Lecture Notes in Mathematics

Edited by A. Dold and B. Eckmann

Subseries: Institute for Mathematics and its Applications, Minneapolis
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The Mathematics and Physics of Disordered Media

Proceedings, Minneapolis 1983

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The Mathematics and Physics of Disordered Media:

Percolation, Random Walk, Modeling, and Simulation

Proceedings of a Workshop held at the IMA
University of Minnesota, Minneapolis
February 13–19, 1983

Edited by B. D. Hughes and B. W. Ninham

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The Mathematics and Physics of Disordered Media

PREFACE

The successes of the new physics in the 17th and 18th centuries were inextricably interwoven with the discovery of the calculus. Following Newton, Leibniz, and Laplace, the scientific rationalists, in a burst of enthusiasm over the omnipotence of deductive reasoning, made mathematics Big Bird of the Sciences. The orderliness of that God who made this best of all possible deterministic worlds stood revealed. In the words of Descartes, *Cum Deus calculat, fit mundus*!

Then came Gauss and Riemann with non-Euclidean geometries, Cantor with infinite sets and a host of logicians with the axiomatization of mathematics. All of these developments challenged preconceived notions, and many researchers went deeper and deeper into the foundations of mathematics, trying to find The Perch for Big Bird. These hopes, along with the dreams of the rationalists, ended suddenly when Godel showed that any sufficiently rich system of axioms contains undecidable propositions.*

This loss of faith, like the dread acciditas, that dry soul-withering wind which afflicted the good monks of Egypt so many centuries ago, resulted in a crisis of confidence. Coincident with this internal attack on the foundations, one also finds many applied scientists viewing mathematics as irrelevant to the real world. These developments are in no small measure responsible for the present separation between pure mathematics, applied mathematics, and the sciences generally. Unlike their counterparts in nuclear and particle physics, astronomy and space sciences, biology, and computer and earth sciences, who trumpeted their triumphs real or imagined, mathematicians sat mute and musing.

Awareness of the increasing gap between science and mathematics prompted the National Science Foundation to fund the Institute for Mathematics and its Applications (IMA) at Minnesota along with a sister Institute at Berkeley in 1982.

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*These developments have been documented in the challenging and extraordinarily lucid writings of Morris Kline in Mathematics, the Loss of Certainty, Oxford, (1981).

The purpose of the IMA is to facilitate the flow of problems and ideas between scientists and mathematicians.

An exciting glimpse of one bold new shape for the mathematics of the 1980's emerged from a workshop held at the IMA in February 1983. The workshop was devoted to the Mathematics and Physics of Disordered Media. Our attempt to define a charter read as follows:

> One of the fundamental questions of the 1980's facing both mathematicians and scientists is the mathematical characterisation of disorder. Until recently it had been impossible to conceptualize or even to contemplate the possibility that a tractable calculus might emerge. A classic example is that of liquids. This state of matter is intermediate between gases, where characteristic distribution functions are uniform to lowest order, and crystals, where the unperturbed distribution functions are periodic. There is no rigorous mathematical description appropriate to the intermediate irreducibly disordered state. Beyond the simple statement of Lindemann's law there is no theory of melting. The situation is analogous in the field of irregular porous media, ubiquitous in areas as diverse as earth sciences and the food industry.
>
> The last decade has seen the beginnings of a unity of methods and approaches in statistical mechanics, transport in amorphous and disordered materials, properties of heterogeneous polymers and composite materials, turbulent flows, phase nucleation, and interfacial science. All have an underlying structure characterized in some sense by chaos, self-avoiding random walk, percolation and fractals.
>
> Some real progress has been made in understanding random walks and percolation processes on the one hand, and through mean field or effective medium approximations and simulation of liquids and porous media on the other. The subject is directly connected with the statistics of extreme events and important pragmatic areas like fracture of solids, comminution of particulate materials, and flow through porous media.

The key words are fractals, percolation, random walks, and chaos. The realization, so eloquently expounded by Mandelbrot, that the Hausdorff dimension of the length of a real (linear) coast line is not one, is an astonishing one. Things are not what they seem. They depend on how one looks at them. This should not be kept secret, and unquestionably progress in the topics of this Volume will throw new light on renormalization groups, particle physics, and phase transitions.

