assigned the value 0. The probability to find a connected point to $P$ is not equal for all cells of the neighbourhood but is much smaller for the outer cells. We use this by beginning the search at the cells with the highest probability (cf. Fig. 1(b)) and then going outwards to the cells with lower probability of connection.

It is checked if the new links $AP$ and $PB$ have already been found. If not, they are new front links. Otherwise they already were saved as front links and their \textit{front} flag is assigned the value 0. One notices that it is not necessary to look through the entire array of links to check whether $AP$ and $PB$ have already been found. In our algorithm we use an array \texttt{connect} in which we save for each point the links connected to this point. Therefore it is only necessary to check whether the links $AP$ and $PB$ are already saved in the \texttt{connect} arrays of the points $A$ and $B$. If there is still a front link left treat the next one, otherwise the Delaunay random lattice is finished.

Finally the Voronoi tessellation is determined. For each point $P$ all triangles which have $P$ as one site are ordered counterclockwise. The centers of the circumscribing circles of the triangles are connected. The polygon constructed in this way is the Voronoi cell which is dual to the point $P$. In summarized form the algorithm looks like the following:

- Put random points into the region
- Construct the initial triangle
- Construct the Delaunay random lattice. Do the following steps as long as there are front links $AB$ left:

1. Find point $P$ which completes front link $AB$ to a Delaunay triangle. If not possible, $AB$ is a border link.
2. Check if the two new links are already stored as front links. If not they are new front links.

- Construct the Voronoi tessellation by connecting the centers of the circum-scribing circles of all triangles connected to a point.

The computation time $T(N)$ for constructing the VRL random lattice is proportional to the number of points $N$. This is due to the fact that for each point the neighbour points can only be found in the 36-cell neighbourhood.

### 3.2. Poissonian random lattices

In this section we describe an algorithm for generating a random lattice consisting of points with uniformly distributed $x$ and $y$ values. In the limit of infinite lattices this corresponds to a Poisson process (see, e.g., Ref. 13).

The actual generation of a random lattice based on a Poissonian distribution of lattice points has many aspects in common with the approach used in the previous Section 3.1. Different techniques are, however, necessary in some places mainly due to the fact that for the PRL the number of neighbours is not bounded. The algorithm used here is described in detail in Ref. 4 and based on the one proposed in Ref. 5.

#### 3.2.1. PRL algorithm

During the initialization process, a starting triangle is identified and its edges are defined to be active links, similar to the front links of the previous section. Thereafter the list of active links is treated until there are no more active links left. To identify an active link a flag treated is used, which is initialized to zero for every new link found. To generate the random lattice one has then to go through the following steps:

- Take the next active link:
  1. Draw a circle around this link and check if it contains points
  2. If so, choose the one which leads to the largest radius
  3. If not, move the center of the circle perpendicular to the link by a small amount $\epsilon$ dependent on the number of points present in the region. Draw a new circle. Repeat until the circle contains points. Select the one which leads to the smallest radius

- Store the point found as a new site and create two new links by connecting it to the two sites of the considered link.

- Check if these new links already exist. If they do, remove the active attribute, if not append them as new active links

- Remove the active attribute from the considered active link.
Fig. 2. Finding a new point to construct a new triangle starting from one link of an existing triangle. $M_1$, $M_2$ and $M_3$ are centers of the circles, the $C$’s are points of the lattice.

One has to search for every active link the next neighbour in the sense of the Delaunay construction. A way to do this is shown in Fig. 2. A circle is drawn through the endpoints of the link $AB$, its center being the link’s midpoint $M_1$. One has then to check, if there are points inside that circle (e.g., $C_1$). If there are, one has to choose the point which gives the largest radius by drawing a circle determined by the point and the endpoints of the link. If in the beginning there were no points in the circle, one has to move the center of the circle by a small amount $\epsilon$ dependent on the density of points into the direction where the neighbour should be located (e.g., $M_2$, $M_3$), until one or more points are inside the circle (e.g., $C_2$, $C_3$). One chooses then the point giving raise to the circle with the smallest radius. This method is used because testing if a point is inside a circle or not is much faster than the radius calculation.

