Abstract

Talk given at the conference on ‘Inhomogeneous Random Systems’ at the University of Cergy-Pontoise, France, (23 January 2001).

I describe the classic circle-packing problem on a sphere, and the analytic and numerical approaches that have been used to study it. I then present a very simple Markov-chain Monte Carlo algorithm, which succeeds in finding the best solutions known today. The behavior of the algorithm is put into the context of the statistical physics of glasses.

keywords: Monte Carlo Methods; Packing of Circles; Glass Transition

AMS numbers: 00A72; 52C15; 82D30

What is the minimal radius $R_N$ of a sphere allowing $N$ non-overlapping circles of radius $r = \frac{1}{2}$ to be drawn on its surface? In a classic paper, Schütte and van der Waerden [1] reduced this problem to a study of planar graphs: As the sphere has minimal radius, many circles are blocked, i.e. they cannot move. These circles make up the $M \leq N$ vertices of the graph. If two circles are in (blocking) contact, they are connected by an edge.

Schütte and van der Waerden considered all graphs with $M \leq 12$ vertices. Some of these graphs can correspond to a blocked configuration of circles on a sphere of radius $\tilde{R}$, with $R = \min_{\text{graphs}} \tilde{R}$. They were able to determine $R_N$ for $N \leq 12$. For this latter case $N = 12$, e.g., the centers of

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For $N = 13$ spheres, $1 < \frac{R}{d} = \frac{R+1}{2}$ as proven by Schütte and van der Waerden. This means that 13 identical spheres cannot be placed on top of another one, of same size.

The circles are located at the vertices of an icosahedron of side length 1, and lie on a sphere of radius

$$R_{12} = \frac{\sqrt{10 + 2\sqrt{5}}}{4} = 0.951 \ldots$$

(1)

Schütte and van der Waerden [2] were later able to prove that $R > 1$ for $N > 12$. This result (cf figure [1]) implies that 13 spheres of radius 1 cannot be placed on top of another sphere of the same size, and solves a packing problem discussed at least since the time of Newton. The best currently known packing of spheres for $N = 13$ concerns spheres of radius 1 on top of another sphere of radius 1.09111... The corresponding circle arrangement is shown in figure [2] and is almost certainly optimal. Today, it should be easy to enumerate planar graphs on a computer, and to prove this conjecture.

The problem of packing disks on the surface of a sphere has appeared repeatedly in the literature, as there are important applications in mathe-
matics and the natural sciences. Hundreds of papers have been written on this subject (for a partial list of references cf e.g. [3]), most of them improving upper bounds on $R_N$ in the range of $13 < N \simeq 100$. Only for $N = 24$ has a new optimal solution been proven [4].

The problem of $N$ non-overlapping disks on a minimal sphere can be reformulated as a minimization problem of the potential energy of $N$ particles $i = 1, \ldots, N$ on the surface of the sphere of radius 1 with a two-body interaction [5, 6]

$$V = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left( \frac{c}{r_{ij}} \right)^p$$

where $r_{ij}$ is the Euclidean distance between circles $i$ and $j$. Therefore, customary minimization programs (such as the Newton-Raphson method) can be applied to find local - and hopefully global - minima for ever increasing values of $p$. In our first units (circles of radius $\frac{1}{2}$ on a sphere of radius $R$), the minimal radius $R_N$ is given by

$$R_N = \frac{1}{\min_{i,j} r_{ij}}$$

in the limit $p \to \infty$.

Current records were set by Kottwitz [6], who used values of $p$ in the astonishing range of $p = 80$ to $p = 1310720$. Running such a sophisticated Newton-Raphson program is a delicate task as one has to avoid getting trapped in local minima of the potential energy. Nevertheless, the strategy proved to be successful, as a large number of new values for $R_N$ were found, and as these values have so far stood the test of time.

Recently, I have reconsidered the non-overlapping circle problem from the viewpoint of Markov-chain Monte Carlo algorithms. Instead of searching for the minimum of a regularized energy, I move circles during a large number of time steps $t = 1, \ldots, T_{\text{max}}$. At time $t$, a single, randomly chosen circle $i$ is moved a tiny bit into a random direction. Specifically, let us denote the position of $i$ at time $t$ by $\vec{r}_i$, and let the displacement vector be $\delta \vec{r} = (\delta x, \delta y, \delta z)$ with Gaussian random numbers $\delta x$ etc. that have zero mean and variance $\sigma^2 \ll 1$. Then the following move is considered [7]

$$\vec{r}_i \to \vec{r}_i' = \frac{\vec{r}_i + \delta \vec{r}}{|\vec{r}_i + \delta \vec{r}|} R$$

If the move can be performed without violating the constraints, it is accepted, and rejected otherwise. This procedure implements a standard local Metropolis algorithm for a constant stationary probability distribution:
Any non-overlapping configuration of circles should be visited with the same probability.

