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ARTICLE

Monte Carlo Simulation of Fully Markovian Stochastic Geometries

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The interest in resolving the equation of transport in stochastic media has continued to increase these last years. For binary stochastic media it is often assumed that the geometry is Markovian, which is never the case in usual environments. In the present paper, based on rigorous mathematical theorems, we construct fully two-dimensional Markovian stochastic geometries and we study their main properties. In particular, we determine a percolation threshold p_c equal to 0.586±0.002 for such geometries. Finally, Monte Carlo simulations are performed through these geometries and the results compared to homogeneous geometries.

KEYWORDS: Monte Carlo, stochastic media, chord length sampling, Markovian property, percolation, transport through stochastic media

I. Introduction

In the literature, binary stochastic mixtures are particularly studied because of their numerous applications concerning the diffusion of radioactive contaminants in geologic media, the transport in turbulent media for the inertial confinement fusion, or high-temperature gas-cooled reactors. However, for such reactors, as the pebble bed reactor, the double heterogeneity of the fuel particles randomly placed in the core makes a full Monte Carlo simulation impossible. To overcome these geometrical difficulties, several authors[1-3] propose an alternative method that consists of simulating the trajectory of the neutrons by sampling the distributions of chords in different materials. Simple models of stochastic media[4] assume that the chord length distribution inside each material is exponential (i.e. they have Marvokian properties). However, for geometries of importance such as those consisting of randomly placed disks in two dimensions or spheres in three dimensions, this property is not strictly valid outside the disks (or spheres) and never inside, as it was recently shown.[5] Thus, in order to validate chord length sampling methods, it is important to construct a real two-dimensional Markovian geometry (and later a three dimensional one) as it has been done earlier in one dimension[6] for which we have theoretical as well as numerical results (benchmarks).

This paper is the first step of a vast program devoted to the study of Markovian stochastic geometries for transport problems. It focuses on the two-dimensional case for which a rigorous construction exists. Thanks to numerical simulations, the main statistical properties of fully Markovian stochastic geometries will be presented. During this process we also determine with accuracy the percolation threshold for these geometries for the first time. Finally, Monte Carlo simulations of the transport of neutrons through binary stochastic media made of water and air are presented.

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II. Uncolored Geometries

1. Construction

The stochastic geometry is realized according to a procedure described by Switzer in 1964, which is until now the unique way of building two-dimensional Markovian geometries.[7] For the needs of transport physics, the stochastic geometries that we study are generated in a square of side L, itself inscribed in a circle of radius $R = L/\sqrt{2}$ as shown in **Fig. 1**.

The number of random lines in polar coordinates (ρ,θ), where ρ is the length of the perpendicular to the line from the origin and θ is the angle this perpendicular makes with

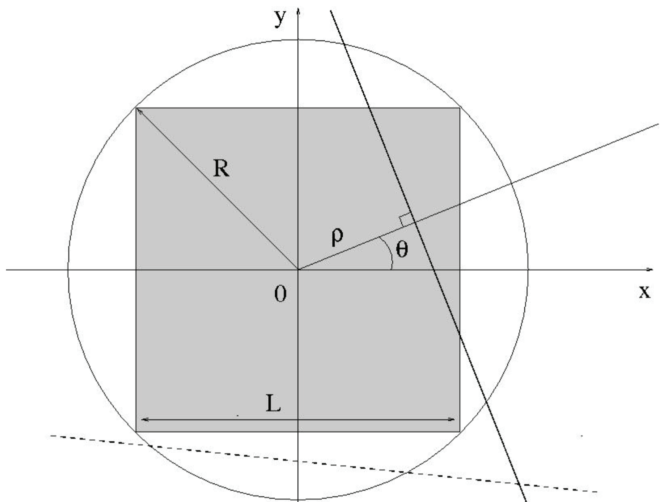

Fig. 1 Geometry construction: the solid line crosses the domain and serves to build the stochastic geometry. The dashed line does not cross the domain and is rejected.