3.2.2. Data structure

The two basic elements of the random lattice, sites and links, are organized as a linked list of special data structures which allow to store the information needed:

```c
SITE{
    POINT p;      /* Coordinates */
    int border;   /* Border Site Flag */
    int nNb;      /* Number of Neighbours */
    NBNODE *pFirstNbNode; /* Address of the First Neighbour Site */
    SITE *pNextSite;  /* The Next Site in the List */
    SITE *pNextSlSite; /* The Next Site in the Current Bin */
};

LINK{
    POINT p1, p2;  /* Coordinates of Constituting Points */
    SITE *pSite1,*pSite2; /* Addresses of these Points */
    int orient;   /* Orientation of the Link */
    char border;  /* Border Link Flag */
    char treated; /* Treated Link Flag */
    LINK *pNextLink; /* The Next Link in the List */
};
```

The site list is initialized only once in the beginning. During the construction of the lattice neighbours are, however, dynamically appended to each site. The address of the first neighbour is given by $p$FirstNbNode. Each appended neighbour is again a structure containing information about the address of the neighbour site and the
link connecting it:

```c
NBNode
    NBNode *pNextNbNode; /* The Next Neighbour Site */
    SITE *pNb; /* Address of the Current Neighbour */
    LINK *pLink; /* Address of the Link Connecting */
}; /* the Site with this Neighbour */
```

In contrast to the arguments given in Section 3.1 one does not know where exactly to find the neighbour site. For the search of this neighbour it is however not acceptable to do a complete search of all points, since this would imply a time behaviour proportional to $N^2$. Alternatively one could use a tree-like structure, where one can identify points in the neighbourhood. Another possibility is to implement binning, i.e., divide the lattice into sublattices so that in each bin one finds on the average the same number of sites. This method has been implemented here. The pointer `pNextSlSite` contains the address of the next site in a considered bin. Thus for each link—on the average—only a fixed number of sites has to be searched. This number should be equal to 5–10 sites per bin, while the 8 neighboring bins are searched for each active link.

During the construction of the lattice the algorithm will encounter situations, where a neighbour found gives raise to new links which have already been found, and are still waiting in the active link list to be treated. In this case one has to mark these links as treated by setting the corresponding flag `treated` in the link structure. Treated links are skipped when processing the link list.

The stopping criterion depends on the problem one is investigating. If there are no periodic boundary conditions, one has to introduce a limit beyond which the algorithm should stop to look for new points. If the problem has periodic boundary conditions, no special stopping criterion is needed.

3.2.3. Speed and memory

The speed of a program depends on the setup of the algorithm and the realization on a given computer. The best performance one could have is $O(N)$, i.e., the order of the computation time $T(N)$ increases linearly with the number of points treated.

To avoid any superfluous calculation the following measures have been taken in this algorithm:

- While creating the lattice one has to check whenever a new neighbour and therefore two links are found, that these links are not yet in the list of active links. To minimize the impact of this task on the time behaviour, each site knows through the structure `NBNode` not only about its neighbours `pNb` but also about the connecting links `pLink`. So only the links already attached to the site have to be searched, a number which is constant on the average.

- Searching potential neighbours, one has to draw circles and move their centers. Care is taken, that the quantity $\epsilon$ by which the centers are moved depends
on the density of points. If one would not account for that, more and more heavy radius calculations would be necessary as the density grows.

With these measures taken the algorithm should have a time behaviour like $O(N)$, since for every point—on the average—a fixed number of calculations and memory allocations are carried out.

These theoretical considerations do, however, not reflect reality. Dynamic memory allocation is intuitively and easily programmable; the computer will on the other hand be obliged to maintain longer and longer lists of allocated memory blocks, so memory allocation time will grow faster than the system size.

That is why in this program memory is allocated in huge blocks from the start. Whenever new memory is needed (for new neighbours or links) it is taken from these “pools”. The computer thus has no additional work to do for maintaining memory allocation tables. Allocating memory in the beginning is in fact possible since one knows that the average number of neighbours for a site is 6. Particularly for large lattices ($N \geq 10,000$) this is very advantageous, since memory management tends to become a substantial part of the calculation time. Allocating memory from the start one has the other advantage that the linking of the lists is not necessary anymore, and this saves memory.

### 3.3. Dynamic Random Lattices

Now we describe a method to calculate a random lattice using a Dynamic Random Lattice algorithm (DRL), which makes it possible to dynamically maintain the random lattice in a simulation. The idea is to start from an existing lattice (e.g., a triangular lattice) and then successively change this lattice by moving the points in order to obtain the final random lattice. The lattice fulfils at all times the Voronoi construction and this ensures that also the final lattice will be a Delaunay random lattice.

