SCALING METHODS



Edited by Yakov Pachepsky David E. Radcliffe H. Magdi Selim



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SCALING METHODS IN SOIL PHYSICS

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Preface

Soil physical properties are needed to understand and manage natural systems spanning an extremely wide range of scales: from microbial habitats to plant root zone environment to field crop productivity to watershed processes to regional weather modeling and global circulation models. Capabilities of soil measurements at those scales are vastly different. This creates a fundamental problem for soil physicists and for multiple users of soil physics data. Many soil data are obtained from small soil samples and cores, monoliths, or small field plots, yet the goal is to reconstruct soil physical properties across fields, watersheds, and landforms, or to predict physical properties of pore surfaces and structure of pore space. The representation of processes and properties at a scale different from the one at which observations and property measurements are made is a pervasive problem in soil physics, as well as in soil science in general. This scale-transfer problem must be solved, in particular, in order:

- To integrate chemical, biological and physical processes affecting soil quality and environmental health
- To describe effectively the coupled fluxes of heat, moisture, gases and solutes across land surfaces
- To establish appropriate soil parameters for describing the long-term fate of pollutants
- To interpret various remote sensing data
- To delineate management zones in agricultural fields
- To estimate water yield and geochemical fluxes in ungauged watersheds
- To understand sources and importance of diversity and patchiness in terrestrial ecosystems
- To provide parameters for estimating biogeochemical trends related to climate change

The multiscale characterization of processes and parameters of soil physics needs to be addressed as a research issue of scale dependencies in soil physical properties and as a practical/operational issue of data assimilation or data fusion in environmental monitoring and prediction.

Scale is a complex concept having multiple connotations reflected in the majority of chapters in this book. A notion of *support* is important to characterize and relate different scales in soil physics. Support is the length, area, or volume for which a single value of soil property is defined and no variations in this and other properties are taken into account. Size of an individual soil sample and size of the discrete spatial element in a soil model are typical examples of supports. The term "resolution" is often used for supports defined in terms of length, and the term "representative elementary volume" is applied for supports defined as volumes. The terms "pixel size" and "grid size" are also used to define support. An area or a volume that is sampled with given support determines the *extent* of measurements. Yet another notion, *spacing*, i.e., distance between sampling locations, is of importance in characterization of the scale of research or an application. Any research of soil physical properties is made with specific support, extent and spacing. If those properties are to be used with different support, extent or spacing, scaling becomes necessary. Scaling is used as a noun to denote a relationship between soil physics data at different scales or as a verb to denote an action of relating such data on different scales. Upscaling (downscaling) usually refers to soil physical properties at a support that is larger (smaller) than the one at which data are available.

Two general approaches to scaling are represented in this book. One approach assumes that a physical model can be invoked or developed to perform scaling. The most prominent examples of

this approach are fractal models and soil-landscape models. Another approach relies on establishing empirical scaling relationships from a large database. Both approaches have obvious advantages and limitations. The accuracy of a scaling can be broadly defined as a correspondence between measured and estimated data for the data set *from which a scaling has been developed*. The reliability of scaling can be assessed in terms of the correspondence between measured and estimated data for the data sets *other than the one used to develop a scaling*. Models in physics-based scaling cannot capture all factors of inherent variability in soils, and therefore scaling is not as accurate in simulating data as an empirical model might be. These models, however, have a potential to be more reliable, whereas the reliability of empirical scaling is essentially unknown. In many cases, empirical scaling in soil physical properties has eventually led to the development of physical models to explain this scaling.

This book is organized across the hierarchy of spatial scales in soils. The first three chapters deal with scaling in properties of soil pore space spanning pore radii range from 10^{-6} to 10^{-2} m. Fractal models of soil physical properties have become popular sources of scaling relationships for those support sizes. Fractal geometry was developed to describe the hierarchy of ever-finer detail in the real world. Natural objects often have similar features at different scales. Measures of these features, e.g., total number, total length, total mass, average roughness, total surface area etc. are dependent on the scale on which the features are observed. Fractal geometry assumes that this dependence is the same over a range of scales, i.e., it is scale invariant within this range. This dependence is used for scaling. To apply fractal geometry, one must have in mind a physical or mathematical model that explains the process involved in formation of fractal features in the objects under study.

In Chapter 1, Perrier and Bird present a pore solid fractal (PSF) model that can be used as a reference model to describe the number-size distributions of soil particles, pores, aggregates and the scaling of measures such as solid–pore interface areas, solid and pore volumes, density and porosity, in soils or in any porous medium exhibiting hierarchical heterogeneities over a broad range of scales. This model provides an explicit geometrical description of scaling in soil structure and leads to deterministic links between the scaling laws of different structural properties and soil hydraulic properties. In Chapter 2, Tarquis, Giménez, Saa, Díaz and Gascó, present an overview of scaling of soil porosity data using multifractal models and configuration entropy. The importance of such scaling methods increases as more two- and three-dimensional data on soil pore space become available; reconstruction of pore connectivity will become feasible, thus opening an avenue to explain and predict preferential flow patterns.

In Chapter 3, Williams and Ahuja show that the assumption of similarity is not crucial for development of an empirical scaling law for soil pore space properties. They propose a one-parameter model of the soil water retention curve that is based on a strong, linear relationship observed between the intercept and slope of a log–log plot of matric potential and soil water content below the air-entry value. Furthermore, for widely different soils this relationship is found to coalesce into one common relationship.

The following three chapters explore scaling in solute diffusion and dispersion in soils using the travel distance as a measure of scale. Chapter 4, by Ewing and Horton, explores scaling laws that emerge from diffusion in porous media with sparsely connected pore spaces, of which soils are an example. Monte Carlo simulations using pore network models, in conjunction with percolation theory, show that, at the percolation threshold, accessible porosity, tortuosity and diffusivity are described by equations that scale with time, distance or proximity to the percolation threshold.

Slightly above the percolation threshold, a different kind of scaling appears. From porosity and diffusivity a residual tortuosity can be calculated, which also shows both kinds of scaling. In Chapter 5, Zhou and Selim examine the notion of scale in soil solute dispersion studies. They present four distinct types of dispersivity–time or dispersivity–distance relationships that are appropriate to describe the relationship between dispersivity and time or distance. These types of scaling were analyzed using simulations and analysis of literature data. In Chapter 6, Perfect demonstrates the

applicability of the power law scaling of dispersivity in geological materials to soils. This scaling law allows him to scale up the dispersivity predicted from water retention properties.

As the scales become coarser and the soil profile is included in the extent of study, two different approaches to the scaling problem can be found in the literature and in this book. One is to assume that the same parameters of soil physical properties can be used at the laboratory sample scale and at the pedon/plot scale. Then an effective averaging procedure can be found to upscale soil properties to the pedon scale. Such an approach is taken in Chapter 7, written by Zhu and Mohanty. They compare commonly used averaging schemes for the hydraulic parameters and compare their capability to generate effective parameters for the ensemble behavior of heterogeneous soils. It appears that the efficiency of the upscaling procedure depends on the degree of correlation between different hydraulic parameters and boundary conditions. Another approach to the transition to the plot/pedon scale is to change the parameter used to characterize the same soil property. A routine example is using a soil water retention curve for the sample scale and field water capacity for the pedon/plot scale to characterize a soil's ability to retain water.

Soils are inherently variable. A model of spatial variability of soil properties has to be known if upscaling is performed by aggregating the additive soil properties. Chapter 8, written by Western, Grayson, Blöschl, and Wilson, provides an introduction to the topic. The authors present a variety of statistical approaches for representing variability and for the spatial scaling of soil moisture, for spatially distributed deterministic modeling of soil moisture patterns at the small catchment scale, and for using remote sensing and topography to interpret variability in soil moisture at larger scales.

The next three chapters outlay specific techniques to model and characterize the variability for scaling purposes. Ellsworth, Reed, and Hudson in Chapter 9 examine the performance of six interpolation methods applied to soil and groundwater solute concentrations. Spacing appears to be an important scale parameter. A nonlinear geostatistical method, referred to as quantile kriging, was found to be optimal for the sparse, clustered sample designs, whereas ordinary kriging and a deterministic calibrated variant of inverse distance interpolation performed the best with dense, regularly spaced sample data. Chapter 10, written by Si, shows opportunities in analyzing space-scale dependencies in soil properties with wavelet analysis that can handle the spatial nonstationarity common in field soils. The localized features and nonstationarity may have significant impacts on modeling soil water flow and chemical transport. The wavelet analysis of the soil hydraulic conductivity and the inverse microscopic capillary length transects exhibits the multiscale variations and localized features seen at different scales.

