Preface

Modern physics is confronted with a large variety of complex spatial structures; almost every research group in physics is working with spatial data. Pattern formation in chemical reactions, mesoscopic phases of complex fluids such as liquid crystals or microemulsions, fluid structures on planar substrates (well-known as water droplets on a window glass), or the large-scale distribution of galaxies in the universe are only a few prominent examples where spatial structures are relevant for the understanding of physical phenomena. Numerous research areas in physics are concerned with spatial data. For example, in high energy physics tracks in cloud chambers are analyzed, while in gamma ray astronomy observational information is extracted from point patterns of Cherenkov photons hitting a large scale detector field. A development of importance to physics in general is the use of imaging techniques in real space. Methods such as scanning microscopy and computer tomography produce images which enable detailed studies of spatial structures.

Many research groups study non-linear dynamics in order to understand the time evolution of complex patterns. Moreover, computer simulations yield detailed spatial information, for instance, in condensed matter physics on configurations of millions of particles. Spatial structures also derive from fracture and crack distributions in solids studied in solid state physics. Furthermore, many physicists and engineers study transport properties of disordered materials such as porous media.

Because of the enormous amount of information in patterns, it is difficult to describe spatial structures through a finite number of parameters. However, statistical physicists need the compact description of spatial structures to find dynamical equations, to compare experiments with theory, or to classify patterns, for instance. Thus they should be interested in spatial statistics, which provides the tools to develop and estimate statistically such characteristics. Nevertheless, until now, the use of the powerful methods provided by spatial statistics such as mathematical morphology and stereology have been restricted to medicine and biology. But since the volume of spatial information is growing fast also in physics and material science, physicists can only gain by using the techniques developed in spatial statistics.

The traditional approach to obtain structure information in physics is Fourier transformation and calculation of wave-vector dependent structure functions. Surely, as long as scattering techniques were the major experimental set-up in order to study spatial structures on a microscopic level, the two-point correlation function was exactly what one needed in order to compare experiment and theory. Nowadays, since spatial information is ever more accessible through digitized images, the need for similarly powerful techniques in real space is obvious.

In the recent decades spatial statistics has developed practically independently of physics as a new branch in statistics. It is based on stochastic geometry and the traditional field of statistics for stochastic processes. Statistical physics and spatial statistics have many methods and models in common which should facilitate an exchange of ideas and results. One may expect a close cooperation between the two branches of science as each could learn from the other. For instance, correlation functions are used frequently in physics with vague knowledge only of how to estimate them statistically and how to carry out edge corrections. On the other hand, spatial statistics uses Monte Carlo simulations and random fields as models in geology and biology, but without referring to the helpful and deep results already obtained during the long history of these models in statistical physics. Since their research problems are close and often even overlap, a fruitful collaboration between physicists and statisticians should not only be possible but also very valuable. Physicists typically define models, calculate their physical properties and characterize the corresponding spatial structures. But they also have to face the 'inverse problem' of finding an appropriate model for a given spatial structure measured by an experiment. For example, if in a given situation an Ising model is appropriate, then the interaction parameters need to be determined (or, in terms of statistics, 'estimated') from a given spatial configuration. Furthermore, the goodness-of-fit of the Ising model for the given data should be tested. Fortunately, these are standard problems of spatial statistics, for which adequate methods are available.

The gain from an exchange between physics and spatial statistics is two-sided; spatial statistics is not only useful to physicists, it can also learn from physics. The Gibbs models used so extensively today in spatial statistics have their origin in physics; thus a thorough study of the physical literature could lead to a deeper understanding of these models and their further development. Similarly, Monte Carlo simulation methods invented by physicists are now used to a large extent in statistics. There is a lot of experience held by physicists which statisticians should be aware of and exploit; otherwise they will find themselves step by step rediscovering the ideas of physicists.

Unfortunately, contact between physicists and statisticians is not free of conflicts. Language and notation in both fields are rather different. For many statisticians it is frustrating to read a book on physics, and the same is true for statistical books read by physicists. Both sides speak about a strange language and notation in the other discipline. Even more problems arise from different traditions and different ways of thinking in these two scientific areas. A typical example, which is discussed in this volume, is the use of the term 'stationary' and the meaning of 'stationary' models in spatial statistics. This can lead to serious misunderstandings. Furthermore, for statisticians it is often shocking to see how carelessly statistical concepts are used, and physicists cannot understand the ignorance of statisticians on physical facts and well-known results of physical research.

