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On the Boolean Model of Wiener Sausages

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Abstract The Boolean model of Wiener sausages is a random closed set that can be thought of as a random collection of parallel neighborhoods of independent Wiener paths in space. It describes e.g. the target detection area of a network of sensors moving according to the Brownian dynamics whose initial locations are chosen in the medium at random. In the paper, the capacity functional of this Boolean model is given. Moreover, the one- and two-point coverage probabilities as well as the contact distribution function and the specific surface area are studied. In $\mathbb{R}^2$ and $\mathbb{R}^3$, the one- and two-point coverage probabilities are calculated numerically by Monte Carlo simulations and as a solution of the heat conduction problem. The corresponding approximation formulae are given and the error of approximation is analyzed.

Keywords Wiener sausage · Boolean model · Sensor network · Capacity · Volume fraction · Specific surface area · Covariance function · Contact distribution function · Approximation · Heat conduction problem · Finite element method · Monte Carlo simulations · Stochastic geometry

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1 Introduction

A parallel neighborhood of a path of the Brownian motion is named after Norbert Wiener a *Wiener sausage*. This random closed set is used in physics, chemistry, biology and telecommunication to model various phenomena; cf. references in Yang et al. (2000). More complicated random closed sets can be constructed on its basis using the paradigm of *germ–grain models*. For that, a number of random locations in space called *germs* is supplied with random *grains* placed in these locations.

A germ–grain model with the spatially homogeneous Poisson point process of germs and independent identically distributed grains is a *Boolean model*. It is distinguished by the structural simplicity and the availability of analytical formulae for its characteristics; (cf. e.g. Stoyan et al. 1995). Boolean models with convex, polyconvex or smooth grains appear naturally in many applications in materials science, biology and medicine; (cf. e.g. Molchanov 1997). For this reason, most applied papers deal with these very well studied classes of primary grains. Extending the class of possible grains to parallel neighborhoods of fractal sets such as Wiener sausages and providing analytical formulae for the new type of grains would give practitioners more flexibility in modelling rough geometric structures.

Boolean models of Wiener sausages appear in connection with sensor networks (cf. e.g. Shakkottai 2005 and Kesidis et al. 2003). Imagine that sensors scattered initially at random in a non-transparent medium start moving according to the Brownian dynamics. Each sensor can detect a target within a range $r > 0$. The target detection area of such sensor network up to time $T > 0$ forms a Boolean model with the Wiener sausage of radius r as a primary grain. The probability of target detection (also known as the *one-point coverage probability* or *volume fraction* of the Boolean model) in three dimensions is given in Kesidis et al. (2003).

In this paper, we deal mainly with the *two-point coverage probabilities* of the Boolean model of Wiener sausages that are often called the *covariance function*. We give approximation formulae for the covariance function in two and three dimensions based on Monte Carlo simulations and numerical solutions of the heat conduction equation.

In Section 2, preliminaries on Wiener sausages are given. Section 3 deals with the capacity functional of the Boolean model of Wiener sausages connecting it with the initial and boundary value problems for the heat equation. A general representation of the volume fraction, the covariance function and the contact distribution function as values of the capacity functional on particular test sets follows easily. This representation involves an integral of the solution of the heat conduction problem in some region. For the covariance function, this is an exterior of the union of two (possibly overlapping) spheres. If these spheres coincide an explicit analytical solution can be given in any dimension. Nevertheless, in all dimensions excepting three this formula can not be used in practice since it involves integrals of a combination of Bessel functions. Moreover, in general case the corresponding analytical expression is still unknown and has to be assessed numerically. In Section 3.3, a formula for the specific surface area of the Boolean model of Wiener sausages is given. The numerical analysis of the covariance function in two and three dimensions is performed in Section 4 by means of finite element method and by simulation (Sections 4.1 and 4.3, respectively). Simple approximation formulae are provided and the error of approximation is discussed. Results of different computation methods are compared in Section 4.4. We conclude with a brief discussion of open problems.

2 Preliminaries

Let $A \oplus B$ be the pointwise sum of two sets A and B in $\mathbb{R}^d$. For the ball $B = B(o, r)$ of radius $r \geqslant 0$ in $\mathbb{R}^d$ centered at the origin, the set $A_r = A \oplus B(o, r)$ is called the *r-parallel neighborhood of A*. The operation $A \mapsto A_r$ is known as *dilation*. Let us write $V_d(A)$ for the volume of a Borel set $A \subset \mathbb{R}^d$. For any set A, denote $\check{A} = -A$. Let $\omega_d = \pi^{d/2}/\,\Gamma(1 + d/2)$ be the volume of the unit ball in d dimensions.

Let $\{B^x(t), t \geq 0\}$ be the d-dimensional Brownian motion in $\mathbb{R}^d$ with variance $\sigma^2 > 0$ starting at $B^x(0) = x \in \mathbb{R}^d$. Throughout the paper, we assume that $d \geqslant 2$. Given a radius $r > 0$ and a time $T > 0$ we set

$$S^x_{r,T} = \{B^x(t) : 0 \leq t \leq T\} \oplus B(o, r)\,. \tag{2.1}$$

$S^x_{r,T}$ is called the *Wiener sausage*; (cf. e.g. Sznitman 1998, p. 64). It is a random compact set (in the sense of Matheron, see Matheron 1975). We shall write only $S_{r,T}$ for $S^o_{r,T}$ if the Brownian motion starts at the origin. It is known that all moments of the volume $V_d(S_{r,T})$ are finite, see Sznitman (1987).

