Importance of spatial structures in advancing hydrological sciences

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[1] Spatial patterns of land surface and subsurface characteristics often exert significant control over hydrological processes at many scales. Recognition of the dominant controls at the watershed scale, which is a prerequisite to successful prediction of system responses, will require significant progress in many different research areas. The development and improvement of techniques for mapping structures and spatiotemporal patterns using geophysical and remote sensing techniques would greatly benefit watershed science but still requires a significant synthesis effort. Effective descriptions of hydrological systems will also significantly benefit from new scaling and averaging techniques, from new mathematical description for spatial pattern/structures and their dynamics, and also from an understanding and quantification of structure and pattern-building processes in different compartments (soils, rocks, and land surface) and at different scales. The advances that are needed to tackle these complex challenges could be greatly facilitated through the development of an interdisciplinary research framework that explores instrumentation, theory, and simulation components and that is implemented in a coordinated manner.

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1. Introduction

[2] Spatial heterogeneity of land surface and subsurface characteristics, such as soil properties, topography and vegetation that are present over a hierarchy of scales, largely control hydrological processes from the subpore up to the catchment and regional scale [*Blöschl and Grayson*, 2001]. Its proper identification and definition as well as the thoughtful representation of key characteristics in corresponding hydrological models remain a challenge for future research.

[3] In particular, the spatial structure and organization of properties and states exhibit significant control over water related land surface and subsurface fluxes. Examples are manifold and range over several spatial orders of magnitude. For example, subsurface heterogeneity resulting from biologic activity or geological, geomorphological and soil forming processes plays a critical role in the onset as well as the growth and/or decay of instabilities and preferential flow systems in the saturated as well as in the unsaturated zone. Results from numerical simulation, lab and field experiments indicate that both the onset of instabilities and preferential flows and their subsequent growth and decay are intimately related to the spatial structure of the heterogeneities. Without a clearer understanding of the processes that control the onset and propagation of preferential flow systems and instabilities, resultant pattern as well as flow rates and pathways cannot currently be predicted with sufficient accuracy to facilitate management of subsurface water or contaminant flow.

[4] The coupling of surface and subsurface water fluxes and the triggering of preferential flow systems under local saturated conditions is currently recognized as an important mechanism in controlling infiltration processes, runoff generation and water quality related processes at the hillslope and watershed scale [*McDonnell et al.*, 2001; *Zehe and Blöschl*, 2004]. As an example, *Grayson et al.* [1997] analyzed the differences between organized and randomly distributed initial conditions in a rainfall-runoff modeling experiment. Two patterns of initial soil moisture deficits, each with the same second-order statistics, but one spatially random and the other organized by a wetness index, produce very different runoff responses and infiltration pattern to given rainfall intensities.

[5] Hydrological synthesis is needed to develop methods for identifying and characterizing the spatial organization of surface and subsurface properties that are critical for watershed management; for developing methods of representing these structures in hydrological models; and for exploring the utility of the approaches across disparate watersheds. The discussions to follow briefly review different approaches of representing spatial variability, discuss some emerging methods for identifying and quantifying spatial organization and using such information in hydrological models. Finally, the manuscript identifies the key challenges that exist for advancing the incorporation of structural information in hydrological sciences.

2. Representing Spatial Variability

[6] There are different approaches to conceptualize the fact that our natural environment, including aquifers, soils and landscapes, is typically structured at any scale. A common approach is the definition of a "representative

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elementary volume (REV)" [*Bear*, 1972] whereby the structural units and relevant processes associated with a particular length scale can be adequately represented. The mean value of relevant REV properties becomes invariant under translation of the observation scale, and the structural properties can be defined by second-order statistics. If the physical process description at the subscale is well known, a variety of asymptotic methods, such as stochastic methods (e.g., perturbation methods) [*Dagan*, 1989; *Gelhar*, 1993] or volume averaging and homogenization techniques [*Attinger*, 2003; *Lunati et al.*, 2002; *Papanicolaou and Varadhan*, 1981; *Whitaker*, 1999], exist to derive effective descriptions and parameterizations for an equivalent homogeneous medium at the larger spatial scales.