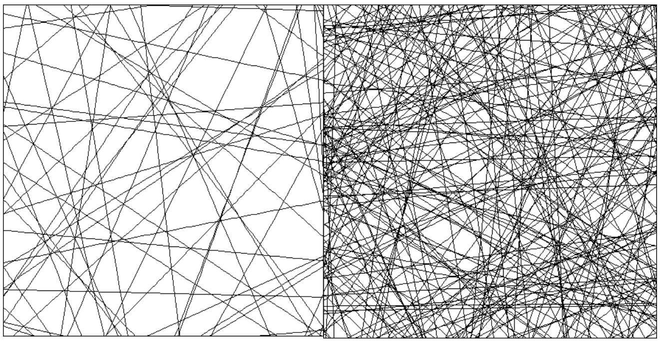

Fig. 2 Examples of uncolored geometries built respectively with L=50 and λ=1 (left); λ=1 and L=200 (right), corresponding to ~60 lines and ~250 lines.

the x axis, is sampled according to a Poisson process.[8] More precisely, the probability p_k that the disk of radius R contains exactly k lines is given by a Poisson law:

$$p_k = \frac{(2R\lambda)^k}{k!} e^{-2R\lambda},$$

where λ is a positive constant (homogeneous to the inverse of a length) that characterizes the density of the Poisson process.

The quantity 2λ/π is the mean number of lines that cross an arbitrary unit segment.[8] This assumption is a key point in Switzer's demonstration and should be kept in mind during the construction of the stochastic geometry. Lines so generated divide the square into convex polygonal cells. Examples of realizations for different intensity of lines are presented in **Fig. 2**. We call that kind of geometry, the uncolored one.

2. Statistical Results

For uncolored geometries Switzer has proven that they have the remarkable property of being Markovian. It means that if we throw a test line in this geometry then this line is cut by the lines already present in segments of independent length. The length *l* of such segments follows an exponential density probability law p(*l*) with mean length $<l>=\pi/(2\lambda)$:

$$p(l) = \frac{1}{<l>} e^{-l/<l>} . \quad (1)$$

Other authors have established various properties of uncolored geometries. Indeed, let us consider an arbitrary polygon in the domain and name N its number of sides, S its perimeter and A its area. Probability laws for these random variables are not known so far but in the limit where the size of the domain tends to infinity, one has for the means:[8]

$$< N >= 4 \qquad < \mathrm{S} >= \frac{2\pi}{\lambda} \qquad < \mathrm{A} >= \frac{\pi}{\lambda^2} . \quad (2)$$

The variance-covariance matrix of the vector (N,S,A) is also known:[9]

$$\begin{pmatrix} \frac{\pi^2-8}{2} & \frac{\pi(\pi^2-8)}{2\lambda} & \frac{\pi(\pi^2-8)}{2\lambda^2} \\ \frac{\pi(\pi^2-8)}{2\lambda} & \frac{\pi^2(\pi^2-4)}{2\lambda^2} & \frac{\pi^2(\pi^2-4)}{2\lambda^3} \\ \frac{\pi(\pi^2-8)}{2\lambda^2} & \frac{\pi^2(\pi^2-4)}{2\lambda^3} & \frac{\pi^2(\pi^2-2)}{2\lambda^4} \end{pmatrix}$$

as well as the first two values of the distribution of the number of sides, that is the proportion of triangle p_3 and quadrangle p_4:[10]

$$p_3 = 2 - \frac{\pi^2}{6} \qquad p_4 = -\frac{1}{3} - \frac{7\pi^2}{36} + \pi^2 \log(2) - \frac{7}{2}\zeta(3)$$

where ζ is the Riemann zeta function.

In order to check how the finite size of the domain influences the distributions of N, S and A (polygons located on the border are truncated) we calculate two distributions: one taking into account internal polygons only (thus not the truncated ones) and one taking into account all the polygons. Monte Carlo simulations were performed for a domain of size L=500 and line density equal to 1 (unless otherwise specified, this is the density value used in our calculations) corresponding to a mosaic of approximately 150,000 polygons. 1,250 geometries were built in order to correctly sample the Poisson distribution of the random lines. Final statistics are thus performed for more than 180 million polygons and are presented in **Tables 1** and **2**. Our simulations are in very good agreement with the theoretical results. We also check that for a domain of size L=500, the border effects are very small. The incertitude on <N> is zero when all the polygons are taken into account since, in this case, each realization of the geometry has exactly four times more sides than polygons.

