# CLUSTERING IN A CONTINUUM PERCOLATION MODEL 

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#### Abstract

We study properties of the clusters of a system of fully penetrable balls, a model formed by centering equal-sized balls on the points of a Poisson process. We develop a formal expression for the density of connected clusters of $k$ balls (called $k$-mers) in the system, first rigorously derived by Penrose [15]. Our integral expressions are free of inherent redundancies, making them more tractable for numerical evaluation. We also derive and evaluate an integral expression for the average volume of $k$-mers. boolean model; cluster properties AMS 1991 SUBJECT CLASSIFICATION: PRIMARY 60D05


## 1. Introduction

We consider systems of fully penetrable (i.e. spatially uncorrelated) equal-sized balls in one, two and three dimensions. In this model, balls of equal size are centered on the points of a stationary Poisson process. Since the balls are allowed to overlap, clusters of various sizes and volumes are formed. We call a cluster comprised of $k$ balls a $k$-mer. This model is a special case of the Boolean model, which replaces the equal-sized balls with random shapes [10].

This is a prototypical model for continuum (off-lattice) percolation $[4,9]$ and has been given a variety of names, including 'fully penetrable spheres', 'overlapping spheres', the 'Swiss-cheese model' and the 'Poisson blob model'. The study of clustering behavior of particles in continuum systems is of importance in phenomena such as conduction in dispersions, flow in porous media, elastic behavior of composites, sol-gel transition in polymer systems, aggregation of colloids and microemulsions, and the structure of liquid water, to mention but a few examples. Certain types of 'connectedness' functions and related quantities have been analytically and numerically determined for this model [1-3, 6-8, 14, 15, 22-26].

In this paper we study certain clustering properties of fully penetrable balls; in particular, we calculate the average number density of $k$-mers and the average

[^0]volume of $k$-mers. Given et al. [6] claimed a general expression for the probability $p_{k}$ that a given sphere lies in a $k$-mer. Their expression was later rigorously proved by Penrose [15], who also included the correct domain of integration and a coefficient that was suppressed by Given et al. In this article we use a constructive paradigm to obtain an equivalent expression for this probability by viewing the centers as a Poisson arrival process. This paradigm is similar to the branching process argument for point processes in the plane, which dates back at least to Gilbert [5]. Our evaluations of this probability are in excellent agreement with direct Monte Carlo simulation.

Given et al. also described an expression for the expected geometrical union volume $v_{k}$ of a $k$-mer. This description is somewhat incomplete and is corrected here. We again find that our expression is in excellent agreement with computer simulations.

The quantities $p_{k}$ and $v_{k}$ are known analytically in one dimension [20]. In higher dimensions, however, these quantities are integrals which cannot be evaluated analytically, and we have to settle for numerical evaluation. We find that the constructive paradigm yields integrals free of the redundancies inherent in Penrose's expression, and so these integrals can be numerically evaluated more efficiently. The effort to perform these numerical integrations increases as $k$ and the number of dimensions increase, and therefore efficient computation of these integrals becomes imperative.

In Section 2 we define the quantities that will be used throughout this report. In Section 3 we consider the calculation of the probability that a particle lies in a $k$-mer, obtaining integral expressions which require numerical evaluation. Finally, in Section 4 we calculate the expected volume of a $k$-mer for any dimension.

## 2. Definition of clustering quantities

We now define the quantities that will be investigated in this article. Our model is a system of fully penetrable equal-sized balls, i.e. balls whose centers are determined by a Poisson process with given rate $\rho$. The common diameter of the balls will be denoted by $\sigma$. The reduced density is defined by

$$
\begin{equation*}
\eta=\rho V_{1}(\sigma) \tag{2.1}
\end{equation*}
$$

where

$$
V_{1}(\sigma)=\frac{\pi^{d / 2}}{\Gamma(1+d / 2)}\left(\frac{\sigma}{2}\right)^{d}
$$