By the DRL algorithm, the VRL random lattice is obtained by moving the points—one by one—to new positions randomly chosen in the cells (cf. Fig. 3(a)) associated to the points (see Figs. 3(a)-(b)). The PRL random lattice is obtained by moving the points to new positions randomly chosen over the entire lattice (see Figs. 3(c)-(d)). The time dependence for the DRL algorithm is more complicated than for the other two algorithms due to the “search” part of the algorithm (see below) and will have the slowest performance in the case of the PRL random lattice and the fastest in the case of the VRL random lattice.

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The total time for computing large lattices will increase more than linearly since the computer will be forced to swap memory pages.
3.3.1. DRL algorithm

We now describe the basic elements of the algorithm (see Refs. 7 and 14 for a more detailed description). When a point is moved from one place to another it is possible to view all the changes of the lattice as link-flip processes. A link-flip process is when, e.g., the link $EP$ in Fig. 4(a) is flipped to $DF$ as in Fig. 4(b). In this case it is a neighbour-loosing process for the points $P$ and $E$, whereas it is a neighbour-gaining process for the points $D$ and $F$. Intuitively, when a point is moved, one follows the trajectory of the point and tests whether a link-flip process will take place. The condition for this to occur is: i) either the point $P$ enters the circumscribing circle of a triangle (corresponding to the points $A$, $B$ and $C$ in Fig. 4(a)), which then implies a neighbour-gaining process (cf. Fig. 4(b)) or, ii) the point $P$ leaves the circumscribing circle for three points (corresponding to the points $D$, $E$ and $F$ in Fig. 4(a), which do not define a triangle), and this implies a neighbour-loosing process (cf. Fig. 4(b)).

Fig. 4. Part of a Delaunay random lattice (a) before and (b) after the point $P$ has been moved. The link-flip process appearing to the left of the point $P$ is a neighbour-loosing process whereas the process to the right is a neighbour-gaining process. The thick lines represent the links of the random lattice whereas the thin lines are the edges of the Voronoi cells.

Even though it is impossible to predict the number of processes that will take place, the full set of changes can always be viewed as consisting of the neighbour-gaining and loosing processes taking place by following the point along its trajectory. It is, however, not necessary to carry out the updating of all the processes along the points trajectory. When a point has to be moved one first removes it from the lattice leaving a lattice with $N-1$ points, and updates the neighbourhood. Then the point is put at its new position, and the location of this new position, i.e., to which triangle it belongs in the lattice, is determined. Since one does not know into which of the existing triangles on the random lattice the point is put, the way this triangle is determined is by a search through the lattice (see Ref. 14). Finally, the point is added and the neighbourhood is updated by carrying out neighbour-gaining and loosing processes. In schematized form the DRL algorithm looks like this:

- Generate a triangular lattice with $N$ points and the topology of a torus (periodic boundary conditions)
- For all points $P$ on the lattice do:
  1. remove the point $P$ and the links to its neighbours
  2. calculate/update the new links
  3. put the point $P$ at a new (randomly chosen) position
  4. search through the Delaunay random lattice with $N-1$ points and locate in which triangle the new point belongs
5. add the point $P$ and calculate/update the new links followed by neighbour flipping processes (cf. Fig. 3)

### 3.3.2. Data structure

The random lattice algorithm is implemented using a dynamic pointer structure. For each point a SITE structure (see below) is defined where information associated to the site is stored. Included in this information is a nearest-neighbour pointer list NN. For each site in this list there is a pointer referring to the location of the original site itself, so that the information associated to a site is only stored once. The sites and nearest neighbour linked lists are organized as follows:

```c
SITE {
    POINT p; /* coordinates */
    int n; /* point number */
    int q; /* coordination number */
    NN *pNN; /* pointer to first Nearest Neighbour */
};

NN {
    SITE *pSite; /* pointer to the site */
    CIRCLE circle; /* circumscribing circle */
    int pos; /* position relative to the site */
    NN *pNN; /* pointer to the Next Neighbour */
};
```

The updating of the lattice when a flip process takes place is carried out by rearranging the pNN pointers in the nearest-neighbour pointer lists. When a new triangle appears or an old one disappears information on the circumscribing circles is updated and stored in the NN nearest-neighbour pointer list (cf. Ref. 14).