3 Boolean Model of Wiener Sausages

Assume $\varphi = \{x_n\}_{n=1}^{\infty}$ to be a stationary Poisson point process in $\mathbb{R}^d$ with intensity $\lambda > 0$ (see e.g. Stoyan et al. 1995 for more details). Consider an independent identically distributed collection of Wiener sausages $\{(S_{r,T})_n\}_{n=1}^{\infty}$ (each starting at the origin) which are independent of the process φ. Introduce the *Boolean model* Ξ *of Wiener sausages* (Fig. 1) by putting

$$\Xi = \bigcup_{n=1}^{\infty} \big(x_n + (S_{r,T})_n\big). \tag{3.1}$$

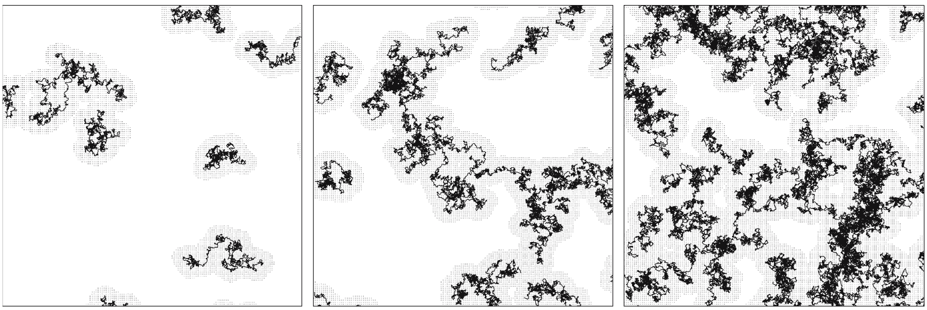


Fig. 1 Three realizations of Boolean models of Wiener sausages for $T = 10$ and $r = 1$. The intensity λ is chosen to fit volume fractions 0.25, 0.5 and 0.75, respectively

Since $\mathrm{E}\, V_d(S_{r,T} \oplus B(o, r')) = \mathrm{E}\, V_d(S_{r+r',T}) < \infty$ for all $r' > 0$, Ξ is a random closed set (see Stoyan et al. 1995). The isotropy of $S_{r,T}$ and stationarity of φ imply that Ξ is stationary and isotropic. It means that the probability distribution of Ξ is invariant with respect to rigid motions.

3.1 Capacity Functional, Volume Fraction and Covariance Function

The *capacity functional* $T_\Xi(C) = P(\Xi \cap C \neq \emptyset)$ for all compact $C \subset \mathbb{R}^d$ plays the same role in the theory of random sets as the distribution function of random variables in the classical probability theory. Namely, it defines the distribution law of Ξ uniquely. It is known that the capacity functional of the Boolean model is given by

$$T_\Xi(C) = 1 - e^{-\lambda\, \mathrm{E}\, V_d(S_{r,T} \oplus \check{C})} \tag{3.2}$$

for all compact C; cf. Stoyan et al. (1995).

Following Spitzer (1964), we can compute the expected volume of $S_{r,T} \oplus \check{C}$ using Fubini's theorem as

$$\mathrm{E}\, V_d\left(S_{r,T} \oplus \check{C}\right) = \int\limits_{\mathbb{R}^d} \mathrm{P}\left(x \in S_{r,T} \oplus \check{C}\right) dx = \int\limits_{\mathbb{R}^d} \mathrm{P}\left(\tau^x_{C \oplus B(o,r)} \leq T\right) dx\,, \tag{3.3}$$

where $\tau^x_A = \inf\{s > 0 : B^x(s) \in A\}$ is the first hitting time of a Borel set A for the Brownian motion starting at $x \in \mathbb{R}^d$. Introduce the notation $u(t, x) = \mathrm{P}\left(\tau^x_{C\oplus B(o,r)} \leq t\right)$, $x \in \mathbb{R}^d$, $t \geqslant 0$. Kolmogoroff and Leontowitsch (1933), Hunt (1956) and Doob (1955) showed that $u(t, x)$ is the unique bounded solution to the following heat conduction problem:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\sigma^2}{2} \triangle u, && t > 0,\ x \in \mathbb{R}^d \setminus (C \oplus B(o, r)), \\ u(0, x) &= 0, && x \in \mathbb{R}^d \setminus (C \oplus B(o, r)), \\ u(t, x) &= 1, && t \geqslant 0, x \in \partial(C \oplus B(o, r))\,. \end{aligned} \tag{3.4}$$

For arbitrary compact sets C the problem (3.4) has to be solved by numerical methods. In some special cases (for instance, if $C = \{o\}$) an analytical solution is given in Berezhkovskii et al. (1989). This is the expected volume of the Wiener sausage:

$$\begin{aligned} \mathrm{E}\, V_d(S_{r,t}) = \omega_d r^d &+ \frac{d(d-2)}{2} \omega_d \sigma^2 r^{d-2} t \\ &+ \frac{4d\, \omega_d\, r^d}{\pi^2} \int\limits_0^\infty \frac{1 - e^{-\frac{\sigma^2 y^2 t}{2r^2}}}{y^3 \left(J^2_\nu(y) + Y^2_\nu(y)\right)}\, dy, \qquad d \geqslant 2, \end{aligned} \tag{3.5}$$

where J_ν and Y_ν are Bessel functions of the first and second kind of order $\nu = (d-2)/2$. In three dimensions, this formula simplifies to

$$\mathrm{E}\ V_3(S_{r,t}) = \frac{4}{3}\pi r^3 + 4\sigma r^2\sqrt{2\pi t} + 2\pi\sigma^2 rt\,, \tag{3.6}$$

compare Spitzer (1964).

The *volume fraction* p_Ξ of the Boolean model Ξ defined by

$$p_\Xi = \mathrm{P}(o \in \Xi) = \mathrm{E}\ V_d(\Xi \cap [0,1]^d)$$

is just the one-point coverage probability of Ξ. It follows from relations $p_\Xi = T_\Xi(\{o\})$, Eqs. 3.2 and 3.5 that

$$p_\Xi = 1 - e^{-\lambda\left(\omega_d r^d + \frac{d(d-2)}{2}\omega_d\,\sigma^2 r^{d-2}T + \frac{4d\,\omega_d\,r^d}{\pi^2}\int\limits_0^\infty \frac{1-e^{-\frac{\sigma^2 y^2 T}{2r^2}}}{y^3\left(J_\nu^2(y)+Y_\nu^2(y)\right)}\,dy\right)}. \tag{3.7}$$

For $d = 3$ this formula can be found in Kesidis et al. (2003).