[7] However, it is more the rule than an exception that an REV cannot be derived within natural systems. Material properties and states often change with spatial scale as a result of structural units of different lengths that are interlaced and nested in a continuous hierarchy. Also, physical and biological processes within structural units often differ significantly (as, for example, turbulent water flow in macropores versus Darcy flow in the soil matrix) and are characterized by intrinsic process length scales that are inconsistent with an REV length scale. To this end, material properties and processes are inherently preasymptotic, rendering a consistent mathematical upscaling framework that requires an equivalent homogeneous media difficult, if not impossible, to obtain.

[8] A concept to handle such multiscale heterogeneity has recently been proposed by *Vogel and Roth* [2003]. Their "scaleway" approach suggests that "structure" at any scale can be separated from "texture," which can be described using effective material properties. Given an appropriate process description within the structural units (e.g., Stokes equation at the pore scale; Richards equation at the continuum scale), the effective properties (or an effective system behavior) at a given observation scale can be derived computationally. To illustrate this concept, *Vogel and Roth* [2003] used X-ray tomography to identify different structural units within a soil column and then used soil bulk density, measured by X-ray absorption as a proxy, for obtaining (hydraulic) properties within different structural units. Using numerical modeling, they showed that the "scaleway" concept resulted in a robust approach, whereby even an approximate knowledge of the continuous form of structural elements with the associated texture properties and process descriptions enabled a reasonable prediction of water flux through the system.

[9] Successful extension of this concept from the soil column to the hillslope and catchment scale represents a hydrological synthesis challenge, as it will require advanced approaches to identify controlling structures and structure forming processes, appropriate upscaling theory, and numerical modeling approaches that incorporate the structural complexities at the watershed scale. It is possible, for example, to translate system behavior (including the effects of structural heterogeneity at one scale) into an effective description for the "textural" properties at the next upper spatial level. Such a translation might best be achieved by developing generalized theoretical scaling concepts, which can transfer the heterogeneous system to preasymptotic scales, and then combining the generalized method with the scaleway concept, where the identification of controlling structural units is one of the essential ingredients.

[10] Several approaches could be invoked for such upscaling, including spatial filtering [*Attinger*, 2003; *Beckie et al.*, 1996]. Spatial filtering divides any heterogeneous model into a filtered or coarse grained model characterized by a filtering length scale and the corresponding residuum. The residuum could serve as an error estimator for the upscaling procedure. The large flexibility of filtering procedures allows for resolving details of processes where necessary and for diminishing spatial resolution where possible. This meets the needs of the scaleway concept of *Vogel and Roth* [2003]. On the catchment scale, *Zehe et al.* [2006] proposed a dynamical upscaling by employing a physically based numerical model structure, that was previously shown to portray hydrological dynamics at different scales. Using the structure and output of the model, they derived constitutive relations for describing subsurface flow and runoff production within a "representative elementary watershed" approach that has previously been introduced by *Reggiani et al.* [1998, 2000].

[11] The development of most efficient "effective" descriptions for surface and subsurface water and solute fluxes at any given scale will initially make use of and advance stochastic averaging and filtering techniques as far as possible. When reaching theoretical (or practical) limits of these approaches, it will be the explicit consideration of structural units including appropriate flow descriptions that will allow to further proceed in any application.

3. Identification and Quantification of Spatial Structures

[12] One major challenge within this framework will be the identification of controlling structures over a range of spatial scales. Such identification could be realized by current developments in geophysical (e.g., ground penetrating radar, or electrical resistance tomography) and remote sensing techniques (e.g., multispectral and hyperspectral imaging, thermography or passive and active microwave) mounted on ground, aircraft, and satellite platforms for mapping horizontal as well as vertical aquifer, soil, and vegetation structures. However, there is still a need for those techniques to be further developed in order to improve their flexibility, reliability and use for interpreting hydraulic properties as well as their spatial and temporal resolutions [*Hubbard and Rubin*, 2005].

[13] Another emerging approach for obtaining surface and subsurface structural information is the use of available knowledge on structure forming processes, such as those associated with the disciplines of pedology, soil biology and geomorphology, to expand limited measurements to a continuous representation of spatial patterns. This approach was recently raised within the scope of "hydropedology" [*Lin*, 2003] and is based on the fact that spatial heterogeneity of nature is typically not the result of some random process but the consequence of certain mass and energy fluxes.