### 3.3.3. Performance

The average computation time of the DRL algorithm can be written as

$$T(N) = O(N(R(N) + S(N) + A(N)))$$

(2)

where $R(N)$ is the average time to remove a point, $S(N)$ the search time and $A(N)$ the time to add a point. For a triangular lattice the coordination number is 6 so $R(N)$ and $A(N)$ would both imply 6 nearest-neighbour operations. From Eq. (2) follows that the average coordination number for a triangulation is 6, so both $R(N)$ and $A(N)$ will on average be approximately constant.

The search time $S(N)$ is proportional to the distance between the old and new position of the point. In the VRL case the new positions of the points are within a fixed distance from the old positions, i.e., $S(N)$ is a constant, and we expect the total time $T(N)$ to scale linearly with $N$, i.e., an $O(N)$ behaviour. For the PRL lattice the search will in the worst case be proportional to the size of the system, i.e., $\sqrt{N}$, leading to an $O(N\sqrt{N})$ behaviour for the computation time.
4. Results

All simulations we report in this section were carried out using Sun Sparc 10 workstations. In Table 1 and Fig. 5 are shown the computation times for the static VRL and PRL algorithms as well as for the dynamic algorithm, denoted here as DVRL and DPRL. For the static version one notices an approximate linear increase in computation time as a function of the number of points \( N \) on the lattice. For large systems the performance is worse due to the fact that almost all the memory of the computer is used. In the VRL case the expression \( T(N) \approx 0.20N \) milliseconds fits the data very well whereas the PRL algorithm is a little slower with the expression \( T(N) \approx 0.24N \) milliseconds providing a good fit.

Table 1. The upper part shows the performance of the VRL algorithm for the VRL random lattice and for the PRL algorithm the PRL random lattice. In the lower part the values for the dynamic algorithm are given for the VRL and PRL random lattice, denoted here as DVRL and DPRL. The times are measured in seconds.

| \# Points, \( N \) | 100  | 1000 | 10,000 | 50,000 | 100,000 | 200,000 | 300,000 |
|-----------------|------|------|--------|--------|---------|---------|---------|
| VRL             | 0.04 | 0.18 | 1.72   | 8.90   | 18.3    | 38.6    | 60.3    |
| PRL             | 0.02 | 0.20 | 2.05   | 11.3   | 23.0    | 47.3    | 73.9    |
| DVRL            | 0.11 | 0.99 | 10.15  | 50.6   | 101.0   | 207     | 308     |
| DPRL            | 0.14 | 1.70 | 29.20  | 264.8  | 713.8   | 1938    | 3476    |

Fig. 5. Computation time for the VRL, PRL and DRL algorithms in order to generate random lattices with \( N \) points. The times are measured in seconds. Also shown are curves representing a linear increase and an \( N\sqrt{N} \) increase in computation time.

For the DRL algorithm one notices a linear relation between execution time and the number of points \( N \) for the VRL random lattice, \( T(N) \approx 1.01N \) milliseconds. In the PRL case the behaviour asymptotically approaches the \( O(N\sqrt{N}) \) behaviour, as discussed in Sec. 3.3.3. An expression of the form \( T(N) = aN(b + \sqrt{N}) \) (with \( a \approx 150 \) ms and \( b \approx 65 \)) follows our curve (cf. Fig. 5), and this has the anticipated \( O(N\sqrt{N}) \) behaviour for large \( N \). When in advance one has a knowledge of the distribution of the points it may be possible to reduce the search time by using “bins” (cf. Sec. 3.2.2), but we have only investigated the general DRL algorithm without using any information about the location of the points.

5. Conclusions

In the present paper we have discussed different algorithms for generating Delaunay random lattices and the associated (dual) Voronoi tessellations. We have described

\[ c \] The linear behaviour of the algorithm is only valid if every bin contains about the same number of points. For distributions of \( x \) and \( y \) values which are not uniform, the binning should be adjusted.

\[ d \] The initialization time for generating the initial triangular lattice where memory for the dynamic pointer structure is allocated is included in the above computation times. This initialization time scales approximately linearly as \( cN \) with \( c \approx 0.157 \) ms.
how the algorithms have been implemented in the C programming language using
dynamic pointer structures.

For the vectorizable random lattice and the Poissonian random lattices we found
that the computation time is roughly linear. When the system size approaches the
memory limit of the computer the time dependence increases more rapidly. We
also discussed a dynamic random lattice algorithm. This algorithm allows for a
random lattice to be maintained during a simulation and can also be used in order
to obtain a random lattice but with a slower time performance than the VRL and
PRL algorithms.

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