The *covariance function* of the isotropic Boolean model Ξ can be introduced by

$$C_\Xi(h) = \mathrm{P}(o, h\cdot u \in \Xi), \tag{3.8}$$

where u is an arbitrary unit vector in $\mathbb{R}^d$ and $h \ge 0$; (see Stoyan et al. 1995 and Molchanov 1997). It follows from Eq. 3.2 and the formula of total probability that

$$C_\Xi(h) = 2p_\Xi - T_\Xi(\{o, h\cdot u\}) = 2p_\Xi - 1 + e^{-\lambda\,\mathrm{E}\ V_d(S_{r,T}\cup(S_{r,T}+h\cdot u))}\,. \tag{3.9}$$

It follows from relations (3.2) and (3.3) that the mean volume

$$\mathrm{E}\ V_d(S_{r,T}\cup(S_{r,T}+h\cdot u)) = \int\limits_{\mathbb{R}^d} \mathrm{P}\left(\tau^x_{B(o,r)\cup B(h\cdot u,r)} \le T\right)\,dx \tag{3.10}$$

in formula (3.9) can be computed by integrating the solution of the heat conduction problem (3.4) where

$$C \oplus B(r,o) = \{o, h\cdot u\} \oplus B(o,r) = B(o,r) \cup B(h\cdot u, r)\,. \tag{3.11}$$

The mean volume in Eq. 3.10 is related to the *covariogram*

$$C_{S_{r,T}}(h) = \mathrm{E}\,V_d(S_{r,T} \cap (S_{r,T} + h\cdot u))$$

of the Wiener sausage $S_{r,T}$ by

$$\mathrm{E}\,V_d(S_{r,T}\cup(S_{r,T}+h\cdot u)) = 2\,\mathrm{E}\,V_d(S_{r,T}) - \mathrm{E}\ V_d(S_{r,T}\cap(S_{r,T}+h\cdot u)) \tag{3.12}$$

where $\mathrm{E}\,V_d(S_{r,T})$ is given in Eq. 3.5.

3.2 Contact Distribution Function

For a compact test set $C \subset \mathbb{R}^d$, $o \in C$, the *contact distribution function* of a random closed set Ξ is introduced as

$$H_C(\rho) = P(d_C(o, \Xi) \leqslant \rho \mid o \notin \Xi), \qquad \rho > 0,$$

where $d_C(x, A) = \min\{\rho \geqslant 0 : (x + \rho C) \cap A \neq \emptyset\}$ is the distance from a point $x \in \mathbb{R}^d$ to a closed set $A \subset \mathbb{R}^d$ measured by "inflating" the test set C. It can be easily shown that

$$H_C(\rho) = P(\Xi \cap \rho C \neq \emptyset \mid o \notin \Xi) = \frac{T_\Xi(\rho C) - T_\Xi(\{o\})}{1 - T_\Xi(\{o\})} ,$$

cf. Stoyan et al. (1995). If Ξ is the Boolean model of Wiener sausages then $T_\Xi(\{o\})$ is given by relation (3.7). The value of $T_\Xi(\rho C)$ can be assessed numerically if C is a general compact set; see the next section for an example of such numerical analysis. However, if C is a unit ball then the *spherical contact distribution function* $H_{B(o,1)}(\rho)$ can be given explicitly, since by Eq. 3.2 we get

$$T_\Xi(\rho B(o, 1)) = T_\Xi(B(o, \rho)) = 1 - e^{-\lambda \mathrm{E}\, V_d(S_{r,T} \oplus B(o,\rho))} = 1 - e^{-\lambda \mathrm{E}\, V_d(S_{r+\rho,T})}$$

which together with relation (3.5) yields the formula

$$H_{B(o,1)}(\rho) = 1 - e^{-\lambda M(d,\sigma^2,r,\rho,T)} ,$$

where

$$M(d, \sigma^2, r, \rho, T) = \omega_d \left((r+\rho)^d - r^d\right) + \frac{d(d-2)}{2} \omega_d \sigma^2 \left((r+\rho)^{d-2} - r^{d-2}\right) T$$
$$+ \frac{4d\,\omega_d}{\pi^2} \left((r+\rho)^d \int_0^\infty \frac{1 - e^{-\frac{\sigma^2 y^2 T}{2(r+\rho)^2}}}{y^3 \left(J_\nu^2(y) + Y_\nu^2(y)\right)}\, dy \right.$$
$$\left. - r^d \int_0^\infty \frac{1 - e^{-\frac{\sigma^2 y^2 T}{2r^2}}}{y^3 \left(J_\nu^2(y) + Y_\nu^2(y)\right)}\, dy \right).$$

3.3 Specific Surface Area

The specific surface area S_Ξ is defined as the mean surface area of Ξ per unit volume. More formally, consider the measure $S_\Xi(B) = \mathrm{E}\, \mathcal{H}^{d-1}(\partial \Xi \cap B)$ for all Borel sets $B \subset \mathbb{R}^d$, where $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional Hausdorff measure. Due to the stationarity of Ξ, the measure S_Ξ is translation invariant. By Haar's lemma, there exists a constant $S_\Xi \in (0, \infty)$ such that $S_\Xi(B) = S_\Xi \cdot V_d(B)$ for all Borel sets B. The factor S_Ξ is called the *specific surface area* of the Boolean model Ξ (cf. Stoyan et al. 1995, p. 235). The following formula (3.13) is well-known for Boolean models with convex compact grains; cf. e.g. Lemma 4.1 of Heinrich and Molchanov (1999). We prove that it holds also in the case of the Boolean model of Wiener sausages whose boundaries are Lipschitz manifolds almost surely in dimensions two and three.