This last statement can be understood as follow: consider a polygon of side n. Since the vertices form a set of null measure, a random line never passes by a vertex. Consequently, the random line divides two sides of the polygon

Table 1 Mean of (N, S, A) and its variance-covariance matrix, obtained for L=500 and λ=1 (uncolored geometry)

	Without borders	With borders	Theory
Nb of edges ($\bar{N}$)	3.99624 (1.9e-04%)	4 (0%)	4
Perimeter ($\bar{S}$)	6.259 (0.12%)	6.27 (0.12%)	6.283
Area ($\bar{A}$)	3.117 (0.25%)	3.129 (0.25%)	3.142
Var(N)	0.9312 (0.021%)	0.9345 (0.021%)	0.9348
Var(S)	28.72 (0.25%)	28.79 (0.25%)	28.97
Var(A)	38.28 (0.51%)	38.51 (0.51%)	38.83
Cov(N,S)	2.920 (0.12%)	2.930 (0.12%)	2.937
Cov(N,A)	2.909 (0.25%)	2.924 (0.25%)	2.937
Cov(A,S)	28.62 (0.38%)	28.74 (0.38%)	28.97

Table 2 Distribution of the number of side N obtained for L=500 and λ=1 (uncolored geometry)

N	Without borders	With borders	Theory
3	0.35638 (0.016%)	0.354948 (0.016%)	0.35507
4	0.38164 (0.023%)	0.381646 (0.022%)	0.38147
5	0.188836 (0.018%)	0.1896 (0.018%)	
6	0.0582633 (0.039%)	0.058732 (0.039%)	
7	0.0125758 (0.086%)	0.0127282 (0.085%)	
8	2.02328e-03 (0.22%)	2.05667e-03 (0.22%)	
9	2.54667e-04 (0.65%)	2.60272e-04 (0.64%)	
10	2.50124e-05 (2%)	2.56742e-05 (2%)	

and by this process increases the number of sides by two. It also separates the polygon in two pieces by a common segment. This segment is a side for each of the two new polygons and the number of sides also increases by two. Thus, when a random line cut a polygon its forms two small polygons and the number of sides increases by four. Since our geometry is an assembly of polygons and since the original "seed" is a square (but it can be any quadrangle), then each realization of the geometry has exactly four times more sides than polygons.

Assured that we have built rigorous Markovian two-dimensional stochastic geometries, we pursue our study by coloring each polygon.

III. Colored Geometries

1. Construction

The isotropic binary mixture where the distribution of chords is Markovian for both materials is based on the uncolored geometry. From now on, each polygon randomly receives a color (here, red and blue). The probability of painting a polygon in red is p and 1-p is thus the probably painting a polygon in blue (while there is no restriction, we limit our study to two colors). This process allows us to obtain, by merging of adjoining polygons of the same color, a new stochastic geometry composed of red and blue polygons. This time, polygons are not always convex and can even have holes as it is shown in **Fig. 3**. In the next section, such geometries will serve to model random stochastic media (red and blue polygons becoming media of different nature).

2. Statistical Properties

Like the uncolored geometry, the colored one is Markovian. Segments of a test line crossing alternatively the red and blue polygons have independent lengths. These lengths are distributed according to exponential laws, with means $\langle l_R \rangle = \langle l \rangle/(1-p) = \pi/(2\lambda(1-p))$ inside the red polygons and $\langle l_B \rangle = \langle l \rangle/p = \pi/(2\lambda p)$ inside the blue ones. To the best of our knowledge, this is the unique theoretical result for these stochastic geometries. We check with accuracy this behavior and evaluate the statistical properties (number of sides N, perimeter S and area A) of the red polygons. We also calculate N_p, the number of "small" (uncolored) polygons which compose a "big" red polygon.

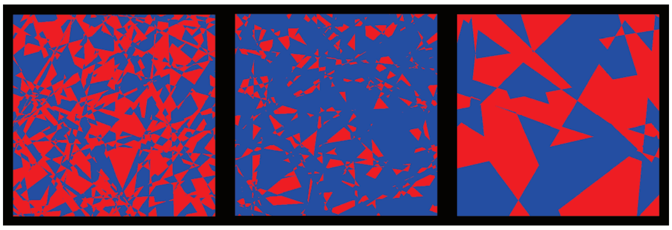

Fig. 3 Examples of colored geometries for a domain of size L=100. λ=1 and p=0.5 (left); λ=1 and p=0.2 (center); λ=0.2 and p=0.5 (right).