is the volume of a ball of diameter $\sigma$ in $d$ dimensions. Finally, the volume fraction of the void phase and particle (ball) phases are respectively given by

$$
\phi_{1}=e^{-\eta} \text { and } \phi_{2}=1-\phi_{1} .
$$

The primary cluster statistics of interest will be $p_{k}$, defined to be the probability a given particle lies in a $k$-mer, and $v_{k}$, the expected volume of a $k$-mer. From these quantities, other cluster statistics used in the literature can be obtained, including the mean number of clusters per unit volume, the probability that a given cluster is a $k$-mer, the mean cluster size, and the average volume of a randomly chosen cluster.

## 3. Probabilities of finding $\boldsymbol{k}$-mers

In this section we calculate the probability $p_{k}$ related to finding $k$-mers in the system. This probability can be computed rather handily in one dimension [20], and Penrose [15] rigorously derived an integral expression for $p_{k}$ in any dimension $d$; however, this integral cannot be calculated analytically and hence requires numerical evaluation. This expression is somewhat simplified by a constructive paradigm, viewing the model as an arrival process. These simplifications allow us to numerically evaluate the probabilities more efficiently.

In $d$ dimensions, a given sphere is a monomer exactly when the sphere of radius $\sigma$ centered at the given sphere contains no other sphere centers, and so

$$
\begin{equation*}
p_{1}=\exp \left[-2^{d} \rho V_{1}(\sigma)\right]=\phi_{1}^{2^{d}} . \tag{3.1}
\end{equation*}
$$

For $k \geqq 2$, Given et al. [6] claimed and Penrose [15] later rigorously proved, in any dimension, that

$$
\begin{equation*}
p_{k}=\frac{\rho^{k-1}}{(k-1)!} \int d r_{2} \int d r_{3} \cdots \int d r_{k} \exp \left[-\rho V_{k}\left(r^{k} ; \sigma\right)\right] I\left(r^{k} ; \sigma / 2\right), \tag{3.2}
\end{equation*}
$$

where for simplicity we take $r_{1}$ to be at the origin, $V_{k}\left(r^{k} ; \sigma\right)$ is the union volume of $k$ spheres with radius $\sigma$ centered at $r^{k}=\boldsymbol{r}_{1} \cdots \boldsymbol{r}_{\boldsymbol{k}}$, and $I\left(\boldsymbol{r}^{k} ; \sigma / 2\right)$ is the indicator function that the union of $k$ spheres with centers at $r_{k}$ and radius $\sigma / 2$ is connected. (Given et al. suppressed all prefactors and the indicator function in their expression.)

We now use a constructive approach to obtain an equivalent expression for (3.2). This approach will yield integrals without redundancies and hence will be more efficient for numerical integration.

Theorem 1. The probability $p_{k}$ that a given particle is part of a $k$-mer is given by

$$
\begin{equation*}
p_{k}=\sum_{1=k_{0}<\cdots<k_{i}=k} p_{k}\left(k_{0}, \cdots, k_{i}\right), \tag{3.3}
\end{equation*}
$$

where

$$
\begin{align*}
p_{k}\left(k_{0}, \cdots, k_{i}\right)= & c\left(k_{0}, \cdots, k_{i}\right) \int_{B \xi_{1}-k_{0}} d r_{2} \cdots d r_{k_{1}} \\
& \times \int_{C\left(k_{0}, k_{1}\right)^{k_{2}-k_{1}}} d r_{\left(k_{1}+1\right)} \cdots d r_{k_{2}}  \tag{3.4}\\
& \times \cdots \int_{C\left(k_{i-2}, k_{i-1}\right)^{k_{i}-k_{i-1}}} d r_{\left(k_{i-1}+1\right)} \cdots d r_{k} \exp \left[-\rho V_{k}\left(r^{k} ; \sigma\right)\right]
\end{align*}
$$

and

$$
c\left(k_{0}, \cdots, k_{i}\right)=\frac{\rho^{k-1}}{\left(k_{1}-k_{0}\right)!\cdots\left(k_{i}-k_{i-1}\right)!} .
$$

