1: On the Fundamentals of Hydrological Sciences

GÜNTER BLÖSCHL

Institute for Hydraulic and Water Resources Engineering, Vienna University of Technology, Vienna, Austria

Although there is no universal theory in hydrology that starts from first principles, the various branches of hydrology show numerous common threads. They relate to the nature of the processes including their space–time variability, the general principles of hydrological measurements, and the types of methods for representing hydrological processes in a quantitative way, either statistically or deterministically. The purpose of this article is to provide some common ground for this Encyclopedia to highlight the particularities of the hydrological sciences.

WHAT ARE THE FUNDAMENTALS IN HYDROLOGY?

Hydrology is the science that deals with the waters above and below the land surfaces of the Earth; their occurrence, circulation and distribution, chemical and physical properties, and their interaction with their environment, including their relationship to living beings (NRC, 1991). Owing to its central focus on water, the science of hydrology holds a unique place in the field of earth system science, intimately intertwined with other water-related disciplines such as meteorology, climatology, geomorphology, hydrogeology, and ecology. As an applied science, hydrology is highly relevant to the management of the world's water resources and water quality and for the prediction and mitigation of water-related natural hazards such as floods and droughts. Thus, hydrology is an exciting field of study.

What now are the theoretical underpinnings of hydrology, what are the fundamentals? In many disciplines, a treatise on the fundamentals starts with a universal "big picture" theory on which there is consensus among scientists. From theory one would then move into the specific questions of how to measure, how to conceptualize more specific processes and how to model them. The theory would give guidance on all of these and would be further developed on the basis of feedbacks from them. Hydrology is different in this respect from some other natural sciences. There is no universal theory of hydrology that starts from first principles. There are different concepts for different parts of the hydrologic cycle and different spatial and temporal scales. The various branches of hydrology, however, do show remarkable parallels. The nature of hydrological variability is remarkably similar for different processes and the measurement techniques available to probe them have similar characteristics as well. Both have distinctly shaped the descriptive and predictive methods that have evolved in this discipline over the years and they ultimately control the accuracy of hydrological predictions. The common threads of the various hydrological subdisciplines may hence be a useful starting point for a presentation of fundamentals in the hydrological sciences. These are the subject of **Part 1: Theory, Organization and Scale** of this Encyclopedia. The objective of Part 1 and this chapter in particular, is to provide some common ground for the remainder of the Encyclopedia and to bring out some of the hydrological concepts that are common to them.

HYDROLOGICAL PROCESSES – WATER CYCLES AND WHY ORGANIZATION IS AN ISSUE

The most influential concept in hydrology has undoubtedly been the water cycle that links the movement of water on the Earth's surface with subsurface waters and water in the atmosphere. It not only provides a general layout

Encyclopedia of Hydrological Sciences. Edited by M G Anderson.

of the main mechanisms but also allows formulation of how much water there is in the different compartments (in the atmosphere, on the land surface, and in the subsurface) and how fast the exchange takes place (*see* **Chapter 2, The Hydrologic Cycles and Global Circulation, Volume 1**; **Chapter 25, Global Energy and Water Balances, Volume 1**; **Chapter 29, Atmospheric Boundary-Layer Climates and Interactions with the Land Surface, Volume 1**; **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**; **Chapter 103, Terrestrial Ecosystems, Volume 3**; and **Chapter 173, Global Water Cycle (Fundamental, Theory, Mechanisms), Volume 5**). Obviously, the movement of water is more complex than an exchange of water between different boxes. In fact, one could argue that there are many water cycles, as water moves around at many space and time scales. There is a multitude of different pathways (*see* **Chapter 4, Organization and Process, Volume 1**; **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**; **Chapter 80, Erosion and Sediment Transport by Water on Hillslopes, Volume 2**; and **Chapter 113, Hyporheic Exchange Flows, Volume 3**). Water may fall as rain in the same regions as it is evaporated, a process termed *local moisture recycling*, and water may remain much longer in the ground in some places than in others, so there are huge differences in the time scales as well. The global water cycle is linked to the global energy cycle through evapotranspiration on the land surface. Understanding the water cycle is also a key element in understanding fluxes of matter (e.g. nutrients, sediments) that are driven by the water fluxes (*see* **Chapter 79, Assessing Uncertainty Propagation Through Physically based Models of Soil Water Flow and Solute Transport, Volume 2**; **Chapter 80, Erosion and Sediment Transport by Water on Hillslopes, Volume 2**; and **Chapter 96, Nutrient Cycling, Volume 3**).