The meeting drew together mathematicians, pure and applied, chemists, chemical engineers, physicists, computer scientists, materials and polymer scientists and statisticians from industry and academia. An honored guest was John M. Hammersley, an Oxford Mathematician who invented the subject of percolation theory thirty years ago. Unlike most mathematical terms, percolation needs no explanation. It means exactly what it means in good old-fashioned English. Another pioneer, Elliott Montroll, was unable to attend because of illness, but nonetheless has co-authored two of our papers.

This very diverse group of scientists found themselves speaking the same language. Progress does seem to be in the air on the difficult problem of developing a calculus to describe chaotic and random systems. Most things in nature are chaotic and random. Mathematical constructs such as Cantor sets, and continuous non-differentiable functions, hitherto considered to be highly abstract and far from the real world, loom large in these recent developments, but in a nice comprehensible way. Perhaps after all and in the longer view, mathematicians <u>are</u> on the right track. Have a good read.

Barry Hughes George Sell
Barry Ninham Hans Weinberger

June 1983

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THE MATHEMATICS AND PHYSICS OF DISORDERED MEDIA

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RANDOM PROCESSES AND RANDOM SYSTEMS:

AN INTRODUCTION

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ABSTRACT

We introduce and review a number of topics drawn from the theories of random processes and random systems. In particular we address the following subjects: random walks in continuous spaces and on lattices; continuum limits of random walks and stable distributions; master equations, generalized master equations and continuous-time random walks; self-avoiding walks on lattices; percolation theory; steady-state and transient transport in random lattices; and diffusion and conduction in heterogeneous continua.

Table of Contents

Introduction

The present article has been written with several purposes in mind. The first is that it should serve as a self-contained introduction, suitable for a wide audience, to some of the topics discussed from a more specialized point of view in other articles in this volume. The second is that it should be useful as a review, and a guide to the primary literature. However, the main thrust of the article is the development of two distinct themes, random processes and random systems, which are gaining increasing importance in the physical sciences. In Part A of the article, we emphasize models in which random processes and random systems have discrete structure. Part B is devoted to transport problems in disordered continua.

Overview of Part A

The notion of a random process, as we see it, grows from an attempt to describe microscopically complex processes by statistical equations of evolution. A prototypical example is the erratic Brownian motion of dust particles or pollen grains in solution due to collisions with solvent molecules. Although above the quantum mechanical level, the process is entirely deterministic, the motion of each grain is sufficiently erratic that it may be taken as random (with the simplest model being that of a "random walk", as discussed in sections 1 to 4). The random processes which have been most extensively and successfully studied are those which possess no memory effect, or very simple memory effects. Much harder and less well understood are problems with strong memory effects, exemplified by the problem of a self-avoiding walk (section 5).

By modelling a physical phenomenon as a random process, we usually are adopting the view of a natural phenomenon as a drama played out on a fairly simple and uniform stage, but with a random script. The direct antithesis of this view is what we call the random system, in which the script is written out and orderly, but the stage setting is chaotic. The simplest physical example of a random system is an irregular porous medium. If fluid flows steadily through the voids in the medium, the streamlines are fixed in space, but tortuous due to the spatial variation in local geometry and topology. Percolation theory (section 6) gives a precisely formulated mathematical model, in the context of which random geometry and topology can be investigated quantitatively. It can be generalized to predict the hydraulic or electrical resistance, or other steady-state transport properties of a random system, as outlined for lattice systems in section 7; transport in random continua is deferred to Part B. Many fundamental outstanding questions in this area remain to be resolved.

While the notions of random process and random system, as we have outlined them, are apparent opposites, it is now known that for successful modelling of important physical phenomena the two concepts must be fused together. For example, in the dispersion (speading) of a blob of dye convected through a porous medium, the effects of tortuousness of the streamlines (random system) compete with diffusion between streamlines (random process). We discuss simple models for random processes in random systems in section 8.