The workshop 'Statistical Physics and Spatial Statistics' took place at the University of Wuppertal between 22 and 24 February 1999 as a purely German event. The aim was simply to take a first step to overcome the above mentioned difficulties. Moreover, it tried to provide a forum for the exchange of fundamental ideas between physicists and spatial statisticians, both working in a wide spectrum of science related to stochastic geometry. This volume comprises the majority of the papers presented orally at the workshop as plenary lectures, plus two further invited papers. Although the contributions presented in this volume are very diverse and methodically different they have one feature in common: all of them present and use geometric concepts in order to study spatial configurations which are random.

To achieve the aim of the workshop, the invited talks not only present recent research results, but also tried to emphasize fundamental aspects which may be interesting for the researcher from the other side. Thus many talks focused on methodological approaches and fundamental results by means of a tutorial review. Basic definitions and notions were explained and discussed to clarify different notations and terms and thus overcome language barriers and understand different ways of thinking.

Part 1 focuses on the statistical characterization of random spatial configurations. Here mostly point patterns serve as examples for spatial structures. General principles of spatial statistics are explained in the first paper of this volume. Also the second paper 'Stationary Models in Stochastic Geometry - Palm Distributions as Distributions of Typical Elements. An Approach Without Limits' by Werner Nagel discusses key notions in the field of stochastic geometry and spatial statistics: stationarity (homogeneity) and Palm distributions. While a given spatial structure cannot be stationary, a stationary *model* is often adequate for the description of real geometric structures. Stationary models are very useful, not least because they allow the application of Campbell's theorem (used as Monte Carlo integration in many physical applications) and other valuable tools. The Palm distribution is introduced in order to remove the ambiguous notion of a 'randomly chosen' or 'typical' object from an infinite system.

In the two following contributions by Martin Kerscher and Karin Jacobs et al. spatial statistics is used to analyze data occurring in two prominent physical systems: the distribution of galaxies in the universe and the distribution of holes in thin liquid films. In both cases a thorough statistical analysis not only reveals quantitative features of the spatial structure enabling comparisons of experiments with theory, but also enables conclusions to be drawn about the physical mechanisms and dynamical laws governing the spatial structure.

In Part 2 geometric measures are introduced and applied to various examples. These measures describe the morphology of random spatial configurations and thus are important for the physical properties of materials like complex fluids and porous media. Ideas from integral geometry such as mixed measures or Minkowski functionals are related to curvature integrals, which characterize connectivity as well as content and shape of spatial patterns. Since many physical phenomena depend crucially on the geometry of spatial structures, integral geometry may provide useful tools to study such systems, in particular, in combination with the Boolean model. This model, which is well-known in stochastic geometry and spatial statistics, generates random structures through overlapping random 'grains' (spheres, sticks) each with an arbitrary random location and orientation. Wolfgang Weil focuses in his contribution on recent developments for inhomogeneous distributions of grains. Physical applications of Minkowski functionals are discussed in the paper by Klaus Mecke. They range from curvature energies of biological membranes to the phase behavior of fluids in porous media and the spectral density of the Laplace operator. An important application is the morphological characterization of spatial structures: Minkowski functionals lead to order parameters, to dynamical variables or to statistical methods which are valuable alternatives to second-order characteristics such as correlation functions.

A main goal of stereology, a well-known method in statistical image analysis and spatial statistics, is the estimation of size distributions of particles in patterns where only lower-dimensional intersections can be measured. Joachim Ohser and Konrad Sandau discuss in their contribution to this volume the estimation of the diameter distribution of spherical objects which are observed in a planar or thin section. Rüdiger Hilfer describes ideas of modeling porous media and their statistical analysis. In addition to traditional characteristics of spatial statistics, he also discusses characteristics related to percolation. The models include random packings of spheres and structures obtained by simulated annealing. The contribution of Helmut Hermann describes various models for structures resulting from crystal growth; his main tool is the Boolean model.