Table 3 Mean of (N_p, N, S, A) and its variance-covariance matrix, obtained for L=500, λ=1 and p=0.5 (colored geometry)

	Without borders	With borders	With mirrors
Nb of polygons ($\bar{N}_P$)	2.315 (0.028%)	2.326 (0.028%)	2.39402 (8.9e-04%)
Nb of edges ($\bar{N}$)	5.139 (0.018%)	5.155 (0.017%)	5.24735 (4.8e-04%)
Perimeter ($\bar{S}$)	10.19 (0.13%)	10.25 (0.13%)	10.4422 (8.9e-04%)
Area ($\bar{A}$)	7.242 (0.26%)	7.309 (0.26%)	7.5572 (1.5e-03%)
Var(N_P)	6.987 (0.13%)	7.047 (0.13%)	7.97904 (1.1e-03%)
Var(N)	12.81 (0.14%)	12.92 (0.13%)	14.5651 (8.4e-04%)
Var(S)	128.0 (0.28%)	129.1 (0.28%)	141.103 (3.7e-04%)
Var(A)	242.1 (0.55%)	245.4 (0.55%)	276.789 (3.6e-04%)

Besides both manners already mentioned to treat the finiteness of the domain (taking into account or not polygons at the border) we add a third (empirical) one. This time, the border acts like a mirror, doubling the size of a polygon when it touches the border. This manner to proceed compensates the truncation of the polygons located at the border, assuming that such a polygon extends beyond the border of a typical size given by its own size. Results of our Monte Carlo simulations for the colored geometries, realized in the same condition as the uncolored one (1,250 samples), are presented in **Table 3**.

When p approaches a critical value p_c (the percolation threshold as we will see in the next section) some red polygons extend through the whole domain. The size of such polygons and the way to handle border effects play then a crucial role as shown in **Fig. 4**.

Thus, given that the mean size of the red polygons must diverge when p tends to p_c, the mirror method describes better the geometry in the neighborhood of p_c (as expected, the method that ignores the polygons at the border has the wrong behavior).

3. Excursion in Percolation

(1) Infinite Domains

If the domain spans across the whole plane, then for the probability p of coloring a red polygon, there exists a critical value p_c, named percolation threshold, such that:[11)]

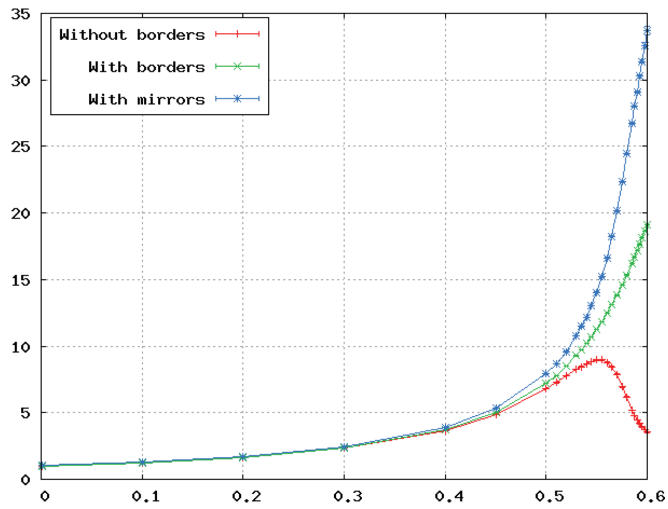

Fig. 4 Mean number of uncolored polygons $<N_p>$ versus the probability p for the three treatments of the border effects