Proposition 3.1 *The specific surface area of* Ξ *in* $\mathbb{R}^d$ $(d = 2, 3)$ *is equal to*

$$S_\Xi = \lambda \,\mathrm{E}\, \mathcal{H}^{d-1}(\partial S_{r,T}) e^{-\lambda \,\mathrm{E}\, V_d(S_{r,T})}, \qquad r > 0, \tag{3.13}$$

where the mean volume $\mathrm{E}\ V_d(S_{r,T})$ *is given in Eq. 3.5 and*

$$\begin{aligned}\mathrm{E}\,\mathcal{H}^{d-1}(\partial S_{r,T}) &= d\omega_d r^{d-1} + \frac{4d^2\,\omega_d\, r^{d-1}}{\pi^2}\int_0^\infty \frac{1-e^{-\frac{\sigma^2 y^2 T}{2r^2}}}{y^3\left(J_\nu^2(y)+Y_\nu^2(y)\right)}\,\mathrm{d}y \\ &\quad + d\omega_d\sigma^2 r^{d-3} T\left(\frac{(d-2)^2}{2} - \frac{4}{\pi^2}\int_0^\infty \frac{e^{-\frac{\sigma^2 y^2 T}{2r^2}}}{y\left(J_\nu^2(y)+Y_\nu^2(y)\right)}\,\mathrm{d}y\right)\end{aligned} \tag{3.14}$$

is the mean surface area of the Wiener sausage. In three dimensions, formula (3.13) simplifies to

$$S_\Xi = 2\pi\lambda\left(2r^2 + 4r\sigma\sqrt{2T/\pi} + \sigma^2 T\right) e^{-2\pi\lambda r\left(2/3r^2 + 2\sigma r\sqrt{2T/\pi} + \sigma^2 T\right)}. \tag{3.15}$$

Proof Since Ξ is isotropic, and since the boundary of the Wiener sausage is a $(d-1)$–dimensional Lipschitz manifold almost surely (cf. Rataj et al. 2006, Corollary 4.1) we can use the relation

$$S_\Xi = -\frac{d\,\omega_d}{\omega_{d-1}} C'_\Xi(0) \tag{3.16}$$

to get S_Ξ; (cf. e.g. Stoyan et al. 1995, p. 204). The covariance function (3.9) rewrites

$$C_\Xi(h) = 2p_\Xi - 1 + (1-p_\Xi)^2 e^{\lambda C_{S_{r,T}}(h)}, \qquad h \geqslant 0\,.$$

Its first derivative in zero is given by

$$C'_\Xi(0) = \lambda C'_{S_{r,T}}(0) e^{-\lambda \,\mathrm{E}\, V_d(S_{r,T})}\,. \tag{3.17}$$

It is shown in Černý and Rataj (2006) that

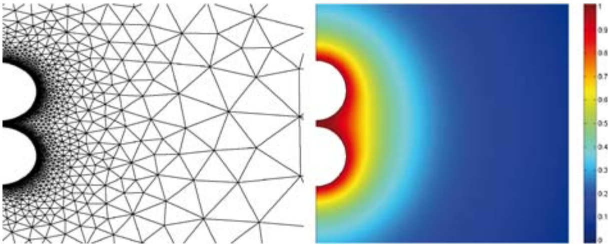
$$C'_{S_{r,T}}(0) = -\frac{\omega_{d-1}}{d\,\omega_d}\,\mathrm{E}\,\mathcal{H}^{d-1}(\partial S_{r,T}), \qquad r > 0. \tag{3.18}$$

The analytical formula (3.14) together with its simplified counterpart for $d = 3$ is given in Rataj et al. (2006). Combining expressions (3.16), (3.17), and (3.18) yields the result (3.13). Its special case (3.15) in three dimensions follows from formula (3.6) of this paper and relation (2.3) of Rataj et al. (2006). □

4 Numerical Assessment of the Covariance Function

As far as it is known to the authors, it is difficult to find an explicit analytical solution to Eq. 3.4 on the complement of the union of two spheres. Hence, numerical methods can be used to solve Eq. 3.4 and get a graph of the covariance function C_Ξ. In Section 4.1, we perform this numerical analysis by means of the finite element method (fem, for an introduction see Braess 2001; Ciarlet 2002, and references quoted therein). Alternatively, a large number of Monte Carlo simulations of Wiener sausages can lead to precise estimates of C_Ξ as it is done in Section 4.3.

Fig. 2 Zoom of the used fem mesh (*left*) and corresponding computed solution u (*right*) of Eq. 3.4 for $d = 2, \sigma = 1, r = 1, h = 2.2$ and $t = 100$



The MATLAB- and FEMLAB-Code which was used to compute the results below by the Monte Carlo simulations resp. the finite element method can be downloaded from the web.[1]

4.1 Numerical Solution of the Heat Conduction Problem

For $d = 2, 3$ we used the finite element method to compute an approximate solution u of Eq. 3.4. To solve the problem efficiently we used rotational and axial symmetry in 3D resp. axial symmetries in 2D to reduce the complexity of problem (3.4). Furthermore, we restricted the resulting problem to a bounded domain Ω_h with $\max_{x,y\in\Omega_h} |x - y| > 10(2 + h)$ for $r = 1$, $0 \leq h \leq 20$, and $0 \leq t \leq 100$. This domain is large enough to provide the same numerical results for the problem (3.4), (3.11) solved in Ω_h. For discretisation we used a graded mesh with minimal mesh size $h_{\min} = 0.015$ along the boundary of the balls $B(o, r)$, resp. $B(h \cdot u, r)$ and a mesh grading of 1.3, i.e. the rate how the mesh size grows as $|x|$ tends to infinity. A zoom of the resulting finite element mesh is shown in Fig. 2 for $r = 1$ and $h = 2.2$. As ansatzspace we used globally continuous, piecewise polynomials of degree 4 and an adaptive timestepping scheme. These calculations were done by using the software package FEMLAB/COMSOL (Funken 2003) or can be done by adapting Alberty et al. (1999).