The topics discussed in Part A represent a somewhat arbitrary selection from an enormous body of work contained in the mathematical, physical, chemical, and engineering literatures. We have avoided wherever possible the discussion of problems which require a knowledge of the deeper concepts and technicalities of contemporary probability theory. Extensive references are given, with a distinct bias towards the applied literature and no attempt to place the topics discussed in the broader contexts of Markov processes and their derivatives, Markov random fields, and so on. Even within the applied literature, we make no claim to bibliographic completeness. A recent random walk bibliography [L.H. Liyange, C.M. Gulati and J.M. Hill, "A bibliography of applications of random walks in theoretical chemistry and physics", Advances in Molecular Relaxation and Interaction Processes 22 (1982), 53-72] lists almost 300 references, and yet represents but the tip of the iceberg. It is hoped that the references supplied here will prove sufficient to guide the reader into those parts of the literature which arouse his or her interest.

We draw to the reader's attention the existence of published proceedings of a number of recent conferences on random processes and random systems*. A clear introduction to some of the concepts and applications of random walk theory has been given by G.H. Weiss ["Random walks and their applications", Amer. Scientist 71 (1983) 65-71], and a delightful account of the historical antecedents of random walk theory, entitled "A wonderful world of random walks", has been compiled by E.W. Montroll and M.F. Shlesinger, and appears in a volume dedicated to M. Lax, edited by H. Falk and published by the Physics Department of City College of the City University of New York. A compendium of papers edited by N. Wax, Selected Paper in Noise and Stochastic Processes (New York, Dover, 1954) remains valuable, but gives no idea of the wealth of developments which were shortly to follow. Some aspects of the theory of homogeneously disordered systems, from the perspective of solid state physics, form the subject of a major book by J.M. Ziman entitled Models of Disorder (Cambridge University Press, 1979). Three important collections of papers on modern theoretical and numerical approaches to thermodynamic critical phenomena contain survey articles which are relevant to the problems of self-avoiding walk, percolation, and conduction in random systems: Numerical Methods in the Study of Critical Phenomena, ed., J. Della Dora, J. Demongeot and B. Lacolle (Berlin, Springer-Verlag, 1981); Monte Carlo Methods in Statistical Physics, ed. K. Binder (Berlin, Springer-Verlag, 1979); and Real-Space Renormalization, ed. T.W. Burkhardt and J.M.J. van Leeuwen (Berlin, Springer-Verlag, 1982).

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* (a) The proceedings of the Symposium on Random Walks and Their Application to the Physical and Biological Sciences (National Bureau of Standards, Gaithersburg, Maryland, 1982), published as a special issue of the Journal of Statistical Physics (Volume 30, No. 2, 1983); some additional papers presented at the symposium will be appearing in an American Institute of Physics Conference Proceedings Volume edited by M.F. Shlesinger and B.J. West.

(b) "Percolation Processes and Structures", Annals of the Israel Physical Society, Vol. 5, ed. G. Deutscher, R. Zallen and J. Adler, (Bristol, Adam Hilger, 1983); this volume contains articles by several contributors to the present volume (Hammersley, Halley and Redner) and many others.

(c) Electrical Transport and Optical Properties of Inhomogeneous Media, ed. J.C. Garland and D.B. Tanner, AIP Conference Proceedings, Vol. 40 (New York, American Institute of Physics, 1978).

(d) Disordered Systems and Localization, ed. C. Castellani, C. Di Castro and L. Peliti, Lecture Notes in Physics Vol. 149 (Berlin, Springer-Verlag, 1982).

(e) Macroscopic Properties of Disordered Media, ed. R. Burridge, S. Childress and G. Papanicolaou, Lecture Notes in Physics, Vol. 154 (Berlin, Springer-Verlag, 1982).

(f) Ill-condensed Matter, ed. R. Balian, R. Maynard and G. Toulouse (Amsterdam, North-Holland, 1979).