In Chapter 11, Kumar shows that a model of spatial variability can be established that spans several scales. Such a model can be used to relate measurements of soil properties made at multiple scales with different measurement techniques. Typically, several regions of fine-scale measurements of limited coverage are embedded within coarse-scale measurements of larger coverage. Consequently, in regions at the fine scale that are devoid of measurements, inferences about the statistical variability can be made only through conditional simulation. This chapter describes a conditional simulation technique that utilizes measurements at multiple scales and its application to remote sensing data of soil moisture.

Soil properties are known to be related to landscape position; scaling at field, landscape or regional scales can take advantage of soil-landscape relationships. Chang and Islam in Chapter 12 present a stochastic framework for characterizing the steady-state soil moisture distribution in a heterogeneous-soil and -topography field under the influence of precipitation and evaporation. Upscaling is accomplished by applying a perturbation method and spectral techniques to a stochastic partial differential equation that depends on three main factors: the heterogeneity of soil properties, the variability of topography and the change of mean soil moisture. Results suggest that topography (soil properties) controls soil moisture distributions when the area is dominated by coarse-texture (fine-texture) soil or by soils with small (large) correlation lengths of topography.

Timlin, Pachepsky, and Walthall in Chapter 13 use spatial autoregression and terrain variables to estimate water holding capacity across a field over a range of spacings. Slope and tangential

curvature were found to be significant predictors of surface water holding capacity and spacing had an optimum value. A good correspondence was found between predicted water holding capacity and measured corn grain yields across the field.

High-density data other than topography can be used to define soil properties at field or landscape scales. Chapter 14, written by Morgan, Norman, Molling, McSweeney, and Lowery, presents an overview of measurement techniques available for that purpose. The authors have built a hierarchical example of using data sets of different availability in a model to predict crop yield. They found that at the field scale the USDA soil survey information alone will not be adequate for data needs. Augmenting soil survey information with methods such as inverse modeling to infer soil properties from spatially dense data and landscape survey sensors improves the horizontal resolution required for input in biophysical crop productivity models.

In Chapter 15, Tsegaye, Crosson, Laymon, Schamschula, and Johnson show that temporal highdensity data on rainfall can be used along with basic soil and vegetation properties to downscale remote sensing measurements of soil moisture made at coarse scales. An artificial neural network trained with three sources of input, i.e., high-density rainfall data, coarse scale spatial data on soil moisture, and fine-scale soil and vegetation data, generates values of soil moisture contents at a fine scale. Performance of the neural network becomes worse as the difference increases between coarse-scale and fine-scale supports. It still can be sufficient for applications in which temporal aggregation can be made to match the coarse spatial scale of remote sensing data.

Upscaling and downscaling need to be applied in projects at the field scale where both regional and sample-scale observations appear to be useful to provide input for specific predictions. This book contains several case studies of this type. Chapter 16, written by Cassel and Edwards, explores accumulating and using information about plant response to soil mechanical impedance at sample, plot, field and regional scales. These authors emphasize that research and management questions as well as the relevant soil physical properties are different at different scales. They demonstrate how a management problem at the field scale can be addressed by using regional data to find a probable solution, using field scale data to define soil parameters controlling the usefulness of the proposed solution, and upscaling plot and small-sample scale data to tailor the management practice to a particular combination of soil physical properties.

In Chapter 17, Mulla, Gowda, Birr, and Dalzell describe applications of process-based models to simulate nitrate losses from agricultural fields across a wide range of spatial scales. The authors observe that, as spatial scale becomes coarser, upscaling and aggregation lead to progressively larger uncertainty of model input data. Using simple mass balance equations appears to be more appropriate at the coarsest spatial scale than mechanistic modeling. The performance of spatial upscaling techniques does not seem to depend as much on the magnitude of upscaling as on the relative similarity between the smaller units being upscaled and the larger unit. Chapter 18, written by Seyfried, examines techniques to combine remote sensing data on vegetation with hydrologic modeling. The techniques involve upscaling point-scale soil water models, the incorporation of scale and spatial variability effects on model parameters and the measurements used as input and for model testing, delineating vegetation types, and inferring leaf area index from the vegetation index. Soil mapping units, used in the model to delineate the critical deterministic variability of soil water content, aggregate LANDSAT remote sensing pixels sufficiently that vegetation cover type and vegetation index are effectively described within mapping units while delineating differences among them. Finally, Chapter 19 by Lin and Rathbun shows that the scaling concept can be used to integrate knowledge and data on soil hydrologic properties and regimes in a self-consistent system of concepts and techniques.

The quest of soil physicists to bridge scales is by no means unique. Many scientific disciplines strive to relate observation and models from different scales. One of the closest to soil physics disciplines is represented by Chapter 20, written by Faybishenko, Bodvarsson, Hinds and Witherspoon. The chapter presents a panoramic view of scaling problems in large and complex subsurface volumes of unsaturated fractured rock. Using several examples from experimental investigations in fractured basalt and tuff, the authors show how the concept of the hierarchy of scales becomes instrumental in measuring and modeling flow transport processes. For a given scale, boundary conditions can be defined from studies at a coarser scale whereas determining model parameters requires information from a finer scale. This chapter illustrates the wide opportunities for interdisciplinary cross-pollination in approaching the scale conundrums.

This book does not contain all available ideas, conceptual approaches, techniques or methodologies for scaling of soil physical properties. The list of suggested reading at the end of this preface, as well as references in individual chapters, will help the interested reader. Scaling of soil physical properties is a burgeoning field, responding to the increasing need in environmental modeling and prediction and to the progress in remote sensing technologies to estimate environmental parameters at large scales, in spatially intensive methods to measure indirect indicators of soil physical properties, in *in situ* measurement techniques to obtain small-scale soil data, and in integration of georeferenced data collected at various scales. The contributions in this volume by some of the pioneers in the field represent a broad spectrum of techniques developed and tested to facilitate the use of soil physics data in a wide variety of soil–land–earth-related applications.

> Y.A. Pachepsky D.E. Radcliffe H.M. Selim

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1 The PSF Model of Soil Structure: A Multiscale Approach

E.M.A. Perrier and N.R.A. Bird

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I. INTRODUCTION

Many papers and books have been written about fractals in general and fractals in soil science in particular^{1,2} in the past decade. Central to this theme are the notions of a multiscale structure and a scaling symmetry imposed on this structure. The PSF (pore solid fractal) model is a development of this theme, representing a generalization of the fractal models currently used to model soil structure. While accommodating these models as special, albeit degenerate, cases, it overcomes

some of their shortcomings, providing a geometrical, unified framework which exhibits broad poresize and particle-size distributions, and permitting structure to be modeled over a much wider range of scales and indeed to arbitrarily small scales. In the second section of this chapter we shall review some of the issues that arise in the fractal modeling of soil structure. In the third section we define the PSF model as a simplified but concrete representation of multiscale organizations of pores and solids occurring in soils, which reduces to a fractal model when strict self-similarity occurs at every scale. In the fourth section, we give a comprehensive list of the properties of the PSF model arising from previous studies³⁻⁶ and infer possible deterministic dependencies between different real soil scaling properties. In the concluding section of the chapter, we give an overview of possible extensions of the PSF approach to more complex types of structures, which cannot be analyzed mathematically but by simulation and pore network modeling.

II. FROM FRACTAL SCALING TO A MULTISCALE MODEL OF SOIL STRUCTURE

A. FRACTALS: A THEORY OF MEASURE AND POWERLAW SCALING LAWS

Fractal geometry has brought new concepts to the search for a better quantification of scaledependent soil characteristics. Scaling effects have been observed for a long time in soil physics, for example, soil bulk density varying with the sample size (Figure 1.1a), specific surface areas varying as a function of observation scale, or an increasing number of small voids revealed with increased resolution. There may be different ways to cope with the technical difficulties that such effects produce on measurements.⁷ Fractal theory suggests that these scaling phenomena may be more the rule than the exception and can be explained by an underlying multiscale structure. Similar but theoretical measurements made on a large set of very simple mathematical objects - generated by iterative copies of simple patterns at successive scales — give the same type of results as those obtained on many natural objects. A measure appears to be no longer a single number, nor a mean value within a confidence interval, but a function of scale. In the simplest fractal case, associated with self-similarity at every scale, this function is a powerlaw, and the powerlaw exponent — i.e., the slope of the associated straight line in a log-log plot — depends only on the so-called fractal dimension D of the object (Figure 1.1a). Many formulae of the same type have been derived for different types of measures M (lengths, surfaces, volumes, densities, etc.). A very simple example is the measure of the mass M of a sample of size L which, for a solid mass fractal structure, varies as a power law of L:

$$M_I = M_0 L^D \tag{1.1}$$

This does not mean that we forget the actual and classical value of the measure at a given scale (e.g., M_0 for L = 1) to compare different objects measured at the same resolution, but the fractal dimension D appears to be a key parameter, a second fundamental descriptor of the measure.