4.2 Approximation Formulae

In the following we shall give an approximation $\widetilde{C}_\Xi$ for the covariance function C_Ξ given in Eq. 3.8 for some fixed volume fraction p_Ξ, namely

$$C_\Xi(h) \approx \tilde{C}_\Xi(h) := 2p_\Xi - 1 + (1 - p_\Xi)^{\kappa(h,t)}\,, \tag{4.1}$$

with $\kappa(h, t)$ given by Eqs. 4.5 and 4.6 below. Let $d = 2, 3$ and

$$A_r(h, t) := \mathrm{E}\ V_d(S_{r,t} \cup (S_{r,t} + h \cdot u)) = V_d(B(o, r) \cup B(h \cdot u, r)) + \int\limits_{\mathbb{R}^d\setminus(B(o,r)\cup B(h,r))} u(t, x)\, dx\,, \tag{4.2}$$

(compare Eq. 3.10) where $u(t, x)$ denotes the solution of Eq. 3.4 for some given $h \geq 0$, $r > 0$ and $C \oplus B(r, o)$ as in Eq. 3.11. For some given volume fraction p_Ξ of the

[1] http://www.mathematik.uni-ulm.de/numerik/staff/funken/software

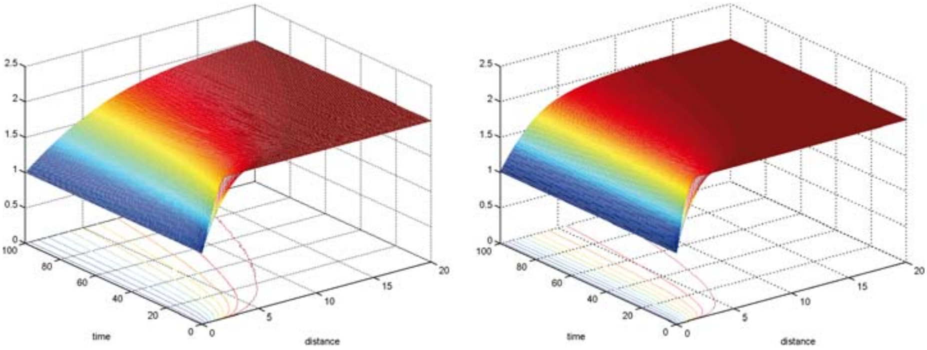


Fig. 3 Computed approximation of $A_r(h,t)/A_r(0,t)$ in 2D (*left*) resp. 3D (*right*) for $r = 1$, $0 \le h \le 20$ and total times $0 \le t \le 100$

Boolean model Ξ we substitute λ implicitly defined by Eq. 3.7 in Eq. 3.9 which leads to

$$C_\Xi(h) = 2p_\Xi - 1 + (1 - p_\Xi)^{A_r(h,t)/A_r(0,t)}\,.$$

For $t = 0$ and $d = 2$ analytic calculations of $V_d(B(o,r) \cup B(h \cdot u, r))$ give

$$\frac{A_r(h,0)}{A_r(0,0)} = \kappa(h,0) := \begin{cases} \frac{2}{\pi}\left(\pi - \arccos\left(\frac{h}{2r}\right) + \frac{h}{2r}\sqrt{1 - \left(\frac{h}{2r}\right)^2}\right), \text{if } h \le 2r\,, \\ 2, \text{otherwise}\,, \end{cases} \tag{4.3}$$

resp. for $d = 3$

$$\frac{A_r(h,0)}{A_r(0,0)} = \kappa(h,0) := \begin{cases} \frac{1}{2}\left(\frac{h}{2r}\right)^3 - 2\left(\frac{h}{2r}\right)^2 + \frac{5}{2}\frac{h}{2r} + 1, \text{if } h \le 2r\,, \\ 2, \text{otherwise}\,. \end{cases} \tag{4.4}$$

For $t > 0$ and $d = 2, 3$ a closed formula for $A_r(h,t)/A_r(0,t)$ is not known to the authors. In the following we give some approximation $\kappa(h, \nu(t))$ (computed by the finite element method and some elementary postprocessing) to the quotient $A_r(h,t)/A_r(0,t)$ (Fig. 3), where we used the scaling invariants of $A_r(h,t)/A_r(0,t)$ w.r.t. the radius r,

$$\frac{A_r(h,t)}{A_r(0,t)} \approx \kappa(h,t) = \begin{cases} \left(\frac{h}{\nu(t)}\right)^3 - 3\left(\frac{h}{\nu(t)}\right)^2 + 3\frac{h}{\nu(t)} + 1, \text{if } h \le \nu(t)\,, \\ 2, \text{otherwise}\,, \end{cases} \tag{4.5}$$

with

$$\nu(t) = \begin{cases} 2.998\,t^{0.3991} + 2.991, d = 2\,, \\ 3.744\,t^{0.2182} + 1.454, d = 3\,. \end{cases} \tag{4.6}$$

Using Eq. 4.1 with Eq. 4.3 or 4.4 resp. Eqs. 4.5 and 4.6 gives an approximation formula for the covariance function C_Ξ. For $p_\Xi = 0.75$, $r = 1$, $0 \le h \le 20$ and $0 \le t \le 100$ numerical calculations show (see Fig. 4) that pointwise in 2D the absolute