One of the fascinating observations on hydrological processes is their astounding variability at all scales, in both space and time. At the smallest scales of interest in hydrology, water fluxes and composition may vary between individual pores of the soil, and climate and hydrological processes vary over continental scales as well. Infiltration may vary over seconds and groundwater tables may vary over decades and more. Within these limits, variability abounds (*see* **Chapter 3, Hydrologic Concepts of Variability and Scale, Volume 1**, **Chapter 7, Methods of Analyzing Variability, Volume 1**). Virtually any quantitative approach to this problem requires the selection of a limited set of spatial and temporal scales. Any particular choice of time and space scales has a major influence on which aspects of this hydrological variability are perceived (*see* **Chapter 8, Fractals and Similarity Approaches in Hydrology, Volume 1**; **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**; and **Chapter 134, Downward Approach to Hydrological Model Development, Volume 3**).

Hydrological variations are driven by variations in physiographic factors such as climate, soils, vegetation, topography, geology, as well as by human activity. These externally driven variations then propagate through hydrological systems (Sivapalan *et al.*, 2001), leading to an extremely rich variety of hydrological patterns apparent at different temporal and spatial scales, in different physical settings. This means that the patterns of variability are linked to their causal processes. Although Schumm (1991) notes that due to nonlinearities multiple processes can lead to the same form, patterns and form should be able to provide an indication of the processes that have led to them. Examining patterns will hence assist in making more representative measurements and more accurate predictions (*see* **Chapter 8, Fractals and Similarity Approaches in Hydrology, Volume 1**, **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**).

The drivers also imply that the variability one encounters in hydrology is usually not fully random but organized in various ways (Gutknecht, 1993). Types of organized variability include continuity (Baird, 1996) in time and space which is often related to storage processes. Another type is the presence of zones with boundaries between them (Woo, 2004). Still another type of organization that seems to exist at all scales is preferential flow – in the voids of the soil, in macropores, and in both porous and hard rock aquifers at a range length-scales (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**; **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**; and **Chapter 147, Characterization of Porous and Fractured Media, Volume 4**). On the land surface, preferential flow occurs from micro rills to streams in the landscape (Rinaldo *et al.*, 1993). The counterpart to preferential flow in the time domain is episodic behavior, that is, a concentration of activity over short periods or events in a range of processes including runoff, erosion, and sediment transport. Other types of organization include self-similar organization, where small-scale variability looks similar to large-scale variability; the observation that extremes or outliers occur more often than would be expected on the basis of standard statistical distributions (Hurst, 1951; Mandelbrot and Wallis, 1968); and periodic variability at diurnal, annual, and multiannual scales (*see* **Chapter 3, Hydrologic Concepts of Variability and Scale, Volume 1**). Clearly, these organized patterns are linked to the processes that drive and modulate them.

The presence of spatial and temporal organization in hydrologic variability has important ramifications for measurements. If it were not for surface runoff concentrated in streams, it would be almost impossible to measure the water flowing from a catchment area. On the other hand, preferential flow in the soils and aquifers tends to make point samples unrepresentative. Organization also has important ramifications for representing the variability in a quantitative way. The presence of organization or patterns in hydrological systems has been seen as an indication that they are, what Dooge (1986) refers to as *middle number systems* or *systems of intermediate complexity*. In these systems, there are too many components to be dealt with by classical (deterministic) mechanics and just not enough components to be dealt with by statistical methods similar to those of statistical mechanics. Thus in hydrology, both statistical and deterministic methods are appropriate depending on the type of variability one means to capture as well as the questions one asks. This type of system behavior also means that interactions of processes will be important at many scales (*see* **Chapter 4, Organization and Process, Volume 1**) such as interactions between surface water and groundwater (*see* **Chapter 113, Hyporheic Exchange Flows, Volume 3**); between soils, vegetation, and the atmosphere (*see* **Chapter 12, Co-evolution of Climate, Soil and Vegetation, Volume 1**); between land surface hydrology and terrestrial ecosystems at large (*see* **Chapter 101, Ecosystem Processes, Volume 3**, **Chapter 103, Terrestrial Ecosystems, Volume 3**); between evaporation and flood generation (*see* **Chapter 122, Rainfall-runoff Modeling: Introduction, Volume 3**; Sivapalan *et al.*, 2005); between floods and stream morphology (*see* **Chapter 86, Measuring Sediment Loads, Yields, and Source Tracing, Volume 2**); between snow processes and boundary-layer atmospheric processes (*see* **Chapter 160, Energy Balance and Thermophysical Processes in Snowpacks, Volume 4**); between catchment hydrology and soil development (*see* **Chapter 4, Organization and Process, Volume 1**); and between runoff and landscape evolution (*see* **Chapter 4, Organization and Process, Volume 1**). Not all the feedbacks will be apparent to an observer, as often observations are limited to a set of scales that reveal only a few of the many processes that are present in the hydrological environment (*see* **Chapter 6, Principles of Hydrological Measurements, Volume 1**, **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**).

