# Equivalence of the void percolation problem for overlapping spheres and a network problem



1983 J. Phys. A: Math. Gen. 16 3071

(http://iopscience.iop.org/0305-4470/16/13/031)

J. Phys. A: Math. Gen. 16 (1983) 3071-3075. Printed in Great Britain

# Equivalence of the void percolation problem for overlapping spheres and a network problem

Alan R Kerstein

Thermofluids Division, 8523, Sandia National Laboratories, Livermore, California 94550, USA

Received 18 February 1983, in final form 19 April 1983

**Abstract.** The percolation problem for the complement of the union of randomly located, overlapping spheres is shown to be equivalent to a bond percolation problem on the edges of the Voronoi tesselation of the sphere centres. This result provides a convenient definition of cluster size, and therefore of the critical exponents, for this problem. It also provides an efficient algorithm for Monte Carlo computation of the percolation threshold and the critical exponents.

## 1. Introduction

Most percolation problems studied to date involve a regular lattice from which sites or bonds are removed according to some random process. A noteworthy exception is the percolation problem for overlapping circles or spheres with randomly located centres, an intensively studied problem which is equivalent to a percolation problem on an irregular lattice, or network, whose sites are the circle or sphere centres. A variety of methods have been employed to compute the percolation thresholds and the critical exponents for the two-dimensional and three-dimensional versions of this problem (Pike and Seager 1974, Haan and Zwanzig 1977, Gawlinski and Stanley 1981, Vicsek and Kertész 1981, Kertész and Vicsek 1982).

Here we analyse a percolation problem for which no underlying network, regular or irregular, is defined *a priori*, namely the percolation problem for the region of space which is the complement of the union of randomly located spheres. The region of space thus defined is the 'allowed region' in the hard-sphere Lorentz model used to study diffusive transport (Götze *et al* 1981, Masters and Keyes 1982), so its connectedness properties are of particular interest. A Monte Carlo calculation of the percolation threshold for this problem has provided an estimate of 0.966 for the critical volume fraction (Kertész 1981). The critical exponents for this problem were not considered.

It is shown here that the percolation problem for the hard-sphere Lorentz model is equivalent to the percolation problem for a certain subset of the edges of the Voronoi tesselation (Santalo 1976) of the sphere centres. Since the latter problem is a network percolation problem, cluster size, and therefore the critical exponents, are defined in the usual manner. Furthermore, the usual Monte Carlo methods for computing the percolation threshold and the critical exponents for networks are applicable. This approach is preferable to direct analysis of the hard-sphere Lorentz model using a continuum definition of cluster size, such as cluster volume. In particular, computational methods for networks are more efficient than the algorithm employed previously (Kertész 1981) which uses a sequence of auxiliary lattices to obtain successive approximations to the continuum percolation problem.

## 2. Equivalence to a network problem

The phenomenon of percolation is characterised by the divergence of some function of the cluster size distribution, such as the mean cluster size or the size of the largest cluster in the system. In network problems, a cluster is a mutually interconnected set of bonds or sites of the network, and its size is defined as the number of bonds or the number of sites. (If the number of bonds per site is finite and bounded, then these two definitions of cluster size are equivalent with respect to percolation.)

In the present problem, we define the medium to be the union of sphere interiors and the void to be the complement of the medium. For the void percolation problem, no underlying network is defined *a priori*. In the absence of an underlying network, cluster size can be defined only in terms of a continuum quantity such as cluster volume, which is relatively inconvenient for analysis and computations. Here, we show that this difficulty can be overcome using a geometrical construction called the Voronoi tesselation, which provides a suitable network.

A tesselation is a partition of space. The Voronoi tesselation is defined with respect to a given set of points in space. The Voronoi tesselation is the partition of space into regions such that each region is closest to one of the given set of points. In three dimensions, the boundaries of these regions are polyhedra, called the Voronoi polyhedra, and the faces, edges and vertices of the Voronoi tesselation are defined with respect to the set of Voronoi polyhedra (Finney 1970). The Voronoi polyhedra are also known to mathematicians as Dirichlet regions and to physicists as Wigner–Seitz cells (Zallen 1979). Each polyhedron contains exactly one point of the given set, a point which we denote as the 'centre' of the polyhedron since the given set of points in the present application is the set of sphere centres.

The key result of this paper is that vertices of the Voronoi tesselation which are connected by the void are connected by edges of the Voronoi tesselation contained within the void. If cluster size for a connected region of the void is defined as the number of vertices within that region, then this result establishes the equivalence of the void percolation problem to the bond percolation problem for those edges of the Voronoi tesselation which are contained within the void.

The results derived below are valid for spheres of identical radius whose centres are a realisation of any homogeneous random point process in three-dimensional space. The random processes usually considered in the percolation problem for the medium are the Poisson process and its generalisation which incorporates a hard core (Pike and Seager 1974).

Since the geometrical constructs developed below are based on a random distribution of sphere centres, many of the statements below are true 'almost surely,' in the measure-theoretic sense. The statements which require this qualifier are obvious from the context, so it is omitted in what follows.

To establish that vertices of the Voronoi tesselation provide a reasonable measure of cluster size for the void, we prove that each point in the void is connected within the void to some vertex.

*Lemma 1.* A given point in the interior or on the boundary of a Voronoi polyhedron is connected to a vertex by a path which is never closer to the polyhedron centre than is the given point.