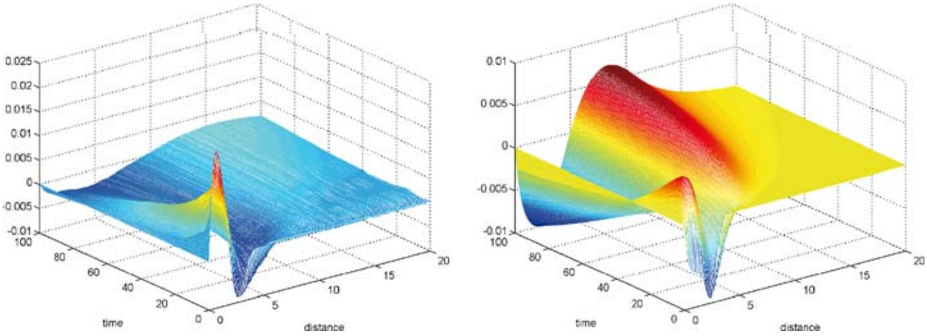


Fig. 4 Estimated relative errors in 2D (*left*) resp. 3D (*right*) of covariance function $|\overline{C}_\Xi(h) - \widetilde{C}_\Xi(h)|/|\overline{C}_\Xi(h)|$ for $p_\Xi = 0.75, r = 1, 0 \le h \le 20$ and total times $0 \le t \le 100$

error $|\overline{C}_\Xi(h) - \widetilde{C}_\Xi(h)| \le 0.0134$, the relative error $|\overline{C}_\Xi(h) - \widetilde{C}_\Xi(h)|/|\overline{C}_\Xi(h)| \le 0.02$ resp. in 3D $|\overline{C}_\Xi(h) - \widetilde{C}_\Xi(h)| \le 0.0063$ and $|\overline{C}_\Xi(h) - \widetilde{C}_\Xi(h)|/|\overline{C}_\Xi(h)| \le 0.01$, where $\overline{C}_\Xi$ is the result of the computation of the covariance function by the finite element approximation.

4.3 Estimation by Monte Carlo Simulation

There are two ways leading to estimates of the covariance C_Ξ from simulations. The first way is to use the definition (3.8) and simulate many realizations of the Boolean model Ξ in a finite observation window estimating the two-point coverage probability from each of them and then averaging over all realizations. The second way is to simulate one Wiener sausage many times and estimate its covariogram. By expressions (3.9) and (3.12), this would lead to an estimate of the covariance C_Ξ. We would prefer the second approach since it leads to more precise results.

In order to do so, simulate N independent copies $\{(S_{r,T,n})_k\}_{k=1}^N$ of the approximated Wiener sausage $S_{r,T,n}$ for sufficiently large approximation parameter n and compute the volume of intersection $S_{r,T,n} \cap (S_{r,T,n} + h \cdot u)$ by averaging over N realizations. To get a realization of $S_{r,T,n}$, we use a piecewise linear approximation $W_i^n(t)$ of each coordinate $W_i(t)$ of $B(t) = B^o(t) = (W_1(t), \ldots, W_d(t))$, where $W_i(t),\ i = 1, \ldots, d$ are standard one-dimensional Wiener processes.

We assume for simplicity $T = \sigma = 1$. Let $Y_0^i = 0$ and $Y_1^i, Y_2^i, \ldots$ be independent sequences of i.i.d. random variables with the distribution $N(0, 1)$, $i = 1, \ldots, d$. Set

$$S_n^i = \sum_{k=0}^{n} Y_k^i$$

to be a special case of the symmetric random walk. Introduce the piecewise linear process $W_i^n(t),\ t \in [0, 1]$ by

$$W_i^n(t) = \frac{S_{k-1}^i}{\sqrt{n}} + \frac{nt - (k-1)}{\sqrt{n}} Y_k^i, \qquad t \in \left[\frac{k-1}{n}, \frac{k}{n}\right). \tag{4.7}$$

Following the well-known invariance principle of Donsker (cf. e.g. Billingsley 1999, Theorem 8.2) it holds

$$W_i^n(t),\ t \in [0,1] \xrightarrow{\mathcal{D}} W_i(t),\ t \in [0,1], \qquad n \to \infty, \qquad i = 1, \ldots, d. \tag{4.8}$$

In other words, the approximations $W_i^n(t)$, $i = 1, \ldots, d$ converge in distribution to independent standard Wiener processes W_i on $[0, 1]$. It follows

$$B^n(t) = \left(W_1^n(t), \ldots, W_d^n(t)\right),\ t \in [0,1] \xrightarrow{\mathcal{D}} B(t),\ t \in [0,1].$$

Set $S_{r,1,n} = \{B^n(t) : t \in [0,1]\} \oplus B(o,r)$ for any $n \in \mathbb{N}$. Let us show that the covariance function of the Boolean model with primary grain $S_{r,1,n}$ approximates C_Ξ as n tends to infinity. It suffices to prove the following

Proposition 4.1 *It holds*

$$C_{S_{r,1,n}}(h) \to C_{S_{r,1}}(h), \qquad n \to \infty, \qquad h \geqslant 0. \tag{4.9}$$

First we need the following auxiliary result.

Lemma 4.1 *Let $\{Y_i\}_{i \in \mathbb{N}}$ be a sequence of i.i.d. random variables with $Y_i \sim N(0,1)$. Then, the inequality*

$$\mathrm{P}\left[\max_{1 \le k \le n} |S_k| \ge x\right] \le 2\,\mathrm{P}[|S_n| \ge x/2], \qquad x \geqslant 0$$

holds for $S_k = Y_1 + \ldots + Y_k$, $k = 1, \ldots, n$.