Part 3 considers one of the most prominent physical phenomena of random spatial configurations, namely phase transitions. Geometric spatial properties of a system, for instance, the existence of infinite connected clusters, are intimately related to physical phenomena and phase transitions as shown by Hans-Otto Georgii in his contribution 'Phase Transition and Percolation in Gibbsian Particle Models'. Gibbsian distributions of hard particles such as spheres or discs are often used to model configurations in spatial statistics and statistical physics. Suspensions of sterically-stabilized colloids represent excellent physical realizations of the hard sphere model exhibiting freezing as an entropically driven phase transition. Hartmut Löwen gives in his contribution 'Fun with Hard Spheres' an overview on these problems, focusing on thermostatistical properties.

In many physical applications one is not interested in equilibrium configurations of Gibbsian hard particles but in an ordered packing of finite size. The question of whether the densest packing of identical coins on a table (or of balls in space) is either a spherical cluster or a sausage-like string may have far-reaching physical consequences. The general mathematical theory of finite packings presented by Jörg M. Wills in his contribution 'Finite Packings and Parametric Density' to this volume may lead to answers by means of a 'parametric density' which allows, for instance, a description of crystal growth and possible crystal shapes.

The last three contributions focus on recent developments of simulation techniques at the interface of spatial statistics and statistical physics. The main reason for performing simulations of spatial systems is to obtain insight into the physical behaviour of systems which cannot be treated analytically. For example, phase transitions in hard sphere systems were first discovered by Monte Carlo simulations before a considerable amount of rigorous analytical work was performed (see the papers by H. Löwen and H.-O. Georgii). But also statisticians extensively use simulation methods, in particular MCMC (Markov Chain Monte Carlo), which has been one of the most lively fields of statistics in the last decade of 20th century. The standard simulation algorithms in statistical physics are molecular dynamics and Monte Carlo simulations, in particular the Metropolis algorithm, where a Markov chain starts in some initial state and then 'converges' towards an equilibrium state which has to be investigated statistically. Unfortunately, whether or not such an equilibrium configuration is reached after some simulation time cannot be decided rigorously in most of the simulations. But Elke Thönnes presents in her contribution 'A Primer on Perfect Simulation' a technique which ensures sampling from the equilibrium configuration, for instance, of the Ising model or the continuum Widomn-Rowlinson model.

Monte Carlo simulation with a fixed number of objects is an important tool in the study of hard-sphere systems. However, in many cases grand canonical simulations with fluctuating particle numbers are needed, but are generally considered impossible for hard-particle systems at high densities. A novel method called 'simulated tempering' is presented by Gunter Döge as an efficient alternative to Metropolis algorithms for hard core systems. Its efficiency makes even grand canonical simulations feasible. Further applications of the simulated tempering technique may help to overcome the difficulties of simulating the phase transition in hard-disk systems discussed in the contribution by H. Löwen.

The Metropolis algorithm and molecular dynamics consider each element (particle or grain) separately. If the number of elements is large, handling of them and detecting neighbourhood relations becomes a problem which is approached by Jean-Albert Ferrez, Thomas M. Liebling, and Didier Müller. These authors describe a dynamic Delaunay triangulation of the spatial configurations based on the Laguerre complex (which is a generalization of the well-known Voronoi tessellation). Their method reduces the computational cost associated with the implementation of the physical laws governing the interactions between the particles. An important application of this geometric technique is the simulation of granular media such as the flow of grains in an hourglass or the impact of a rock on an embankment. Such geometry-based methods offer the potential of performing larger and longer simulations. However, due to the increased complexity of the applied concepts and resulting algorithms, they require a tight collaboration between statistical physicists and mathematicians.

It is a pleasure to thank all participants of the workshop for their valuable contributions, their openness to share their experience and knowledge, and for the numerous discussions which made the workshop so lively and fruitful. The editors are also grateful to all authors of this volume for their additional work; the authors from the physical world were so kind to give their references in the extended system used in the mathematical literature. The organizers also thank the 'Ministerium für Schule und Weiterbildung, Wissenschaft und Forschung des Landes Nordrhein-Westfalen' for the financial support which made it possible to invite undergraduate and PhD students to participate.

Wuppertal *Klaus Mecke*
Freiberg *Dietrich Stoyan*
June 2000