Conversely, because many measures obtained on natural objects appear also as straight lines in a log(measure) vs. log(scale), such as solid–void interface areas or masses of soil samples, this suggests that many soils can be considered as fractal objects, even if we are ignorant of the genesis of the natural object, and even if the scaling behavior can be observed only over a narrow range of scales.

In addition, the same type of fractal conceptual model may be extended from a theory of measures to the simple characterization of number-size distributions for a collection of objects. Because the cumulative number-size distribution of the holes in a lacunar fractal model such as a Sierpinski carpet or a Menger sponge varies as a powerlaw, by extension⁸ termed as fractal a collection of objects with a cumulative number size distribution $N[\ge r]$ varying as a powerlaw of the size, r



FIGURE 1.1 Scaling measures and distributions: a) density data (clay soil [From Chepil, W.S., Soil Sci., 70, 351, 1950.]) fitted by a powerlaw model and associated log/log data fitted by a linear model; b) aggregate size distribution (From Perrier, E.M.A. and Bird, N.R.A., *Soil Tillage Res.*, 64, 91, 2002. With permission); c) particle size distributions from several soils. (From Bird, N.R.A., Perrier, E., and Rieu, M., *Eur. J. Soil Sci.*, 55, 55, 2000. With permission.)

$$N[\ge r] \propto r^{-D} \tag{1.2}$$

In a way similar to that applied to measures, when a cumulative distribution of natural objects (e.g., soil particles, pores or aggregates) is fitted by a powerlaw model (Figure 1.1b,c), it is commonly called fractal in the soil science literature despite some formal objections.^{9,10}

For this reason, many soils have been called fractal, due to successful linear regression on log–log plots of many types of data (Figure 1.1). This view is reinforced when the D parameter proves to be a new indicator of structure that discriminates between different types of soil structures or different structural states for the same type of soil.^{11–13}

Sometimes the log–log plot deviates strongly from linearity and making impossible a fractal description. Nevertheless, the measure generally does vary with scale, which means that the concept of a measure viewed as a scaling function remains valid, and deviations from a powerlaw scaling function suggest a more complex, multiscale organization in terms of soil structure.

Even when good linear fits are obtained for log–log plots a degree of caution is needed in their interpretation. The estimation of a D value from such plots is sensitive to data precision and to the type of powerlaw model tested, as illustrated in Figure 1.2. Because this analysis is carried out on



FIGURE 1.2 (a) Density scaling data (Sharpsburg soil [From Wittmus, H.D. and Mazurak, A.P., *Soil Sci. Soc. Am. J.*, 22, 1, 1958.) fitted by Equation 1.17, solid line, or by Equation 1.1, dashed line; (b) two domains in the log–log plot associated with Equation 1.1, that is, two estimated fractal dimensions, similar to Rieu, M. and Sposito, G., *Soil Sci. Soc. Am. J.*, 55, 1231, 1991b.

real data from soils whose type of fractal organization and dimension is obviously unknown *a priori*, the validity of the result is always questionable and research is ongoing to address this issue.

B. DIFFERENT MEANINGS FOR "THE" SOIL FRACTAL DIMENSION AND SEARCH FOR LINKS

A major problem occurs when using fractal dimensions to quantify and classify soils because fractal dimensions may be derived from independent fractal interpretations of different observed scaling laws. If one chooses arbitrarily one type of fractal interpretation, and if the associated fractal dimension appears as a good parameter to discriminate between different soils from a practical point of view and in a particular operational study, this is useful; the meaning of the fractal dimension D may not matter in this specific, limited context. However the different fractal interpretations of scaling measures or distributions can lead to confusion if we mix different soil classifications based on indicators having the same name D but of different origin and meaning.

A key question is: are there some links or no links between the fractal dimensions used in soil science?^{14–20} The more we find such links, the closer we are to the goal of a unified theory. Our aim is to clarify this point to at least avoid misuses, and also to investigate how far a single scaling process may apply to different properties of the same soil structure, in order to establish whether links between different types of structural scaling properties exist. If the possibility of links is corroborated by a theoretical model, the aim is to look for validation through appropriate

experiments, in order to infer missing structural characteristics from measured ones, or hydraulic properties from structural properties.

A way to proceed is to move from a mere conceptual fractal model of scaling measures or size distributions to a geometrical model representing simultaneously the different components of soil structure. Rieu and Sposito led pioneering work in that direction²¹ by considering a mass fractal model including theoretical links between different powerlaw scaling properties. For instance, the fractal dimension D derived from the powerlaw density scaling law was theoretically the same as the D associated with the powerlaw pore-size distribution and consequently the same as the D that appeared in their expression for the water retention curve.

C. THE PSF APPROACH: A GEOMETRICAL, MULTISCALE MODEL OF SOIL STRUCTURE

With the PSF approach, we follow that of Rieu and Sposito and move from a purely conceptual fractal model of a particular scaling property (for instance, a Von Koch curve to model a fractal interface surface between solids and pores in, for example, References 22 and 23) to an explicit geometrical model of an entire soil structure (Figure 1.3). Whereas the traditional solid mass fractal represents a powerlaw pore-size distribution embedded in a conceptual solid space, which vanishes when the model is developed towards arbitrary small scales (and conversely for a pore mass fractal model), the PSF is a more general approach that represents pore and solid distributions, and that includes previous cases as limiting cases. Because it is a geometrical approach, from any assumption on the spatial arrangement of one phase one can derive consequences for the other phase, the boundary between the two phases and other related properties.

Beyond the search for geometrical coherence, the PSF approach is defined first as a multiscale approach, to be open to future developments where self-similarity may occur only over a limited range of scales.



FIGURE 1.3 From independent fractal models and interpretations of powerlaw curve-fitting of scaling measures or distributions to a fractal model of a very porous object.

III. THE PSF MODEL

A. DEFINITION

The PSF model can potentially describe any multiscale porous medium. It is based on the iterative partitioning of a bound region in a space of Euclidean dimension d. We start with a representative region R of linear extent L, which is divided into three sets P, S and F (Figure 1.4a). The sets P and S represent pore and solid phases, respectively, which are considered to be well identified at any given level of resolution — for example, as white and black parts in an initially nonbinarized image of a porous medium. F represents the undefined "gray" complement where an increased resolution is needed to identify again P and S components. At each resolution level, i.e., at each iteration i in the modeling process, new P, S and F components appear within the F set, and the proportion occupied by these components is defined in a general way by probabilities p_i , s_i , and f_i respectively.

At level i = 1, the initial region R can be depicted as a square (d = 2) or a cube (d = 3) composed of n subregions of linear size $r_1 = \alpha L$, so

$$n = \alpha^{-d} \tag{1.3}$$

where α is called the similarity ratio, and np_1 subregions belong to P, ns_1 subregions belong to S, and nf_1 subregions belong to F.

At level i = 2, the set F is partitioned in a geometrically similar way yielding new pore and solid structures and a new set F composed of nf_1nf_1 regions of size $r_2 = \alpha^2 L$. At each level i,

 $> r_1 = L\alpha$

$$r_i = \alpha^i L \tag{1.4}$$



FIGURE 1.4 (a) Definition of the PSF approach: multiscale formalism. P: pore set, probability p_i ; S: solid set, probability s_i ; F: fractal set, probability f_i ; (b) the PSF model generalizes mass fractal models.

This process is repeated *T* times. The resulting multiscale structure is composed of the pores and particles (sets *P* and *S*) generated at each iteration over the range of scales $(r_i)_{1 \le i \le T}$ and a set *F* composed of

$$n^T \prod_{i=1}^{i=T} f_i$$

subregions of size $r_T = \alpha^T L$.