Proof Using arguments similar to (Billingsley 1999, p. 256), one can prove the following variant of Etemadi's inequality:

$$\mathrm{P}\left[\max_{1 \le k \le n} |S_k| \ge x\right] \le \mathrm{P}[|S_n| \ge x/2] + \max_{1 \le k \le n} \mathrm{P}[|S_k| \ge x/2], \qquad x \geqslant 0.$$

Since $S_k \sim N(0,k)$, it is easy to see that for any $k = 1, \ldots, n$

$$\mathrm{P}[|S_k| \ge y] = \frac{1}{\sqrt{2\pi}} \int\limits_{\mathbb{R} \setminus (-y/\sqrt{k},\, y/\sqrt{k})} e^{-z^2/2}\, dz \leqslant \mathrm{P}[|S_n| \ge y], \qquad y \geqslant 0.$$

Hence, it holds

$$\max_{1 \le k \le n} \mathrm{P}[|S_k| \ge x/2] = \mathrm{P}[|S_n| \ge x/2],$$

and the lemma is proved. □

Proof of Proposition 4.1 Since the mapping $A \mapsto V_d(A \oplus B(o,r))$ is continuous in the Hausdorff metric (see the proof of Stachó 1976, Theorem 3), we have by the mapping theorem for convergence in distribution (Billingsley 1999, Theorem 2.7)

$$V_d(S_{r,1,n}) \xrightarrow{\mathcal{D}} V_d(S_{r,1}), \qquad n \to \infty.$$

Our aim is to show that

$$\mathrm{E}\, V_d(S_{r,1,n}) \to \mathrm{E}\, V_d(S_{r,1}). \tag{4.10}$$

This convergence holds if $V_d(S_{r,1,n})$, $n = 1, 2, \ldots$ are uniformly integrable random variables (Billingsley 1999, Theorem 3.5). A sufficient condition for the uniform integrability is

$$\sup_{n\in\mathbb{N}} \mathrm{E}(V_d(S_{r,1,n}))^2 < \infty. \tag{4.11}$$

We can write

$$V_d(S_{r,1,n}) \leq \omega_d(r + \max_{t\in[0,1]} |B^n(t)|)^d \leq \omega_d\left(r + \sum_{i=1}^{d} \max_{t\in[0,1]} |W_i^n(t)|\right)^d.$$

Since the distributions of $|W_i^n(t)|,\ i = 1, \ldots, d$ are identical we get

$$\begin{aligned}\mathrm{E}(V_d(S_{r,1,n}))^2 &\leq \omega_d^2\, \mathrm{E}\left[r + \sum_{i=1}^{d} \max_{1\leq k\leq n} \frac{|S_k^i|}{\sqrt{n}}\right]^{2d} \\ &= \omega_d^2 \sum_{\substack{k_0,\ldots,k_d\geqslant 0:\\ k_0+\ldots+k_d=2d}} \frac{(d+1)!}{k_0!\ldots k_d!} r^{k_0} \prod_{i=1}^{d} \mathrm{E} \max_{1\leq k\leq n} \left(\frac{|S_k|}{\sqrt{n}}\right)^{k_i},\end{aligned}$$

where $S_k \overset{\mathcal{D}}{=} S_k^i \sim N(0, k)$. Using Lemma 4.1, we get the upper bound

$$\begin{aligned}\mathrm{E} \max_{1\leq k\leq n} \left(\frac{|S_k|}{\sqrt{n}}\right)^m &= \frac{1}{n^{m/2}} \int_0^\infty \mathrm{P}\left[\max_{1\leq k\leq n} |S_k| \geq x^{1/m}\right] dx \\ &\leq \frac{2}{n^{m/2}} \int_0^\infty \mathrm{P}[|S_n| \geq x^{1/m}/2]\, dx = \frac{2^{m+1}}{n^{m/2}} \int_0^\infty m y^{m-1}\, \mathrm{P}[|S_n| \geq y]\, dy \\ &= \frac{2^{m+1}}{n^{m/2}}\, \mathrm{E}\, |S_n|^m \leqslant m!\, 2^m, \quad m \in \mathbb{N},\end{aligned}$$

where the latter inequality follows from the fact that $S_n \sim N(0, n)$. Hence, condition (4.11) is verified, and the convergence (4.10) of mean volumes holds.

We can proceed in the same way and show that

$$\mathrm{E}\, V_d(S_{r,1,n} + h \cdot u) \to \mathrm{E}\, V_d(S_{r,1} + h \cdot u),$$

$$\mathrm{E}\, V_d(S_{r,1,n} \cup (S_{r,1,n} + h \cdot u)) \to \mathrm{E}\, V_d(S_{r,1} \cup (S_{r,1} + h \cdot u))$$

as $n \to \infty$. Together with Eq. 3.10 we get relation (4.9), and Proposition 4.1 is proved. □

Remark 4.1 According to the invariance principle of Donsker, Proposition 4.1 holds (with slight changes in the proof) for any choice of symmetric random walk S_n^i in Eq. 4.7. We choose the random variables Y_n^i standard normally distributed to reduce the error of approximation and increase the speed of convergence of the algorithm.

Relation (4.9) together with the law of large numbers allow us to estimate the covariance function of the Boolean model Ξ from sufficiently many approximations $S_{r,T,n}$. In Fig. 5, such estimates are given in two and three dimensions. For $T = 1$,

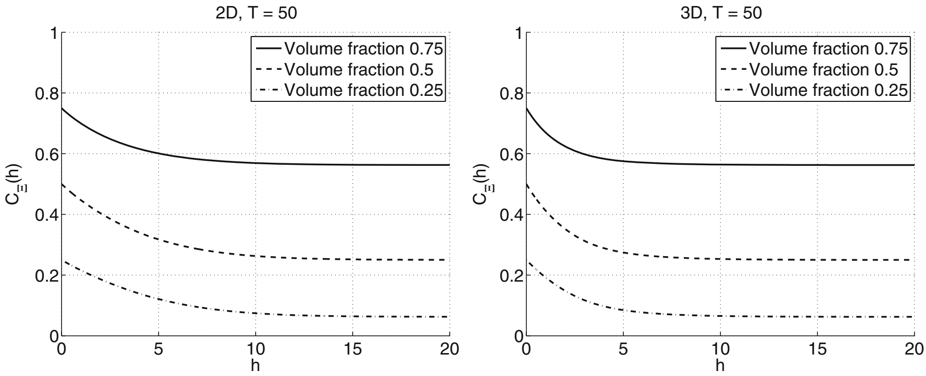


Fig. 5 Estimated covariance functions of the planar and spatial Boolean model of Wiener sausages with $r = 1$ and total time $T = 50$. In each case, the intensity λ is chosen to fit volume fractions 0.25, 0.5 and 0.75, respectively. Estimates for $T = 1$ and $T = 10$ are similar and therefore are omitted here

$T = 10$ and $T = 50$, 10,000 approximations of Wiener sausages with $r = 1$ were simulated. To evaluate the volume of $S_{r,T,n}$ and its covariogram numerically, realizations of Wiener sausages have to be discretized on a quadratic (cubic) grid in $\mathbb{R}^2$ ($\mathbb{R}^3$), and the number of pixels (voxels) belonging to $S_{r,T,n}$ has to be counted. Hence, besides the error of the approximation of the Wiener sausage, the discretization error occurs.