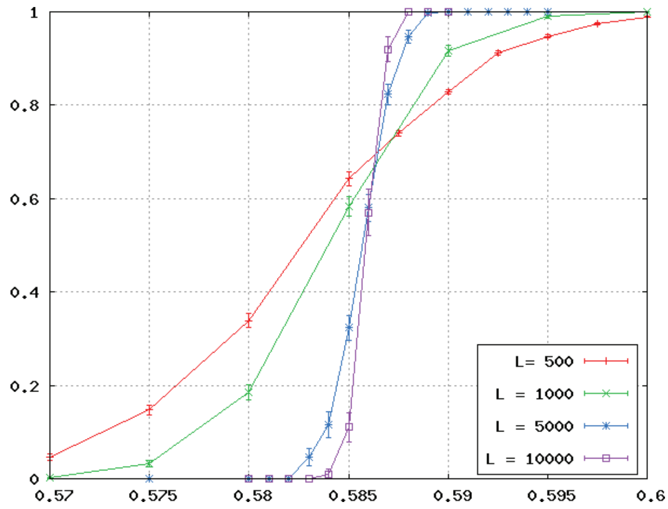

Fig. 5 Probability that the system percolates versus p, for different sizes of the domain

- if $p< p_c$, almost surely no red polygon has an infinite size;
- if $p>p_c$, there exists almost surely a unique red polygon having an infinite size.

Furthermore by noting θ(p) the probability that the polygon containing the origin of the frame is red and has an infinite size, then:

- if $p< p_c$, $\theta(p)=0$,
- if $p> p_c$, $\theta(p)>0$.

Besides, in the case of a triangular network (where $p_c =1/2$) the behavior of θ(p) when p approaches p_c (for $p> p_c$) is known and goes as a power-law in $(p - p_c)^{5/36}$ (the constant 5/36 is a critical exponent usually noted β in the literature.[11]) This critical exponent is suspected to be universal and thus independent of geometrical details.

Note that, since our simulations deal with finite domains, they only allow us to determine an interval where p_c lies.

(2) Evaluation of p_c

We consider that the system percolates if a red polygon hit two opposite edges of the domain. Indeed, under the mirror hypothesis of Section III. 2 this polygon extends to infinity.

We test this condition on several geometries in order to determine the percolation threshold. **Figure 5** shows that this probability goes from 0 to 1 on an interval that becomes smaller as the size of the domain increases. Due to high cost of computer time for huge geometries, our statistics decrease when the size of the domains grows. For L=500 we average over 1,000 geometries, for L=1,000 over 600 geometries, for L=5,000 over 300 geometries and for L=10,000 over 100 geometries. From **Fig. 5** it is reasonable to take the value of p_c at the middle of the interval p_c=0.586, the corresponding error being of 0.25%. Therefore we obtained the following result: for two-dimensional Markovian geometries the percolation threshold is: p_c=0.586±0.002.

(3) Evaluation of the Critical Exponent

To estimate θ(p) one has to verify that the percolating polygon also contains the origin of the frame. **Figure 6** shows the behavior of θ(p) for two different sizes of the domain.

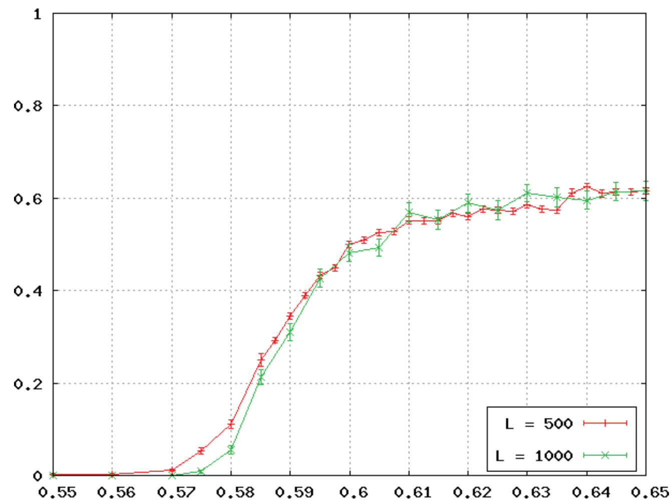

Fig. 6 Probability θ(p) that the red polygon containing the origin has an "infinite" size versus p

Fits were performed for the geometry of size L=500 where we have more points at our disposal. Two ranges of values of p were tested for the fits. The first one between p_c and 0.65, and the second one between 0.6 and 0.65. The second range contains only the values of p for which the probability of percolation is 1. Indeed, this last choice is motivated by the fact that for p < 0.6 border effects, clearly visible in **Fig. 6**, may confuse the fit. The greatest value of p is 0.65 for both cases, a compromise between the need of having points for the fit and the fact that θ(p) is defined only in the neighborhood of p_c. Results are presented in **Table 4** and indicate that under the second hypothesis, the values of the critical exponent are compatible with that of a universal critical exponent equals to 5/36≈0.139.