In this expression $k_{0}=1, k_{i}=k, B_{i}=B_{\sigma}\left(\boldsymbol{r}_{i}\right)$, the sphere with radius $\sigma$ centered at $\boldsymbol{r}_{i}$, and

$$
C(k, l)=\left(B_{k+1} \cup \cdots \cup B_{l}\right) \backslash\left(B_{1} \cup \cdots \cup B_{k}\right) .
$$

Proof. To establish Theorem 1, we employ a paradigm which 'constructs' a $k$-mer by counting the ways that $k$ spheres could form a single cluster. We begin with a given particle centered at $r_{1}$. To form a $k$-mer, there can be no more than $k-1$ particles which overlap $B_{\sigma / 2}\left(r_{1}\right)$; suppose the actual number is $k_{1}-1 \leq k-1$. Then these centers $r_{2}, \cdots, r_{k_{1}}$ must then all lie in $B_{\sigma}\left(r_{1}\right) \equiv B_{1}$.
If there are particles remaining, then $n_{2}-n_{1}$ of these centers, where $n_{2} \leqq k$, must lie in $B_{2} \cup \cdots B_{n_{1}}$. However, by construction, they cannot lie in $B_{1}$ and so these centers $\boldsymbol{r}_{n_{1}+1}, \cdots r_{n_{2}}$ must lie in $C\left(1, k_{1}\right) \equiv C\left(k_{0}, k_{1}\right)$. Continuing this process, we can 'construct' $k-1$ particles which are all connected to $\boldsymbol{r}_{1}$. To ensure that this cluster is a $k$-mer, we must finally ensure that there are no other centers within $V_{k}\left(r^{k} ; \sigma\right)$ except for the already determined centers $\boldsymbol{r}_{1}, \cdots \boldsymbol{r}_{\boldsymbol{k}}$. Since the particle centers are determined by a Poisson process with density $\rho$, we see that the probability that a $k$-mer has the configuration determined by $1<k_{1}<\cdots<k_{i}$ is given by (3.4). Summing over all possible configurations, we finally obtain Theorem 1.
We illustrate this paradigm by calculating $p_{3}$. There are two ways that a cluster containing a particle centered at $r_{1}$ could exist: the two centers $r_{2}$ and $r_{3}$ could both lie in $B_{1}$, or only one center $r_{2}$ in $B_{1}$ and one more center in $B_{2} \backslash B_{1}$. To ensure that the cluster has only three particles, the regions $V_{3}\left(r^{3} ; \sigma\right)$ must be otherwise empty for both cases. We conclude that

$$
p_{3}=\frac{\rho^{2}}{2!} \int_{B_{1}} d r_{2} \int_{B_{1}} d r_{3} \exp \left[-\rho V_{3}\left(r^{3} ; \sigma\right)\right]+\rho^{2} \int_{B_{1}} d r_{2} \int_{B_{2} \backslash B_{1}} d r_{3} \exp \left[-\rho V_{3}\left(r^{3} ; \sigma\right)\right] .
$$

Similarly, we find that $p_{4}$ is given by

$$
\begin{aligned}
p_{4}= & \frac{\rho^{3}}{3!} \int_{B_{1}} d r_{2} \int_{B_{1}} d r_{3} \int_{B_{1}} d r_{4} \exp \left[-\rho V_{4}\left(r^{4} ; \sigma\right)\right] \\
& +\frac{\rho^{3}}{2!} \int_{B_{1}} d r_{2} \int_{B_{1}} d r_{3} \int_{\left(B_{2} \cup B_{3}\right) \backslash B_{1}} d r_{4} \exp \left[-\rho V_{4}\left(r^{4} ; \sigma\right)\right] \\
& +\frac{\rho^{3}}{2!} \int_{B_{1}} d r_{2} \int_{B_{2} \backslash B_{1}} d r_{3} \int_{B_{2} \backslash B_{1}} d r_{4} \exp \left[-\rho V_{4}\left(r^{4} ; \sigma\right)\right] \\
& +\rho^{3} \int_{B_{1}} d r_{2} \int_{B_{2} \backslash B_{1}} d r_{3} \int_{B_{3} \backslash\left(B_{1} \cup B_{2}\right)} d r_{4} \exp \left[-\rho V_{4}\left(r^{4} ; \sigma\right)\right] .
\end{aligned}
$$