In the simplest case, where the iterative process is strictly self-similar, we restrict ourselves to constant p, s and f probabilities at each level i,

$$p + s + f = 1$$
 (1.5)

and to simplify further the definition and the subsequent calculations, we may consider constant p, s and f proportions instead of probabilities at each level.

Thus the PSF multiscale definition includes that of a fractal set *F* defined by successive iterations, creating at each level *i* $(nf)^i$ subregions of linear size $r_i = \alpha^i L$. We note that F is in fact a so-called prefractal set when the total number T of iterations is finite. The fractal dimension of F is given by

$$D = \frac{\log(nf)}{\log(1/\alpha)} \tag{1.6}$$

It is clear that, in the PSF multiscale approach, a pure fractal structural model is only the particular case where strict self-similarity occurs across a broad range of scale. Our following mathematical results have been obtained only in this case and should be considered as a useful, idealized reference case for future extensions.

B. GENERATING **PSF** STRUCTURE MODELS

1. Different Geometrical Patterns

Examples of different PSF structures are provided in References 3 and 4. The simplest originates from Neimark,²⁴ who described a multiscale percolation system (Figure 1.5a) with black and white sites randomly distributed on a regular grid as in standard percolation theory, then smaller black and white cells appearing with increasing resolution. Figure 1.5b exhibits a variant where the cells exhibit irregular polygonal shapes (generated by a Voronoi tesselation around randomly distributed seed points, with an extension to three-dimensional polyhedral shapes in Figure 1.5k). In Figure 1.5c the pores are located at each level around the solids in a way that has been shown³ to be equivalent to the version where pores and solids have a symmetrical geometry; the equivalence relates to the global, fractal or nonfractal, measures and distributions and not to the topology or connectivity, which is obviously quite different.

2. With Only Pores or Only Solids

The PSF model includes two special cases: when s = 0, the PSF reduces to a solid mass fractal and when p = 0, the PSF reduces to a pore mass fractal (Figure 1.4b). The PSF approach is thus a generalization of previous studies made about mass fractal models, with solid mass fractals used mainly in soil science, and pore mass fractals used mainly in geology. The two cases can occur whatever the geometrical pattern (Figures 1.5d,e,f). If *T* goes to infinity these two special cases yield a total void (the porosity equals 1) and a total solid structure (the porosity equals 0) respectively and hence cease to function as practical models of porous media. Thus the fractal domain must be



FIGURE 1.5 The PSF model of soil structure can model different geometrical patterns: (a) is built upon a regular grid whereas (b) uses an irregular polygonal grid (Figures 1.5a,b [From Perrier, E., Bird, N., and Rieu, M., *Geoderma*, 88, 137, 1999.]) and in (c) the pores are located "around" the solids. (d) and (e) exhibit, respectively, pure solid and pore mass fractals to be compared with (a). (f) shows a solid mass fractal to be compared to the pore/solid composition in (c). (g) and (h) are, respectively, associated with (f) and (a) where the fractal (gray) set has been replaced by a solid phase at the last level representing the lower cutoff of scale. Similarly, (i) is associated with (c), but the fractal set at the last level has been replaced by a mixture of pores and solids. (j) and (k) are three-dimensional versions of (a) and (b), again with a mixture of pores and solids at the last level.

bounded and, in the first case, the resulting prefractal set F at level T is *de facto* associated with the solid phase (e.g., the gray phase in Figure 1.5f becomes black in Figure 1.5g), and with the pore phase in the second case.

3. With Lower Bound or No Lower Bound

In the PSF approach, there is no necessity for a lower cutoff of scale in order to model realistic porosities. When infinite iterations are carried out, the PSF remains a valid model for a porous medium, the porosity of which has been shown to depend only on the *p* and *s* parameters as follows:

$$\phi_{PSF} = \frac{p}{p+s} \tag{1.7}$$

A PSF model can easily match any experimental porosity value while representing a broad distribution of pores and solids of different sizes — the properties of which will be given later on in the chapter.

Nevertheless, we will generally introduce a lower bound in the PSF model because we consider that there should be a lower cutoff of scale in real porous media; thus we have a finite number of iterations T and a resulting prefractal set F. In order to complete the description of a porous medium we must identify this set with the solid phase (Figure 1.5h), the pore phase or a combination of both phases. The treatment of the set F is important in determining the scaling behavior of density and porosity. Indeed, with the inclusion of a lower bound to the PSF it is possible to cover a range of monotonic scaling behavior from increasing density and decreasing porosity through constant density and porosity to decreasing density and increasing porosity with increasing sample size.⁶

C. FRAGMENTATION OF A PSF STRUCTURE

In the first studies about the PSF model of soil structure, we considered only the distributions of pores and solid and related measures that could be made on a soil sample, but we did not consider the distribution of aggregates that may result from incomplete fragmentation of the sample. In fact, a fragmentation process is partly independent of the underlying structure. For example, a fractal number size distribution of fragments may result from a very simple, multiscale fragmentation process applied to a homogeneous bulk material.²⁵ We showed later⁵ that the superimposition of a self-similar fragmentation process of dimension D_{frag} on a PSF structure of fractal dimension D leads to a generalization of previous results obtained in soil science, with the novel and realistic feature that both aggregates and particles are released during the fragmentation process. As illustrated in Figure 1.6, one keeps $(1 - x_{frag})$ unfragmented aggregates within the F subparts of the PSF model, and one defines a fragmentation fractal dimension as:

$$D_{frag} = \frac{D \bullet Log(nfx_{frag})}{Log(nf)}$$
(1.8)

IV. INFERRING DETERMINISTIC LINKS BETWEEN SEVERAL SCALE-DEPENDENT SOIL PHYSICAL PROPERTIES

A. LINKS BETWEEN DIFFERENT SCALING STRUCTURAL PROPERTIES

In this section we provide a list of mathematical results obtained for the self-similar PSF model in previous studies, using unified notations.



FIGURE 1.6 The PSF model generalizes fractal models for soil fragmentation, for example, where p = 7/16, s = 3/16, f = 6/16, $x_{frag} = 4/6$. (From Perrier, E.M.A. and Bird, N.R.A., Soil Tillage Res., 64, 91, 2002.)

1. Pore and Particle Size Distributions

It has been shown⁴ that the number $N_s[r = r_i]$ of solid particles of size r_i in a PSF structure is:

$$N_{s}\left[r=r_{i}\right] = \frac{s}{f} \left(\frac{r_{i}}{L}\right)^{-D}$$
(1.9)

and that the cumulative number $N_s[r \ge r_i]$ of solid particles of size greater than r_i is:

$$N_{s}\left[r \ge r_{i}\right] = ns \left(\frac{\left(\frac{r_{i}}{L}\right)^{-D} - 1}{nf - 1}\right)$$
(1.10)

For $r_i \ll L$ we obtain, in a simplified and continuous version, the following approximation:

$$N_{s} \left[\geq r \right] \propto \left(\frac{r}{L} \right)^{-D} \tag{1.11}$$

In a totally symmetrical way, the number N_p of pores of size r_i is given by:

$$N_{P}\left[r=r_{i}\right] = \frac{p}{f}\left(\frac{r_{i}}{L}\right)^{-D}$$
(1.12)

and, if $r_i \ll L$

$$N_{P}\left[\geq r\right] \propto \left(\frac{r}{L}\right)^{-D} \tag{1.13}$$

Equations 1.11 and 1.13 commonly define a fractal number-size distribution of solids and pores, as previously reported (see, for example, Equation 1.2).

2. Aggregate or Fragment Size Distributions

When a constant probability x_{frag} of fragmentation is considered to apply at each scale on a PSF structure (Figure 1.6), it has been shown⁵ that the number $N_{frag}[r = r_i]$ of fragments of size r_i is:

$$N_{frag}\left[r=r_{i}\right] = \left(1-x_{frag}+\frac{s}{f}\right)\left(\frac{r_{i}}{L}\right)^{-D_{frag}}$$
(1.14)

where the fragmentation dimension $D_{frag} \rightarrow D$ when $x_{frag} \rightarrow 1$.

In the PSF approach, the fragments are a mix of porous aggregates and particles, as in real fragmentation experiments.

If $x_{frag} = 1$, the fragmentation is complete; all the fragments represent primary particles and Equation 1.14 reduces to Equation 1.9.