Table 4 Fits of the numerical values of θ(p) by the function $c(p-p_c)^a$

	Exponent a	Factor c	χ^2
Reduced sample (0.6 - 0.65)			21 points
$p_c = 0.585$	0.150 +/- 5.8%	0.94 +/- 2.8%	13.9
$p_c = 0.586$	0.145 +/- 5.8%	0.93 +/- 2.8%	13.8
$p_c = 0.587$	0.140 +/- 5.8%	0.92 +/- 2.7%	13.8
Total sample (p_c - 0.65)			26 points
$p_c = 0.585$	0.211 +/- 5.3%	1.14 +/- 3.9%	87.9
$p_c = 0.586$	0.196 +/- 4.6%	1.09 +/- 3.2%	65.7
$p_c = 0.587$	0.173 +/- 4.1%	1.02 +/- 2.5%	49.5

IV. Monte Carlo Transport Simulations

Transport of neutrons in Markovian geometries is carried out thanks to the Monte Carlo transport code TRIPOLI-4®[a] developed and validated at Commissariat à l'Energie Atomique (CEA).[12] Since the code accepts only three dimensional geometries, we extend the previous 2D Markovian geometries in the vertical direction. Each random line now corresponds to a random vertical plane. The geometry so constructed is bounded in the z direction by two horizontal planes. The geometry remains Markovian since any straight lines that hit two consecutive planes has still an exponential distribution (which now depends on the angle between the direction of the line and the horizontal plane.) However, this geometry is not isotropic any more, since there is long channel in the vertical direction. This way of proceeding was used by Zuchuat and al[6] to pass from the 1D statistics to the 3D computational geometry, comparisons between planar geometry and benchmarks were then possible.

The size of the horizontal domain is 15×15 cms with a density of lines equal to 1 in order to insure a sufficient number of cells (there are as many cells as polygons) in the box. The binary stochastic medium is composed of air (with a filling fraction set to p) and water with boron (filling fraction 1-p), such a composition being used to model boiling water reactor. The problem investigated in this section is the longitudinal transmission and reflection through the stochastic medium. We also investigate whether the stochastic medium can be correctly modeled by an effective uniform medium made of air and water in the proportion p and 1-p. A punctual source of neutrons with incidence direction parallel to the x axis is placed at the center of the left boundary face. Reflecting boundary conditions were applied on all the transverse faces. Simulations were performed with three different filling fractions, p=0.25, p=0.5 and p=0.75 and statistics collected from a thousand geometries in each case. Results are presented in **Table 5** and show a statistically significant difference (of about 12% when p=0.25, and of 7% when p=0.5) between stochastic geometries and homogeneous ones.

[a] TRIPOLI-4® is a registered trademark of CEA.

Table 5 Transmission (T) and reflection (R) for three different compositions

p	Stochastic		Homogeneous	
	T	R	T	R
0.25	0.272 (1.2%)	0.386 (0.4%)	0.238 (0.2%)	0.394 (0.1%)
0.5	0.463 (1.0%)	0.358 (0.7%)	0.432 (0.1%)	0.377 (0.1%)
0.75	0.669 (0.7%)	0.277 (1.3%)	0.6899 (0.067%)	0.283 (0.2%)

V. Conclusion

In the first part of this paper we have presented some results concerning the statistical properties of a binary Markovian mixture in the plane, constructed according to the process envisioned by Switzer. In particular, the mean number of cells and of sides, as well as the mean perimeter and area of the colored polygons have been numerically evaluated. Subsequently, the percolation property of the tiling has been investigated and a value of percolation threshold of 0.586±0.002 found. The simulation value of the critical exponent is compatible with the theoretical value of 5/36. Finally, we showed the feasibility of a neutron transport simulation on such a binary Markovian mixture by the Monte Carlo method, and showed that taking into account the randomness nature of the problem can make a difference in the evaluation of transport properties, such as transmission and reflection in a slab composed of a mixture of water and air. Future works will concern the comparisons between transport trough Markovian geometries and non-Markovian 2D media (made of randomly placed disks as in Donovan and Danon[1] for instance) and the construction of real Markovian three dimensional geometries based on random planes.

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