With sufficient patience one can obtain similar expressions in terms of these subintegrals for the higher $p_{k}$. The inherent difficulty with this procedure is parameterizing the domains of integration. Once this is accomplished, however, this expression eliminates all redundancies and hence lends itself to more efficient numerical integration.
3.1. Two-dimensional results. The integrals determining $p_{k}$ require knowledge of $V_{k}\left(r^{k} ; \sigma\right)$, the union area of $k$ circles of equal radius. To calculate $V_{k}$, it is sufficient to obtain expressions for the intersection of $j$ circles for $j \leqslant k$. Kratky [12] showed that the area of intersection of four or more circles can be reduced to a linear combination of the areas of intersection of two and three circles. Using this result, we can evaluate the integrands of the above integrals exactly, and then use numerical integration to finally obtain the $p_{k}$.

Figure 1 shows theoretical predictions of $p_{2}, p_{3}$ and $p_{4}$ and direct Monte Carlo simulation of these quantities. As we see, simulation and theory are in excellent agreement.

At low densities, the first few coefficients of the series expansions $p_{2}, p_{3}$ and $p_{4}$ around $\eta=0$ agree with the series expansions in Haan and Zwanzig [9]. $\dagger$ Recall that the reduced density $\eta$ is defined by (2.1).
3.2. Three-dimensional results. Kratky [13] also stated that the intersection volumes of five or more spheres of equal radius can be expressed as a linear combination of intersection volumes of two, three and four spheres. The volume of the intersection of three spheres $[17,19,21,27]$ and four spheres [11] are known analytically. Using these results, we can again evaluate the integrands of the above integrals analytically and then numerically obtain the $p_{k}$.

A graph comparing the theoretical predictions of $p_{2}, p_{3}$ and $p_{4}$ in three dimensions to computer simulations is shown in Figure 2. Again, at low densities,

[^1]

Figure 1 . The probability that a particle lies in a $k$-mer (i.e., $p_{k}$ ) in two dimensions. The solid dots are simulation data


Figure 2. The probability that a particle lies in a $k$-mer (i.e., $p_{k}$ ) in three dimensions. The solid dots are simulation data


Figure 3. The probability $p_{3}(\zeta ; d)$ for $d=1,2,3$, and $\infty$. We see that $p_{3}(\zeta ; d)$ approaches its long-range value as $d$ increases
the first few coefficients of the series expansions of $p_{2}, p_{3}$ and $p_{4}$ around $\eta=0$ agree with the series expansions in Haan and Zwanzig [9].
3.3. Other results and approximations. As mentioned previously, the $p_{k}$ are known analytically in one dimension and are given by $p_{k}=k \phi_{1}^{2}\left(1-\phi_{1}\right)^{k-1}$. Also, Penrose [16] has shown, for fixed $\zeta=2^{d} \eta$ and $k \geqslant 1$, that

$$
\lim _{d \rightarrow \infty} p_{k}(\zeta ; d)=\frac{k^{k-2}}{(k-1)!} \zeta^{k-1} \mathrm{e}^{-k \xi} \equiv p_{k}(\zeta ; \infty) .
$$

As we see in Figure 3, the graphs of $p_{3}(\zeta ; d)$ tend toward this limiting value as $d$ increases. This same qualitative behavior occurs for $k=2$ and $k=4$.
Using heuristic reasoning, Roach suggested that $p_{k}$ can be approximated by

$$
\begin{equation*}
p_{k} \approx p_{1}\left(1-p_{1}\right)^{k-1}, \tag{3.5}
\end{equation*}
$$

where $p_{1}$ is given in (3.1). In two dimensions, this formula indeed provides a good approximation to $p_{2}, p_{3}$ and $p_{4}$ for small to medium values of $\phi_{2}$. In three dimensions, (3.5) turns out to be an excellent approximation of $p_{2}, p_{3}$ and $p_{4}$ for $\phi_{2}<0.05$; however, its accuracy declines as $\phi_{2}$ increases above this threshold.