Overview of Part B

In Part B we turn to problems of transport and conduction in random continua. Our discussion is phrased in terms of the diffusion problem, though a number of other problems, including thermal and electrical conduction, electric permittivity and magnetic permeability are mathematically equivalent to the diffusion problem. In the main we focus on the application of variational methods to obtain rigorous bounds on overall diffusion rates. The presentation relies heavily on the reader's physical intuition and common sense - we take it for granted throughout that the passage to samples of infinite size will not lead to grief, and that the details of the boundary conditions at the sample surfaces do not matter so long as a given overall flux or concentration gradient in the diffusing species is maintained. The literature cited is a sampling rather than a list of the work that has been published; the intent is to convey some feeling for the different ways in which information about the structure of the material may be given, and for the methods by which such knowledge may be converted into calculable bounds.

In section 1 we define the effective diffusion coefficient and state the basic variational inequalities. Section 2 introduces the remarkable bounds discovered by Hashin and Shtrikman, which are known to be the best obtainable for an isotropic two-phase material if only the volume fraction of the phases is given. The use of spatial correlations to obtain better bounds is the subject of Section 3, and Section 4 discusses bounds for systems of particles, especially the overlapping spheres model of Weissberg. Bounds derived from information on other bulk properties of the material are described in section 5. We conclude with a brief discussion of Brownian motion in large groups of interacting particles, and obtain an upper bound on the relative velocity of two solute species subject to uniform external forces.

One topic is absent from Part B: percolation. Even far from any percolation threshold, as portions of the material in question become impermeable to the diffusing species, the lower bound on the effective diffusion coefficient goes to zero; even though the upper bound remains useful, this precludes any rigorous statement about percolation thresholds or how they are approached.

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PART A: DISCRETE MODELS

1. Random Walks and Random Flights

The problem of "random walk" was first posed, but not solved, in a letter written to Nature in 1905 by Karl Pearson [1]:

> "A man starts from a point O and walks ℓ yards in a straight line; he then turns through any angle whatever and walks another ℓ yards in a second straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + \delta r$ from his starting point O.
>
> The problem is one of considerable interest....".

A rather informal asymptotic solution of this problem in the limit of large n had been given twenty-five years earlier by Lord Rayleigh [2] in a paper on the addition of sound waves of equal amplitude but random phase, as Rayleigh pointed out in his own letter to Nature [3], duly acknowledged by Pearson [4]. An integral representation of the solution valid for arbitrary values of n was provided almost immediately by Kluyver [5], and contributions to the necessary mathematics were also made by Markoff [6]. Lord Rayleigh returned to the problem in 1919 [7], expanding on earlier analyses of Pearson's problem, and developing the three-dimensional generalization, which he called "random flight".

To present-day scientists much of the analysis associated with the Pearson and Rayleigh problems, as we present it below, is straightforward, while probabilists would readily identify it as a particularly simple case of the well-studied general problem of addition of independent random variables, and perhaps assign it very little importance. However the random walk or random flight concept has been most fruitful in a wide variety of different fields, as may be gauged from major reviews of the field [8,9,10], and the terminology transcends linguistic barriers - Problem des Irrwanderns [11] to the Teutonic, marche aléatoire to the Francophiles. (For the lattice analogue of the Rayleigh-Pearson problem, Pólya, used herumwandernde Punkte and Irrfahrt [12], and promenade au hasard [13].)

Let $P_n(\vec{x})$ denote the probability density function for the position $\vec{x}$ of a random walker (or aviator) in the E-dimensional continuum after n steps (displacements) have been made. The steps are taken to be independent random variables and we write $p_n(\vec{x})$ for the probability density function for the nth step. Then the evolution of the random walk is governed by the equation

$$P_{n+1}(\vec{x}) = \int p_{n+1}(\vec{x} - \vec{x}')\, P_n(\vec{x}')\, d^E\vec{x}'. \tag{1.1}$$

The implicit assumption of translational invariance, embodied in the simple convolution in Eq. (1.1), ensures that the formal solution of the problem is easily constructed using Fourier transforms (characteristic functions [14] to probabilists). Let

$$\tilde{P}_n(\vec{q}) = \int e^{i\vec{q}\cdot\vec{x}}\, P_n(\vec{x})\, d^E\vec{x} \tag{1.2}$$

and

$$\tilde{p}_n(\vec{q}) = \int e^{i\vec{q}\cdot\vec{x}}\, p_n(\vec{x})\, d^E\vec{x}\ . \tag{1.3}$$