If s = 0 there are only porous aggregates made of monosized particles and Equation 1.14 reduces to the formula established for the number $N_A[r = r_i]$ of aggregates from solid mass fractal theory:

$$N_{A}\left[r=r_{i}\right] = \left(1-x_{frag}\right)\left(\frac{r_{i}}{L}\right)^{-D_{frag}}$$
(1.15)

For the cumulative number of aggregates or fragments, when $r_i \ll L$, we obtain the approximation,

$$N_{frag} \left[\ge r \right] \propto \left(\frac{r}{L} \right)^{-D_{frag}} \tag{1.16}$$

which commonly defines a fractal number size distribution of fragments, aggregates or particles.

3. Mass, Density/Porosity Scaling

The mass M (of the solid phase) in a PSF structure scales as a function of the sample size L as follows:⁶

$$M_{L} = L^{d} \rho_{PSF} + \left(\rho_{r} - \rho_{PSF}\right) \left(\frac{L}{r}\right)^{D} r^{d}$$
(1.17)

where

$$\rho_{PSF} = \left(\frac{s}{p+s}\right)\rho_s$$

is the density of the PSF model when the model is developed *ad infinitum*, ρ_s is the density of the solid phase, where ρ_r is the density of the F parts of size *r*.

Let us note that, when s = 0, that is, in the special case of a solid mass fractal model, $\rho_{PSF} = 0$, and only in that case, Equation 1.17 reverts to the classical powerlaw

$$M_L = M_r \left(\frac{L}{r}\right)^D$$

given by Equation 1.1.

From Equation 1.17, the bulk density is given by:

$$\rho_L = \rho_{PSF} + \left(\rho_r - \rho_{PSF}\right) \left(\frac{L}{r}\right)^{D-d}$$
(1.18)

and, similarly, the porosity of the PSF follows as:

$$\phi_L = \phi_{PSF} + \left(\phi_r - \phi_{PSF}\right) \left(\frac{L}{r}\right)^{D-d}$$
(1.19)

Except in the special cases already quoted, the PSF is not a mass fractal, but in every case its mass, porosity and density are scaling functions, expressed in terms of the sample size, or observation scale, L, and resolution level, or yardstick scale, r.

The above expressions are generalizations of those developed for mass fractal models, incorporating the extra fitting parameters ρ_{PSF} and ϕ_{PSF} .

4. Solid-Pore Interface Area Scaling

It has been shown³ that the area S of the pore solid interface in a PSF structure of size L scales as a function of the resolution r as a logarithmic function when D = d - 1, and when $D \neq d - 1$, and $ps \neq d - 0$ as:

$$S_{L} = \frac{ps}{p+s} \frac{2dn^{-d}}{(1-n^{-d}f)} (L^{d-1} - \left(\frac{L}{r}\right)^{D} r^{d-1})$$
(1.20)

and that Equation 1.20 becomes a simple powerlaw scaling function

$$S_L \propto \left(\frac{L}{r}\right)^D S_r$$

if and only if D > d-1 and the number T of iterations is high enough, for the first term in the right-hand side then becomes negligible.

A similar result holds for the two special mass fractal cases (when p = 0 or s = 0).

5. Overview Discussion

A self-similar PSF structure can model at the same time:

- A (fractal) powerlaw pore size distribution and a (fractal) powerlaw particle size distribution, the exponents of which involve the same *D*
- A fractal pore-solid interface of dimension D when D > d 1
- A (fractal) powerlaw fragment or aggregate size distribution involving a dimension D_{frag} where $D_{frag} < D$, and $D_{frag} \rightarrow D$ when the fragmentation process is complete
- A fractal mass for the solid or the pore space in two special cases and, in the general case, mass, density or porosity scaling laws involving exponent D (and at least one additional parameter)

The equations derived for the PSF are identical to or generalize previous equations derived for classical fractal models of soil physical properties. Thus, in many cases, they can be used in the same context and will provide the same fits and estimated fractal dimensions as in previous studies (e.g., Figure 1.1) except when a generalized equation introduces one more parameter to fit (Figure 1.2).

The PSF approach allows us to establish, then to check, a list of coherent, theoretical links, on a geometrical basis, between separate studies and estimated fractal dimensions. If a comprehensive set of data were available on the same soil, the theoretical links inferred by the PSF equations could be validated, and the fractal behavior of a certain class of soils could be better established. Moreover, a general scaling trend exhibited simultaneously by a large set of complementary data would appear more reliable than a collection of independent, log–log plots, each of them leading to the estimation of a fractal dimension without "cross validation."

B. LINKS BETWEEN STRUCTURAL AND HYDRAULIC SCALING PROPERTIES

In the same vein, the PSF approach allows us to check or to establish theoretical links between structural and hydraulic properties in soils. The main link relies on the physically based, though very simplified, capillary model that has been used for a long time to associate the water retention curve or the hydraulic conductivity curve with the pore-size distribution. This association integrates more complex, but deterministic, links between structure and dynamics at a microscopic scale, and should at least account for the connectivity of the pore network,^{26,27} especially with regard to the crucial effect of water paths on the hydraulic conductivity, and also on the hysteresis of the water retention curve.

Nevertheless, in a first modeling approach, working as many other authors, one could introduce mere weighting coefficients accounting for tortuosity or connectivity in the calculation of a hydraulic conductivity curve from a pore-size distribution (for example, References 21 and 28). One can look again, mainly for trends in a one-to-one association between a water retention curve and a pore-size distribution. Using the latter point of view, we obtained an analytical expression for the water retention curve in a PSF model, the first interest of which lies in the comparison with previous theoretical expressions obtained using the same assumptions. Two expressions were available to model the water retention curve in a fractal soil (Equations 1.21 and 1.22). By establishing Equation 1.21,

$$\frac{\theta}{\theta_{\max}} = \left(\frac{h_{\min}}{h}\right)^{d-D}$$
(1.21)

where θ is the volumetric water content and *h* is the capillary pressure. Tyler and Wheatcraft²⁹ gave a fractal interpretation of the widely used Brooks and Corey³⁰ empirical expression, whereas Rieu and Sposito²¹ obtained a different expression in the same context:

$$\theta + 1 - \theta_{\max} = \left(\frac{h_{\min}}{h}\right)^{d-D}$$
(1.22)

Then Perrier³¹ showed that only Equation 1.22 applied on a mass fractal model and that the general equation for the water retention curve associated with any fractal pore-size distribution has the following general expression:

$$\theta + A - \theta_{\max} = A \left(\frac{h_{\min}}{h}\right)^{d-D}$$
 where $h_{\min} \le h \le h_{\max}$ (1.23)

where A is the upper limit of the fractal porosity³² and Equation 1.23 has two special cases (Equation 1.21 when A = 1 and Equation 1.22 when $A = \theta_{max}$).

By finally establishing the following expression for the water retention curve in the selfsimilar PSF model:

$$\theta = \theta_{\max} - \phi_{PSF} \left(1 - \left(\frac{h_{\min}}{h} \right)^{d-D} \right) \quad \text{where} \quad h_{\min} \le h \le h_{\max} * \tag{1.24}$$

Bird et al.⁴ gave a geometrical interpretation of Equation 1.23 that has several implications as regards the links between hydraulic and structural data. Let us consider the exponent D that can be estimated from a fit of Equation 1.24 to water retention data. This D value could give the mass or the density or the porosity scaling exponent involved in Equations 1.17, 1.18, and 1.19, using a PSF theory generalizing that of Rieu and Sposito.²¹ The value of D could also give the exponent of the particle-size distribution, using a PSF theory that shows that the particle- and the pore-size distributions scale in an identical way.

Conversely, as illustrated in Figure 1.7, the value of D estimated from simple measures of particle sizes and masses, obtained from mechanical sieving, could give the exponent in Equation



FIGURE 1.7 Structural data scaling vs. hydraulic data scaling, example, where the value of D calculated from the particle size distribution (a) of a silty clay loam (Ariana soil [From Rieu, M. and Sposito, G., *Soil Sci. Soc. Am. J.*, 55, 1231, 1991b.]) is used to predict the water retention curve (b). (From Bird, N.R.A., Perrier, E., and Rieu, M., *Eur. J. Soil Sci.*, 55, 55, 2000. With permission.)

^{*} Let us note that the condition $h_{\min} \le h \le h_{\max}$, associated with a limited range of scale over which a fractal structure exists, applies to Equations 1.21 and 1.22. In Equation 1.21 $h_{\max} = \infty$.