Given the total runtime T, the maximal shift distance $h_{\max}$ for which the covariogram $C_{S_{r,T}}$ was computed is given by

$$h_{\max} = 2 \cdot F_{0,T}^{-1}(0.99),$$

where $F_{0,T}^{-1}$ is the quantile function of the normal distribution $N(0, T)$. This value $h_{\max}$ yields a good empirical upper bound for the range of dependence of the covariance function C_Ξ. It means that $C_\Xi(h) \approx p_\Xi^2$ is approximately constant for $h > h_{\max}$.

4.4 Comparison of Results

We now compare the numerical calculations by the finite element method (Section 4.1) versus the Monte-Carlo simulation (Section 4.3) with respect to efficiency and accuracy.

Table 1 shows run times for both approaches to compute the covariance function $C_\Xi(h)$ for $r = 1$ and total times $T = 1$, $T = 10$, and $T = 50$ in two and three

Table 1 Computing times for 1,000 Monte Carlo simulations and one finite element run to approximate the covariance function $C_\Xi(h)$ for $r = 1$ and total times $T = 1$, $T = 10$, and $T = 50$

	Monte Carlo simulations		Finite element method	
	2D	3D	2D (s)	3D (s)
$T = 1$	1 h 8 min	19 h 53 min	17.85 s	19.15 s
$T = 10$	2 h 13 min	65 h 8 min	18.46 s	19.45 s
$T = 50$	4 h 20 min	180 h 33 min	18.76 s	20.06 s

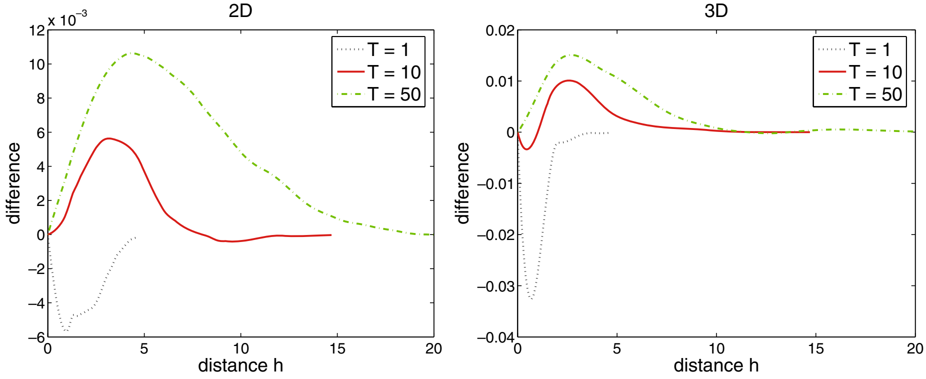


Fig. 6 Differences in approximations of $A_r(h,t)/A_r(0,t)$ by the finite element method (see Section 4.1) and the Monte Carlo simulation (see Section 4.3) in 2D (*left*) resp. 3D (*right*) for $r = 1$ and total times $T = 1$, $T = 10$ and $T = 50$

dimensions. Since adaptive time-stepping was used for the fem, the run time increases only slightly with increasing T. The run time of the Monte Carlo method for $T = 1$ corresponds roughly to 230 evaluations by the fem for different h. Due to rotational symmetry and the reduction of dimension, the run times for 2D and 3D using the fem are almost the same. In contrast, the Monte Carlo simulations in 3D are much more time consuming. The run time depends on several factors such as efficiency of implementation, programming language, computer, to mention a few but not all; we believe, however, that the trend in Table 1 shows the overall efficiency of the fem.

In Fig. 6 we depict the difference between the approximation of $A_r(h,t)/A_r(0,t)$ by the finite element method and the Monte Carlo simulations in 2D and 3D. Asymptotically both methods seem to converge to the same limit, namely 2. Preasymptotically the maximal difference for $T = 10$ is less than 0.006 in 2D and less than 0.01 in 3D. Additional numerical experiments, where we decreased the mesh-size for the fem, did not give smaller deviations which suggests that the fem is more accurate than the Monte Carlo simulation.

To summarize, the comparison of the numerical performance of the finite elements method (fem) and the Monte Carlo simulation shows clear advantages of the fem. Hence, fem can be recommended for the computation of the covariance function of the Boolean model of Wiener sausages.

5 Open Problems

Beside the covariance function and the contact distribution function, there are many other quantities in stochastic geometry describing the geometrical properties of the Boolean model. As an example, *specific intrinsic volumes* (cf. e.g. Schneider and Weil 2000) can be mentioned including the volume fraction, the specific surface area and the specific Euler–Poincaré characteristic. They describe mean curvature properties of Ξ. Formulae for the volume fraction and the specific surface area are given in this paper. It is an open problem to find other $d-1$ specific intrinsic volumes of the Boolean model of Wiener sausages. The core of the problem lies in computing the mean curvature measures of the Wiener sausage explicitly. The first attempt to do that is made in the recent paper Last (2006), where the computation of mean curvature measures is reduced to two *mean curvature functions* of Wiener paths. Unfortunately, the explicit form of these functions is still unknown.

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