Taking the Fourier transform of Eq. (1.1) and using the convolution theorem for the Fourier transform, we deduce that

$$\tilde{P}_{n+1}(q) = \tilde{p}_{n+1}(\vec{q})\, \tilde{P}_n(\vec{q})\ , \tag{1.4}$$

whence

$$P_n(\vec{x}) = \frac{1}{(2\pi)^E} \int e^{-i\vec{q}\cdot\vec{x}}\, \tilde{P}_n(\vec{q})\, d^E\vec{q} \tag{1.5}$$

$$= \frac{1}{(2\pi)^E} \int e^{-i\vec{q}\cdot\vec{x}}\, \tilde{P}_o(\vec{q}) \prod_{j=1}^{n} \tilde{p}_j(\vec{q})\, d^E\vec{q}\ . \tag{1.6}$$

For the problems of Pearson and Rayleigh, the directions of allowed steps are isotropically distributed, and all steps have the same length ℓ , so that

$$p_j(\vec{x}) = \ell^{-E+1} A_E^{-1} \delta(|\vec{x}| - \ell) \tag{1.7}$$

where A_E is the surface area of the hypersphere of unit radius in E dimensions. The radial symmetry enables all of the Fourier transforms to be reduced to single integrals involving Bessel functions if E is even, and trigonometric functions if E is odd and greater than unity (see, e.g., Watson [15] or Bochner and Chandrasekharan [16]). One finds that

$$P_n(\vec{x}) = \frac{1}{2\pi} \int_0^\infty J_0(\rho|\vec{x}|) \{J_0(\rho\ell)\}^n \rho d\rho \tag{1.8}$$

in two dimensions, while in three dimensions

$$P_n(\vec{x}) = \frac{1}{2\pi^2|\vec{x}|} \int_0^\infty \sin(\rho|\vec{x}|) \{ \frac{\sin(\rho\ell)}{\rho\ell} \}^n \rho d\rho \, . \tag{1.9}$$

For large values of n , $P_n(\vec{x})$ converges to a Gaussian or normal distribution, reflecting the central limit theorem of probability theory:

$$P_n(\vec{x}) \sim \{ \frac{En}{2\pi\ell^2} \}^{E/2} \exp(- \frac{En|\vec{x}|^2}{2\ell^2}) \; ; \tag{1.10}$$

an analysis of higher order terms is possible. The explicit evaluation of $P_n(\vec{x})$ for modest values of n is a somewhat harder problem. In <u>three dimensions</u>, Rayleigh [7] gave explicit solutions for $n \leq 4$, Chandrasekhar [17] for $n \leq 6$ and Vincenz and Bruckshaw [18] for $n \leq 8$. The folklore arose, and perhaps persists in some quarters, that the general problem of finding closed-form representations of $P_n(\vec{x})$ in three dimensions for arbitrary $n \geq 2$ is unsolved. However, Treloar [19] was able to derive a general solution almost forty years ago, using methods drawn from sampling theory. (A particularly elegant discussion of the problem along these lines can be found in Feller [20], pp. 32-33.) A direct derivation of Treloar's result from Eq. (1.9) has been given by Dvořák [21]. In the region $|\vec{x}| < n\ell$ where $P_n(\vec{x}) > 0$, it may be written in a variety of equivalent forms, with perhaps the simplest being [21]

$$P_n(\vec{x}) = \frac{1}{4\pi\ell^2|\vec{x}|2^n(n-2)!}\sum_{\nu=0}^{n}(-1)^\nu\binom{n}{\nu}\left[n - 2\nu - \frac{|\vec{x}|}{\ell}\right]^{n-2}\operatorname{sgn}\left[n - 2\nu - \frac{|\vec{x}|}{\ell}\right] .$$

(For computational purposes, a recurrence relation satisfied by $P_n(\vec{x})$ is more efficient when $n > 10$ [21].) The determination of a closed form expression for $P_n(\vec{x})$ in two dimensions is much harder (for reasons discussed in [20], p. 33) and an expression for arbitrary n is apparently not available at present.