1.24 of the variation of the capillary pressure as a function of the water content. Of course we cannot judge the success of the approach on one example, and the log–log fit of the five structural data is less than perfect. But this example, published by Bird et al.,⁴ illustrates the strong principle of the PSF approach, where deterministic links between structural and hydraulic properties could be inferred by a simplified geometrical and physical modeling approach.

V. CONCLUSION AND PERSPECTIVES: TOWARD EXTENDED PSF VIRTUAL STRUCTURES AND PORE NETWORK MODELING

Further work has to be done to validate and to calibrate the PSF model on real data. This will require, at least, the acquisition of pore-, particle- and aggregate-size distributions on the same soil sample to test the validity of the PSF model and to estimate its parameters p,s, (thus f = 1-p-s), n and x_{frag} . The more constraints that will be available, the better, and porosity or density data sets over a large range of scale would be very useful. Then, if successful, PSF virtual soil structures matching real soil samples' properties can be built to conduct numerical experiments.

The formalism developed in the PSF approach to define in a very general way a multiscale porous medium provides scope for further theoretical studies. On the one hand, different geometrical patterns (Figure 1.5) can be created, first to check how far the mathematical results obtained on regular space



FIGURE 1.8 Pore network simulation in a two-dimensional space. (a) and (b) simulation of drainage and imbibition in a mass fractal structure calibrated to represent a given pore size distribution (Ariana soil [From Rieu, M. and Sposito, G., *Soil Sci. Soc. Am. J.*, 55, 1231, 1991b.]); (c) hysteresis of the simulated water retention curves; (d) the simulated hydraulic conductivity curve is unreliable because of the difficulty in modeling the connectivity of the pore network in a two-dimensional space. (From Rieu, M. and Perrier, E., *C.R. Acad. d'Agricul. France*, 80(6), 21, 1994.)



FIGURE 1.9 Pore network simulation in a three-dimensional space (courtesy of Jean-François Delerue). (a) an arbitrary image of a PSF structure exhibiting polyhedral pores over three scale levels; (b) extraction of a pore network: the balls represent the pore location and sizes; (c) simulation of the water retention curve in imbibition.

partitions hold when variations are introduced concerning pore and solid shapes, as well as sizes within each discrete level to match better real variability. Such work has already been done³¹ on two-dimensional computer constructions such as those shown in Figures 1.5g and 1.5i, where analytical expressions Equations 1.22 and 1.24 for the water retention curve proved to give quite successful fits and led to very good estimations of the underlying fractal dimension D of the simulated fractal model structures. This could be extended to other patterns or to three-dimensional fractal models (Figures 1.5j and 1.5k).

On the other hand, using simulations on virtual soil structures, one can account for the effect of the connectivity of the pore network on the hysteresis of the water retention curve (Figure 1.8c) and on the value of the hydraulic conductivity (Figure 1.8d). Such results³³ were obtained directly by applying classical methods in the field of pore network modeling³¹

The novelty involves extracting a pore network (Figure 1.9) from any type of two- or threedimensional porous structure by means of new image analysis tools that have been initially tested on real volumetric images of soils.³⁴ These new algorithms will first allow us to simulate the hydraulic properties of a large set of PSF models, including the hydraulic conductivity, which depends not only on the pore size distribution but also on the geometrical pattern of the structure and on the associated topology of the pore network. The mathematical scaling expressions summarized in this chapter and obtained in the self-similar, fractal case will provide useful limiting cases to check the results of the simulations.

VI. ACKNOWLEDGMENTS

This work is dedicated to the memory of the late Michel Rieu, who initiated and greatly encouraged it.

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2 Scaling and Multiscaling of Soil Pore Systems Determined by Image Analysis

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I. INTRODUCTION

One of the most direct methods of characterizing soil structure is the analysis of the spatial arrangement of pore and solid spaces on images of sections of resin-impregnated soil. Recent technological advances in digital imagery and computers have greatly facilitated the application of image analysis techniques in soil science.^{1,2} Thick sections (soil-blocks) are analyzed by reflected light, and thin sections are analyzed by transmitted light to obtain images from which pores (filled with a resin) and solid spaces can be separated using image analyses techniques.^{3,4} Direct measurements on images together with application of set theory are used to quantify connectivity, size, and shape of pores.⁵ Statistical analyses of the geometry of soil structure can then provide indices of a more general applicability to the characterization of soil structure than any physical property because they can lead to a mechanistic understanding of relationships between geometry of soil structure and soil processes. However, several authors have pointed out that results are a function of image resolution and of the threshold value used to separate pore from solid space.^{6–8}

Scaling of pore systems could potentially be characterized with fractal and multifractal techniques. The fractal approach assumes a hierarchical distribution of mass in space such that at any resolution the fractal structure is seen as the union of subsets similar to the whole. These subsets are either identical (deterministic fractal) or statistically identical (stochastic fractal). In this instance a single fractal dimension serves to characterize the mass distribution.⁹ Fractal techniques have been successfully applied to the characterization of pore systems in soil.^{10–14}

In an object exhibiting multifractal scaling, mass is distributed in a hierarchical pattern as in the fractal case. The whole is formed by the union of similar subsets, but the subsets are related to the whole through different scaling factors. As a result, multifractal distributions cannot be characterized with a single fractal dimension.¹⁵ The multifractal character of a system is intuitively related to the complexity (deterministic or stochastic) of the processes generating it. Multifractal scaling has been found in rock pore systems¹⁶ and suggested as possible in soils based on the distribution of pore sizes^{17,18} or on their spatial pattern.^{19–21}

The distinction between fractal and multifractal scaling in soils is needed for modeling links among fractal dimensions and soil processes and properties.^{22,23} Even though comprehensive reviews have been written on fractal models in soil science,^{24–28} there is significantly less information on multifractal techniques as they apply to soils. Thus, the objectives of this work are to review multifractal techniques as they relate to image analysis of the spatial distribution of soil pores, and to discuss potential applications.

II. BACKGROUND

The main purpose of this section is to introduce some of the fractal and multifractal methods used in the context of image analysis of soil structure. A complete account of fractal and multifractal theories can be found, among others, in Feder's²⁹ and Baveye and Boast's books.²⁶

A. BOX-COUNTING METHOD

This methodology is classical in this field and has generated a large volume of work. If a fractal line in a two-dimensional space is covered by boxes of side length δ , the number of such boxes, $n(\delta)$, needed to cover the line when $\delta \rightarrow 0$ is:³⁰

$$n(\delta) = c\delta^{-D_L} \tag{2.1}$$

The length of the line studied (e.g., the pore–solid interface), $L(\delta)$, can be defined at different scales and is equal to $\delta n(\delta)$. At small δ values the method provides a good approximation to the length of the line because the resolution of the image is approached. At larger sizes the difference between $\delta n(\delta)$ and the "true" length increases. Thus, D_L is estimated using small δ values.¹³ The box-counting method is also used to obtain a fractal dimension of pore space by counting boxes that are occupied for at least one pixel belonging to the class "pore."¹³

B. DILATION METHOD

The study by Dathe et al.⁸ is the only published report of this method in soil science. The dilation method follows essentially the same procedure as the box-counting method, but instead of using boxes it uses other structuring elements to cover the object under study, e.g., circles.⁸ The image is formed by pixels, which are either square or rectangular in shape. If circles are used, the measure of scale is their diameter (as is the side length of the box in the box-counting technique). If we want to have the same dilation in any direction, the orthogonal and diagonal increments should be biased by $\sqrt{2}$, which corresponds to the hypotenuse of a square of unit side length.³¹ The length of the studied object is counted by numbers of circles, and then the slope of the regression line between the log of the object length and the log of the object diameter is defined by the relation:

$$L(\delta) = c\delta^{1-D_L} \tag{2.2}$$

Dathe et al.⁸ applied the box-counting and dilation methods to the same images and found nonsignificant differences in the values of the fractal dimensions obtained with both methods. They pointed out, however, that fractal dimensions estimated with both methods are different: the box counting dimension is the Kolmogorov dimension while the dimension obtained with the dilation method is the embedding dimension (Mikowski-Bouligand). For further details see Takayasu's work.³²

C. RANDOM WALK

Fractal methods can also be used to describe the dynamic properties of fractal networks.^{12,33} Characterization of fractals involving space and time is achieved through the use of fractons³¹ or the spectral dimension.³⁴ For example, Crawford et al.³³ related measurements of the spectral dimension *d* to diffusion through soil, associating *d* with the resistance degree to which the network delays the diffusing particle in a given direction.