*Proof.* The given point is contained in some cone whose apex is the polyhedron centre and whose base is a polyhedron face. The point of the cone which is farthest from the centre is a vertex of the face, namely the vertex which is farthest from the line through the centre which is perpendicular to the plane containing the face. Therefore, this vertex is farther from the centre than is the given point. Furthermore, the straight line from this vertex to the given point is the required path.

*Theorem 1.* Every point in the void is connected to some vertex by a path contained in the void.

*Proof.* By definition of the Voronoi tesselation, points in the same Voronoi polyhedron are closer to the centre of that polyhedron than to any other centre. Therefore, if a given point is in the void, then all points in the Voronoi polyhedron containing it which are farther from the centre than the given point are also in the void. By lemma 1, the required path exists.

Next, we show that a set of vertices in the void is connected only if the set is connected by tesselation edges contained in the void. This result establishes the equivalence of the percolation problem for the void to the bond percolation problem for edges contained in the void.

*Theorem 2.* If two vertices are connected by the void, then they are connected within the void by edges of the Voronoi tesselation of the centres.

*Proof.* Consider any path contained within the void which connects the given vertices. This path is modified to obtain a path consisting of tesselation edges. First, each path segment contained within the interior of a Voronoi polyhedron is replaced by its conic projection from the polyhedron centre onto the polyhedron surface. By an argument similar to the proofs of lemma 1 and theorem 1, the modified path segments are contained within the void. By construction, the modified path is contained within the faces of the Voronoi tesselation. Next, each path segment contained within the interior of a face is projected onto the perimeter of that face. The apex of the projection is the intersection of the plane containing the face with the line through the polyhedron centre which is perpendicular to that plane. By similar reasoning as before, the modified path segments are contained within the void. By construction, the modified path consists of edges of the Voronoi tesselation. Since the endpoints of each segment remain fixed at each stage of the construction, each intermediate path, as well as the final path, connects the two given vertices.

Finally, we establish an explicit, computationally convenient criterion to determine whether an edge of the tesselation is contained within the void.

*Theorem 3.* An edge of the tesselation is contained within the void if and only if its point of closest approach to the plane of the adjacent centres (i.e. the centres of the three Voronoi polyhedra sharing the edge) is in the void.

*Proof.* By definition of the Voronoi tesselation, each point of an edge is closer to the three adjacent centres than to any others, and is equidistant from these centres. Due to the latter property, the edge is perpendicular to the plane containing these centres. The point of the edge which is closest to the centres is therefore the point of closest approach to the plane. (The edge may or may not intersect the plane.) If this point is in the void, then by the definition of the void, the entire edge is in the void. The proof of the converse is trivial.

This method for establishing the equivalence of the void percolation problem for overlapping spheres and a network problem is strongly dependent upon the assumption that all sphere radii are identical. Generalisation to spheres of unequal radii is an open question at present. Thus, the existence of a network problem equivalent to the void percolation problem does not follow immediately from the fact that the complementary problem (percolation of the spheres) has an underlying network.

## 3. Computational method

A Monte Carlo method for estimating percolation properties of the network of edges identified in theorem 3 (and hence of the void, by theorem 2) is as follows. First, a set of sphere centres is randomly generated in the usual manner (Pike and Seager 1974). Second, the coordinates of the vertices of the Voronoi tesselation of the centres are computed and each vertex is associated with its four adjacent centres (Bernal and Finney 1967, Finney 1970). The two vertices associated with each triple of adjacent centres are the endpoints of an edge. In the third step, the 'allowed' edges, i.e. edges contained within the void, are identified using the criterion of theorem 3. This criterion is implemented by determining whether a given edge intersects the plane of the adjacent centres and if so, testing whether the distance from the intersection point to the adjacent centres exceeds the specified sphere radius, $r$. If the edge does not intersect the plane, then the test is performed on the vertices which are its endpoints.

The fourth step is to group allowed edges into clusters by identifying pairs of edges sharing a common vertex. The percolation threshold and the critical exponents may then be determined by the usual methods (Pike and Seager 1974).

## Acknowledgment

This research was supported by the Office of Basic Energy Sciences, United States Department of Energy.

## References

Bernal J D and Finney J L 1967 *Discuss. Faraday Soc.* no 43, p 62
Finney J L 1970 *Proc. R. Soc.* A**319** 479
Gawlinski E T and Stanley H E 1981 *J. Phys. A: Math. Gen.* **14** L291
Götze W, Leutheusser E and Yip S 1981 *Phys. Rev.* A**23** 2634
Haan S W and Zwanzig R 1977 *J. Phys. A: Math. Gen.* **10** 1547
Kertész J 1981 *J. Physique* **42** L393
Kertész J and Vicsek T 1982 *Z. Phys.* B **45** 345

Masters A and Keyes T 1982 *Phys. Rev.* A **26** 2129
Pike G E and Seager C H 1974 *Phys. Rev.* B **10** 1421
Santalo L A 1976 *Integral Geometry and Geometric Probability* (Reading: Addison-Wesley)
Vicsek T and Kertész J 1981 *J. Phys. A: Math. Gen.* **14** L31
Zallen R 1979 *Fluctuation Phenomena* ed E W Montroll and J L Lebowitz (Amsterdam: North-Holland) p 177