Many generalizations and extensions of the preceding analyses have been given, and we list but a few here. Barakat has considered the case when the lengths of the steps are randomly distributed [22], and the case when the number of steps taken is a random variable [23]; Nossal and Weiss [24] have examined the case when the distribution of step directions in Pearson's walk is anisotropic; Montroll and West [9] and Hughes, Montroll and Shlesinger [25] have considered generalizations of Pearsons's and Rayleigh's problems in which the lengths of the individual steps are random variables with infinite variances.

2. Random Walks on Lattices

A considerable conceptual simplification in random walk problems is achieved if the walk is confined to a lattice, or discrete space. The simplest example of a discrete space is the E-dimensional hypercubic lattice, which consists of sites having coordinates $\vec{\ell} = (\ell_1,\ell_2,\ldots,\ell_E)$ [ℓ_j integral] with each site connected to its nearest-neighbour sites by a bond. The idea of confining a random walk to a hypercubic lattice occurred to Pólya in 1921 [12], and he asked the following specific question: Is a walker who steps at random between nearest-neighbour sites (with all allowed steps equally likely) certain to return to his starting site? He was able to answer this question: YES if $E = 1$ or $E = 2$, NO if $E \geq 3$, i.e. in sufficiently low dimensions the walk is recurrent or persistent, while in three or more dimensions eventual escape is certain and the walk can be called transient. Pólya's question is but one of a number of questions which are easy to pose and answer for lattice walks, but difficult to discuss for walks in continuous spaces without measure-theoretic analysis. A thorough treatment of many aspects of the theory of random walks on lattices, directed to a mathematical audience, is contained in a book by Spitzer [26]. More applications-oriented discussions may be found in the book by Barber and Ninham [8] and a recent review by Weiss and Rubin [10]. A number of particularly elegant and influential contributions to the field have been made by Montroll and co-workers (e.g. [9] and [27-30]).

Let $P_n(\vec{\ell})$ denote the probability that the walker is at site $\vec{\ell}$ after n steps, and assume without loss of generality that the walker starts at the origin of coordinates, i.e. $P_0(\vec{\ell}) = \delta_{\vec{\ell}\vec{0}}$. Also let $p(\vec{\ell})$ be the probability that any step consists of a vector displacement $\vec{\ell}$. Then

$$P_{n+1}(\vec{\ell}) = \sum_{\vec{\ell}'} p(\vec{\ell} - \vec{\ell}')\, P_n(\vec{\ell}') \,. \qquad (2.1)$$

Introducing discrete Fourier transforms

$$\tilde{P}_n(\vec{\theta}) = \sum_{\vec{\ell}} e^{i\vec{\ell}\cdot\vec{\theta}}\, P_n(\vec{\ell}) \,, \qquad (2.2)$$

$$\lambda(\vec{\theta}) = \sum_{\vec{\ell}} e^{i\vec{\ell}\cdot\vec{\theta}}\, p(\vec{\ell}) \,, \qquad (2.3)$$

we find that

$$\tilde{P}_{n+1}(\vec{\theta}) = \lambda(\vec{\theta})\tilde{P}_n(\vec{\theta}) \quad \text{i.e.,} \quad \tilde{P}_n(\vec{\theta}) = \lambda(\vec{\theta})^n \,, \qquad (2.4)$$

and so

$$P_n(\vec{\ell}) = \frac{1}{(2\pi)^E} \int_B e^{-i\vec{\ell}\cdot\vec{\theta}}\, \tilde{P}_n(\vec{\theta})\, d^E\vec{\theta} \qquad (2.5)$$

$$= \frac{1}{(2\pi)^E} \int_B e^{-i\vec{\ell}\cdot\vec{\theta}}\, \lambda(\vec{\theta})^n\, d^E\vec{\theta} \,. \qquad (2.6)$$

The integral is taken over the first Brillouin zone $B = [-\pi,\pi]^E$. Equation (2.6) gives the formal solution of the random walk problem.

The function $\lambda(\vec{\theta})$ is usually called the structure function by physicists, the terminology being borrowed from the theory of lattice dynamics. For a Pólya walker (which we define to be a walker who steps between nearest-neighbour sites, with all allowed steps equally likely) $\lambda(\vec{\theta})$ reflects the connectivity structure