The determination of *d* is based on random walks, where in each walk the number of steps taken (n_s) and the number of different pore pixels visited (S_n) are computed. At the beginning of the random walk a pore pixel is randomly chosen, then a random step is taken to another pore pixel from the eight pixels surrounding the present one (see Figure 2.1A). If the new pore pixel has not been visited by the random walk, the S_n and n_s are increased by one, otherwise only n_s is increased. The random walk stops when a certain number of null steps (the step goes into a site used previously during the walk) are achieved or the random walk arrives at an edge of the image (for further details see Crawford et al.³³). A graphical representation of these random walks is shown in Figure 2.2. The number of walks and the maximum number of null steps for each walk can vary.³¹ Also a four-connected random walk (Figure 2.1B) can be used instead of eight-connected one.¹²

For each random walk, d is calculated based on the relation:

$$n_s = cS_n^{\frac{d}{2}} \tag{2.3}$$

where c is a constant. The mean value of the d calculated for each walk is the spectral dimension.



FIGURE 2.1 Possible steps taken in a) eight-connected random walk, and b) four-connected random walk. The present position of the pore pixel is marked by an \times , and the arrows indicate the possible next pore pixel.



FIGURE 2.2 A simplified example of one random walk through the pore space. (From Anderson, A.N. et al., *Soil Sci. Soc. Am. J.*, 60, 962, 1996. With permission.)

D. GENERALIZED DIMENSIONS, D_o

In the box-counting technique, a box is counted regardless of the proportion of its area covered with pixels of the pore class. Thus, boxes entirely occupied by pore class pixels have the same weight as boxes containing one pore pixel. On the other hand, generalized dimensions are calculated using the box-counting technique by accounting for the mass contained in each box. An image is divided into n boxes of size δ (n(δ)), and for each box the fraction of pore space in that box, P_i, is calculated:

$$P_i = \frac{\mathbf{m}_i}{M} = \frac{\mathbf{m}_i}{\sum_{i=1}^{\mathbf{n}(\delta)} \mathbf{m}_i}$$
(2.4)

where m_i is the number of pore class pixels and M is the total number of pore class pixels in an image. In this case, the pore space area is the measure whereas the support is the pore space itself. The next step is to define the generating function ($\chi(q, \delta)$) as:

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$$\chi(q, \delta) = \sum_{i=1}^{n(\delta)} \left[\chi_i(q, \delta) \right] \qquad q \in \mathbb{R}$$
(2.5)

where

$$\chi_{i}(q, \delta) = P_{i}^{q} = \left(\frac{m_{i}}{\sum_{i=1}^{n(\delta)} m_{i}}\right)^{q}$$
(2.6)

and $n(\delta)$ is the number of boxes of size δ in the whole image, χ_i is a weighted measure that represents the percentage of pore space in the ith box, and q is the weight or moment of the measure. A log-log plot of a self-similar measure, χ (q, δ), vs. δ at various values for q gives:

$$\chi(q,\delta) \sim \delta^{-\tau(q)} \tag{2.7}$$

where $\tau(q)$ is the qth mass exponent,²⁹ sometimes called the Rényi exponent.³⁵ We can express $\tau(q)$ as:

$$\tau(q) = -\lim_{\delta \to 0} \frac{\log(\chi(q, \delta))}{\log(\delta)}$$
(2.8)

Then the generalized dimension, D_q , can be introduced by the following scaling relationship:³⁵

$$D_{q} = \lim_{\delta \to 0} \frac{\log[\chi(q, \delta)]}{(q-1)\log\delta}$$
(2.9)

and, therefore,

$$\tau(q) = (q-1)D_a \tag{2.10}$$

For the case that q = 1, Equation 2.9 cannot be applied, using instead:

$$D_{1} = \lim_{\delta \to 0} \frac{\sum_{i=1}^{n(\delta)} \chi_{i}(1, \delta) \log[\chi_{i}(1, \delta)]}{\log \delta}$$
(2.11)

The generalized dimensions, D_q , for q = 0, q = 1 and q = 2 are known as the capacity, the information, and the correlation dimensions, respectively.³⁶ The capacity dimension is the boxcounting or fractal dimension. Two images with the same capacity dimension can have different distribution of mass (i.e., different spectra). The information dimension is related to the entropy of the system, whereas the correlation dimension computes the correlation of measures contained in intervals of various sizes. A graph representing the values of D_q vs. q presents a characteristic shape of an inverted S (see Figure 2.3B) in the case of a multifractal measure. Muller et al.³⁷ defined the



FIGURE 2.3 Spectra obtained with a multifractal analysis of the gray-level measure from a soil thin section image: A) spectrum of the fractal dimensions $f(\alpha)$ and B) spectrum of generalized dimensions D_{q} .

width of the multifractal spectra as $w = D_0 - D_1$ and suggested that w could be an important predictive parameter. A greater w means a wider spectrum and a more heterogeneous distribution on the pore space.

When $f(\alpha)$ and τ (q) are smooth functions, we can express³⁸

$$\alpha(q) = -\frac{d}{dq}\tau(q) \tag{2.12}$$

$$f(\alpha(q)) = q\alpha(q) + \tau(q)$$
(2.13)

where Equation 2.13 is obtained by Legendre's transformation. A multifractal measure will show an $f(\alpha)$ curve with a parabolic shape (see Figure 2.3A).

E. The $f(\alpha)$ -Singularity Spectrum

There are several ways to calculate the $f(\alpha)$ -singularity spectrum besides the general methodology of Evertsz and Mandelbrot³⁹ and Feder,²⁹ and the specific techniques of Meneveau and Sreenivasan.⁴⁰ Once the generating function ($\chi(q, \delta)$) has been defined and taking μ_i as:

$$\mu_{i}(q,\delta) = \frac{\chi_{i}(q,\delta)}{\chi(q,\delta)}$$
(2.14)

the coarse Hölder exponent, $\alpha(q)$, and the Hausdorff measure, f(q) are calculated for a series of diminishing box sizes δ and over a range of values of q as:

$$\alpha(q) = \lim_{\delta \to 0} \frac{\sum_{i=1}^{n(\delta)} \mu_i(q, \delta) \log[\mu_i(1, \delta)]}{\log \delta}$$
(2.15)

$$f(q) = \lim_{\delta \to 0} \frac{\sum_{i=1}^{n(\delta)} \mu_i(q, \delta) \log[\mu_i(q, \delta)]}{\log \delta}$$
(2.16)

A relation between f and α is thus established, with q as a parameter. Notice that in the case that q = 1, then f(1) = $\alpha(1) = D_1$. For further details on Equations 2.15 and 2.16 see Chhabra and Jensen.⁴¹

The f(α) vs. α function contains three characteristic points: (α_{\min}) , (α_{\max}) and $f_{\max}(\alpha)$. Some authors used the amplitude, a, of the spectrum, i.e., $a = (\alpha_{\max} - \alpha_{\min})$, to analyze the complexity of a distribution.^{42,43} The amplitude is used in the same way as the width, w, but is a more sensitive parameter because its value is determined by the whole spectrum. Because a larger number of dimensions are needed to define a measure, larger amplitudes imply higher levels of complexity. Notice that the amplitude is determined by the positive (α_{\min}) and negative (α_{\max}) parts of a spectrum. From a probabilistic point of view, the negative part of the spectrum (q < 0) characterizes the rare events, or the values of the measure with lower frequencies (smaller values). As a result, the negative part of a spectrum contains always larger calculation errors (see Equation 2.6), and is typically not used for analyses other than for estimations of the amplitude.

The symmetry of the spectrum provides information on a system. For example, a symmetric spectrum indicates that higher and lower frequencies of events are contributing the same information. An asymmetric spectrum shifted to the right/left area indicates that lower/higher frequencies scale over a larger range than the opposite part of the spectrum.⁴³ The analysis of the symmetry of a spectrum requires a large number of points to assure that errors are minimized. To avoid or minimize calculation errors, some authors select a minimum threshold value of frequency to analyze the negative portion of the spectrum.⁴⁴

Muller and McCauley¹⁶ obtained the $f(\alpha)$ -singularity spectra of simulated Cantor sets using two different scaling ratios, or P_i (weights). The symmetry and width of the simulated spectra increased as the difference in the P_i values increased. Thus, larger amplitude simulates a more diverse and unbalanced hierarchy of pore distribution in the soil.