[14] In order to handle spatial structures within a mathematical, hydrological modeling framework, it would be helpful to reduce the complex and/or incomplete structural

information to a small but meaningful set of numbers. This would not only allow for the direct comparison of different spatial structures, but also provide a handle on the quantification of temporal changes of structures that could possibly be directly related to water, energy and solute transport processes. Examples include the distribution of land use and vegetation characteristics or the highly variable pattern of internal states, such as groundwater levels, soil moisture, surface temperature or plant physiological properties. There are various approaches that could be used for a reduced mathematical description of structural complexity.

[15] 1. Fractal concepts [*Mandelbrot*, 1982] have quite successfully been applied for describing multiscale rainfall properties [*Sivakumar*, 2001] but were so far less helpful in quantifying surface and subsurface water and solute transport processes [*Blöschl and Grayson*, 2001].

[16] 2. The successful quantification of topology using a connectivity function has been introduced in the area of catchment hydrology by *Western et al.* [2001]. Its relevance to gas diffusion and solute transport characterizing topology using Euler characteristics has recently been demonstrated within a series of application by *Vogel and Roth* [1998] and *Vogel et al.* [2002]. Its extension with methods and measures from mathematical morphology, such as Minkowki numbers and functions derived from morphologic erosion [*Vogel et al.*, 2005], provide an extensive set of measures that can relatively easily obtained from detailed two- and three-dimensional imaging technologies.

[17] Changes of these measures over time, indicating changes in the spatial connectivity of, for example, soil moisture, surface temperature, or photosynthetic activity fields, might yield information about system fluxes or system states at the observational scale. For example, surface soil moisture patterns have been shown to be structured during wet periods and randomly distributed under drying conditions [*Grayson et al.*, 1997], which indicates a possible system switch that might be detectable from advanced geophysical or remote sensing technology.

[18] We believe that a synthesis of advanced remote sensing and geophysical techniques, effective descriptions of structure-building processes from neighboring disciplines, and quantification of structures and their temporal changes using methods from mathematical topology will largely enhance progress in predicting hydrological processes at the catchment scale.

4. Challenges for Advancing Hydrological Sciences

[19] This discussion suggests that the use of structural information for improving the description and prediction of hydrological processes is complex, and involves the characterization of properties and processes, the development of scaling techniques and the advancement of further mathematical approaches and technologies. Some of the key components associated with these challenges include the following.

[20] 1. One component is understanding how to appropriately use geophysical and remote sensing data sets to estimate spatial heterogeneity and structures and to monitor fluxes by modern measurement and monitoring networks. Such activities may benefit from close collaborations between hydro(geo)logists, geophysicists, physicists and engineers by linking field measurements from new sensor technologies with new modeling approaches and theories across different spatial scales.

[21] 2. Understanding structure-building processes relevant to hydrological processes will make the integration of neighbor disciplines, such as geology, geomorphology, pedology, (micro)biology, and ecology, essential.

[22] 3. New (up)scaling theories and hydrological modeling concepts embedded into uncertainty estimation frameworks [*Beven et al.*, 2000, 2001; *Schulz and Beven*, 2003] will be needed that can incorporate any information of structural complexity. Implementation of improved watershed modeling approaches should be assisted by progress in modern computer hardware and software as well as communication technology and visualization technologies (e.g., massive parallel and grid computing, data storage, digital image analysis) provided by computer and software scientists.

[23] Most of these challenges can only be approached and solved by an extensive interdisciplinary framework that is implemented in a coordinated way. For example, the availability of three-dimensional soil moisture fields with extremely high temporal and spatial resolution, in conjunction with river runoff measurements from nested gauges and catchment scale evapotranspiration (ET) or trace gas fluxes are currently not available. This is partly due to current limitations in measurement technologies (such as larger-scale ET measurement), but also to due to limited coordination of different disciplines.

[24] Current national and international research initiatives including the establishment of interdisciplinary, long-term and multiscale networks of observatories as well as platforms for terrestrial environmental synthesis offer excellent venues for exploring the instrumentation and theory that are needed to develop this frontier area.

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