In addition to performing the Metropolis algorithm at fixed $R$, I also implemented the “simulated annealing” procedure \cite{8}: Every so often, the radius of the sphere is reduced by a very small amount, if this is possible without introducing overlaps between particles \cite{9}.

I have found that this simple algorithm reproduces the best results known up to date (cf \cite{6}) for $N = 5 \ldots 90$, typically within a few minutes of computer time \cite{10}.

This observation may be of practical interest, as the Monte Carlo algorithm is much simpler than the previous approaches. However, it also underlines the quality of the bounds obtained by Kottwitz, which I have been able to reach, but not to improve on.

In physical terms, the graph giving $R_N$ is the ground state of the system (which does not have to be unique: for $N = 15$, e.g., two best solutions are known \cite{1}). Following Stillinger and Weber \cite{11}, all the other graphs that can be put on the surface of a sphere (with larger radii $\tilde{R} > R_N$) may be called ‘inherent structures’. These are the configurations that the simulated annealing algorithm may get trapped in. If the Monte Carlo algorithm is trapped in a inherent structure at radius $\tilde{R}$, it could by continuity also get trapped by the same inherent structure at a slightly larger radius $R' \approx \tilde{R}$. This means that, in the strict sense, the Monte Carlo algorithm is non-ergodic at least for all $R'$ satisfying

$$\max_{\text{graphs}} \tilde{R} > R' > R_N. \quad (5)$$

In this and similar systems, very little is known rigorously about the number of inherent structures as a function of radius (their density of states), and enumeration methods at small $N$ should be very helpful. For physical applications, the thermodynamic limit $N \to \infty$ is of prime interest. In this limit, $(R' - \tilde{R})/\tilde{R}$ certainly goes to zero. This means that strict ergodicity (on timescales that diverge with $N$) is reinstalled in the thermodynamic limit. Precise understanding of this complicated thermodynamic limit is lacking.

If, in contrast, the simulated annealing algorithm got trapped in a non-optimal state (with $R$ clearly larger than $R_N$) with probability close to one, we would say that the ‘physical’ system of disks on the surface of a sphere had a glassy phase. Such a phase seems to be absent for monodisperse circles. Our findings agree very well with what has been found in monodisperse hard disk and hard sphere systems on two- and three-dimensional tori \cite{12, 13}.
In contrast, there is strong numerical evidence that polydisperse hard disks can be glassy: in a system of hard disks of varying radii on a torus \[12\], a comparable local Monte Carlo algorithm always gets trapped at finite density. Again, it is fundamentally unclear how this observation carries over into the thermodynamic limit. Empirically, diffusion times of particles seem to grow without bounds at a well-defined, finite density.

In these two-dimensional systems, it has been found \[12\] that other Monte Carlo dynamics do not suffer the same slow-down as the local algorithm. These methods also provide strong indications that the glass transition in these two-dimensional models is a purely dynamic phenomenon, which does not manifest itself in equilibrium averages over the stationary probability distribution.

Acknowledgements: I would like to thank L. Santen and S. Tanase-Nicola for helpful discussions.

References

[1] K. Schütte, B. L. van der Waerden, “Auf welcher Kugel haben 5, 6, 7, 8 oder 9 Punkte mit Mindestabstand 1 Platz?” *Math. Ann.* **123**, 96 (1951).

[2] K. Schütte, B. L. van der Waerden, “Das Problem der dreizehn Kugeln” *Math. Ann.* **125**, 325 (1953).

[3] J. H. Conway, N. J. A. Sloane, *Sphere Packings, Lattices and Groups* (Springer, New York, 1993).

[4] R. M. Robinson, “Arrangement of 24 points on a sphere” *Math. Ann.* **144**, 17 (1961).

[5] B. W. Clare, D. L. Kepert, “The closest packing of equal circles on a sphere” *Proc. R. Soc. Lond.* A **405**, 329 (1986).

[6] D. A. Kottwitz, “The densest packing of equal circles on a sphere” *Acta Cryst.* A **47**, 158 (1991).

[7] It is also possible to orthogonalize $\vec{\delta r}$ with respect to $\vec{r}_i$.

[8] S. Kirkpatrick, G. D. Gelatt, M. P. Vecchi, “Optimization by Simulated Annealing” *Science* **220**, 339 (1983).

[9] The resulting algorithm has a few dozen lines and can be obtained on request.
[10] The precision reached was at least 0.01%, and typically 0.0001%. I did not compare the structures obtained with those given in ref. [6]. In some cases, there are exceedingly close contenders for $R_N$. For $N = 61$, e.g., the two best known structures differ by less than $10^{-9}$ in diameter.

[11] F. A. Stillinger, T. A. Weber, “Packing structures and transitions in liquids and solids” Science 225, 983 (1984).

[12] L. Santen, W. Krauth, “Absence of thermodynamic phase transition in a model glass former” Nature 405, 550 (2000).

[13] M. D. Rintoul, S. Torquato, “Metastability and Crystallization in Hard-Sphere Systems” Phys. Rev. Lett. 77, 4198 (1996).