F. THE CONFIGURATION ENTROPY

There are situations in which multifractal methods are not enough to characterize a system entirely. For instance, Beghdadi et al.⁴⁵ used two artificial images with subtle differences to demonstrate that the configuration entropy could separate them, while their multifractal spectra were identical. Another advantage of this parameter is that there is no need to select a range of scales for the calculations.^{45,46} Most of the developments presented here are based in the work of Andraud et al.,^{46,47} who estimated configuration entropies from planar thin sections of gold and sandstone.

The basis of this method is to study the effect of scale in some geometrical quantities, for example, porosity. Estimation of porosity from a binary image implies counting the pixels representing pores and expressing this count as a percentage of the total number of pixels in the image. If an image is divided in an arbitrary number of smaller areas (e.g., boxes) and porosity is estimated in each subarea, a distribution of the measure "porosity" is obtained for the image. The basic idea of local porosity distributions (Local is related to each box into which the image is divided.) is to turn a global measure into a distribution of local measures.⁴⁸ Even though we are focusing on porosity, any geometrical quantity is susceptible to the local concept.

Imagine an image formed by pixels arranged in a square lattice of side *L*. A distribution of local porosity is obtained if this lattice is subdivided in $n(\delta)$ boxes of size δ from $\delta = 1$ to $\delta = L/4$ and in every box the number of pixels belonging to the pore class, N_j, is recorded. (Obviously, δ cannot approach the size of the lattice because the distribution of local porosity would lose meaning.)

The probability associated with a case of j pore pixels in a box of size δ ($p_i(\delta)$) is defined as:

$$p_j(\delta) = \frac{N_j(\delta)}{n(\delta)}$$
(2.17)

where $N_j(\delta)$ is the number of boxes with j pore pixels and $n(\delta)$ is the number of boxes of size δ . In this probability function the value j = 0 has a meaning and should be considered. The configuration entropy, H,⁴⁶

$$H(\delta) = -\sum_{j=0}^{\delta n} p_j(\delta) \log(p_j(\delta))$$
(2.18)

measures the uncertainty associated with the porosity that can be attained by a set of boxes of size δ . Andraud et al.⁴⁷ provided a rigorous connection between the configuration entropy H(δ) and the local porosity concept. This last one was first defined by Boger et al.⁴⁸

Because the underlying probability changes with the number of pixels inside the box ($\delta \times \delta$), H(δ) needs to be normalized for comparing entropy values corresponding to different sizes δ .⁴⁸ This is done through⁴⁷

$$H^*(\delta) = \frac{H(\delta)}{H_{\max}(\delta)}$$
(2.19)

where

$$H_{\rm max}(\delta) = \log(\delta^2 + 1)$$

 $H^*(\delta)$ is called the normalized configuration entropy of the two-dimensional morphology of the image.

Andraud et al.⁴⁷ calculated H^* for two generated images of simple models (Bernoulli site percolation model and Poisson grain model) and two microstructures from experimental images (gold film deposit on a glass substrate and a natural sandstone). Except for the Bernoulli site percolation model (corresponding to a random microstructure), all H* curves have a local maximum at a characteristic length L* (Figure 2.4). The authors concluded that L*, and the curvature of H* around this value, characterize the microstructure. A more heterogeneous structure shows a wider extremum than those in which the pore and solid regions are more compact.⁴⁷

III. PRACTICAL CONSIDERATIONS

The application of a multifractal analysis requires first defining a measure. Several measures can be defined depending on the objective of the study. For instance, the interest could be in the spatial distribution of the gray-levels where any pixel can have an integer value ranging from 0 to 255.^{49,50} Also possible is to define a measure in a binary image in which a pixel can only have a value of 0 or 1. In the latter case the calculation is simpler than with the spectrum of gray-levels.

Barnsley et al.⁵¹ describe a measure for a binary case, which is similar to other probability measures (e.g., Mandelbrot³⁰; Hentschel and Procaccia⁵²) but computationally simpler to implement. When computing boxes of size δ , the possible values of m_i are from 0 to $\delta \times \delta$. So let N_j be the number of boxes containing j pixels of pore space. Equations 2.5 and 2.6 will then be:

$$\chi(\mathbf{q}, \, \boldsymbol{\delta}) = \sum_{i=1}^{\mathbf{n}(\boldsymbol{\delta})} \left(P_i\right)^q = \sum_{i=1}^{\mathbf{n}(\boldsymbol{\delta})} \left(\frac{m_i}{M}\right)^q = \sum_{j=1}^{\delta x \partial} N_j \left(\frac{j}{M}\right)^q$$
(2.20)



FIGURE 2.4 Configuration entropy $(H^*(L))$ as a function of the side length of the measurement cell calculated (L) for random microstructures: a) site percolation image (circles); b) random image with a constant bulk porosity (triangles); c) Poisson grain model (diamonds); and d) experimental image of observed gold film morphology (squares). (From Andraud, C., et al., *Physica A*, 235, 307, 1997. With permission.)

Using the distribution function N_j , calculations become simpler and computational errors are smaller. It is obvious that one should start with j = 1, because j = 0 means that there is no pore mass to account for.

After defining a measure, attention should be paid to the determination of the scales over which a generation function vs. the length is linear when a log–log scale is used, as well as to the range of q's over which the multifractal scaling is valid. For instance, Muller and McCauley¹⁶ found that, from the maximum possible range (1 to 512 pixels), the generation function was linear only between scales of 16 and 128 pixels (four points). This limited range of scales compromises the estimation of parameters through fitting. In Muller and McCauley¹⁶ q spanned from –15 to 15 at steps of 0.1. In a later work, Muller et al.³⁷ used the generalized dimensions D_q to study the effect of image manipulation such as digitization and thresholding. They reduced the range of q from 0 to 5 (covered in increments of 0.2) because they considered that within this range errors are relatively small.

Saucier and Muller⁵³ studied the choice of the scaling range by selecting the range based on the best Chi-square statistics. Recently, Saucier and Muller⁵⁴ proposed a systematic method to choose the scaling range for multifractal analysis and illustrated it with pore space of sedimentary chalks. They described $\chi(q,\delta)$, $\tau(q)$ and D_q and then defined a "global" generating function that was obtained from several samples of equal size, from which the $\chi(q,\delta)$ was previously calculated. The next step is to obtain the global $\tau(q)$ among the intervals that satisfies the well-known multifractality conditions for $\tau'(q)$ and $\tau''(q)$.⁵⁵ The intervals that satisfy these conditions are selected and then the reduced Chi-square of the regression is calculated individually; the one that presents the minimum value in the statistic test applied is selected. They stressed that further work should be done on this methodology. Other issues that require further investigation are whether a relatively small image (e.g., 512×512 -pixel size) is representative of a pore system, and if instead of several replicates in a same image a better resolution can improve the results. Another possible problem is that thresholding could vary among replicates, creating more variation.

IV. SCALING OF PORES IN SOILS AND ROCKS

Among the most commonly estimated fractal dimensions from images of soil pore systems are the mass fractal dimension and the fractal dimension of the pore–solid interface (surface fractal dimension).^{8,12,13,56–63} In more rare cases, the capacity and spectral dimensions have also been estimated.^{12,64} Generalized fractal dimensions have been used to characterize images of preferential flow patterns in field soils. Baveye et al.⁷ used the information dimension (D_I) and the correlation dimension (D_C) to sow the influence of image manipulation on the values of the generalized and of the mass and surface dimensions. This work was the first to apply the concept of generalized dimensions to images of soil profiles, and could be used as a model for studies with images of soil sections.

In the first application of multifractal concepts to images of natural porous media, Muller and McCauley¹⁶ and Muller et al.³⁷ demonstrated that the structure of pore space in sedimentary rocks can be successfully characterized by multifractal analysis. In Muller and McCauley,¹⁶ values of $f(\alpha)$ and their error bars were calculated based on ten replicate images from the same thin section. Differences in texture are reflected in the amplitude of the multifractal spectra ($f(\alpha)$) calculated for each rock (Figure 2.5). Muller et al.⁶⁵ found that the information dimension (D_1) was linearly correlated (positive slope) to air permeability. The authors hypothesized that higher D_1 values



FIGURE 2.5 The $f(\alpha)$ spectra for three different sedimentary rocks reflect different texture of the rocks. (From Muller, J. and McCauley, J.L., *Transport Porous Media*, 8, 133, 1992. With permission.)