## 4. Average volume of $\boldsymbol{k}$-mers

We now consider the average volume of a given $k$-mer. In any dimension, the expected volume of a $k$-mer can be expressed in terms of a conditional expectation on the positions of its $k$ constituent spheres. After giving the general expression for any dimension, we directly calculate the average volume of a $k$-mer $v_{k}$ in one dimension. We then numerically evaluate $v_{k}$ in two and three dimensions.

The average volume of a $k$-mer is the expected volume of the cluster containing a given sphere $r_{1}$ given that the cluster is a $k$-mer. Once again, for simplicity we take $\boldsymbol{r}_{1}$ to be at the origin. From (3.2), given that $k$ particles form a $k$-mer, the conditional probability density function of the locations of the $k$ particles is given by

$$
f\left(r_{2}, \cdots, r_{k}\right)=\frac{\frac{\rho^{k-1}}{(k-1)!} \exp \left[-\rho V_{k}\left(r^{k} ; \sigma\right)\right] I\left(r^{k} ; \sigma / 2\right)}{\frac{\rho^{k-1}}{(k-1)!} \int d x_{2} \int d x_{3} \cdots \int d x_{k} \exp \left[-\rho V_{k}\left(x^{k} ; \sigma\right)\right] I\left(x^{k} ; \sigma / 2\right)}
$$

Since the definition of conditional expectation is

$$
v_{k}=\int d r_{2} \cdots \int d r_{k} V_{k}\left(r^{k} ; \sigma / 2\right) f\left(r_{2}, \cdots, r_{k}\right),
$$

we have the following theorem.
Theorem 2. The expected volume $v_{k}$ of $k$-mers is given by

$$
\begin{equation*}
v_{k}=\frac{\int d r_{2} \cdots \int d r_{k} V_{k}\left(r^{k} ; \sigma / 2\right) \exp \left[-\rho V_{k}\left(r^{k} ; \sigma\right)\right] I\left(r^{k} ; \sigma / 2\right)}{\int d r_{2} \cdots \int d r_{k} \exp \left[-\rho V_{k}\left(r^{k} ; \sigma\right)\right] I\left(r^{k} ; \sigma / 2\right)} \tag{4.1}
\end{equation*}
$$

This is somewhat different than the expression described by Given et al. [6], which suppresses the indicator functions and ignores the conditional expectation and hence the denominator. The integrals in Theorem 2 can be decomposed similarly to the decomposition in Theorem 1 and then numerically evaluated. The results we obtain are again in excellent agreement with computer simulations.

As mentioned in Section 2, the $p_{k}$ and $v_{k}$ can be used to evaluate the average volume of a randomly chosen cluster, denoted by $V(\eta)$. This quantity diverges at the percolation threshold, the infimum of densities at which a cluster of infinite size exists. In other work [18], we have used low-density expansions of $p_{k}$ and $v_{k}$ to approximate $V(\eta)$ and hence estimate the percolation threshold for fully penetrable circles and spheres.

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[^1]:    $\dagger$ The $\rho$ in the two-dimensional results of Table 1 of this reference correponds with our $2 \eta$, their $\rho$ corresponds to our $4 \eta$ in the three-dimensional results, and their $n_{k}$ is equivalent to our $p_{k} / k$. There appears to be a typographical error in this table; the coefficient of $\rho^{4}$ for the $n_{3}$ of circles should be 8.1055 instead of 8.11055 .