FUNDAMENTAL EQUATIONS – ARE THERE ANY?

Yes, there are fundamental equations in hydrology and the most important one is the mass balance of water over a given volume and time interval. This is termed *the water balance equation*. It is so central to hydrology that some observers have noted that the task of hydrology is to solve the water balance equation. The classic example of its application is the estimation of the average evapotranspiration of a catchment over a long period from rainfall and streamflow measurements, but it is widely applied at a range of space and time scales. The water balance equation is the only equation that can be called a *hydrological equation* in its full right and is applicable to the scales hydrologists are interested in.

Another fundamental equation is energy balance, which is mainly used when interfacing with the atmospheric sciences and plays a key role in hydrology in the context of evaporation and snow processes. The remaining balance equation of classical mechanics, momentum balance, is mainly used in representing open channel flow in a fluid mechanics context (*see* **Chapter 5, Fundamental Hydrologic Equations, Volume 1**, **Chapter 135, Open Channel Flow – Introduction, Volume 4**). These balance equations – fundamental as they are – are not sufficient to fully describe the dynamics of hydrologic systems. Hence additional equations, termed *empirical flux laws*, are needed. Most of them have four characteristics:

1. Many of the flux laws used in hydrology are based on flux–gradient type relationships. Examples are Darcy's law (water flux in aquifers – hydraulic potential gradient), Fick's law (matter flux both in aquifers and in surface waters – concentration gradient); the flux-gradient method (vertical water vapor flux in the atmosphere – vapor pressure gradient); and the Chezy equation (water flux in surface waters – energy gradient).
2. Most of them have some element of empiricism, although derivations from more fundamental laws are possible. For example, Darcy's law can be derived from the Hagen–Poiseulle equation for laminar flow in capillaries. The assumptions in the derivations may imply that their applicability is limited to particular conditions, which may not always be clear. Through simplifications additional empiricism may creep in. In the Darcy example, the geometry of soil pores is far more complex than a bundle of tubes. Thus, an empirical element will usually be involved in the flux laws, for example, through empirical parameters in the flux – gradient relationships.
3. Most of the flux laws have been taken from other disciplines such as fluid mechanics, soil physics, and the atmospheric sciences, and hence
4. Many of them apply to the point scale, that is, a sample size that is small relative to the systems hydrologists are interested in. They have been derived for minute control volumes that are amenable to laboratory experiments and the application of continuum mechanics (Hubbert, 1956), rather than for the objects of interest in hydrology (catchments, aquifers, river reaches, regions, etc.). In principle, equations can be formulated for lumped systems at larger scales and catchment models are a good example (*see* **Chapter 10, Concepts of Hydrologic Modeling, Volume 1**). However, repeatable experiments under exactly controlled conditions are not possible at these scales, which challenges the universality of these equations. Another example is the stream order laws of Horton (Horton, 1945) and

other authors that describe the statistical characteristics of the map view patterns of stream networks. While important in fluvial geomorphology they have had limited influence on the hydrological sciences themselves.

Out of the four points listed, the fourth is probably the most important one for hydrology as a science (Blöschl and Sivapalan, 1995). Point scale equations can be straightforwardly extended to catchments, aquifers, reaches, and so on *provided* the boundary conditions are known and the media characteristics are known spatially (e.g. uniform) at the scale of the equations. This means there may be finer scale variability such as grains and voids not resolved by the equations, but at larger scales where the equations apply the media are considered uniform. For example, the mass balance equation for small volumes in aquifers can be combined with Darcy's law, which gives a diffusion type differential equation. It is then possible to use concepts from continuum mechanics to solve for the variable of interest (e.g. hydraulic head), given the initial and boundary conditions (*see* **Chapter 5, Fundamental Hydrologic Equations, Volume 1**).

The challenge in the hydrological sciences is that hydrological systems are never completely uniform in terms of their parameters, fluxes, and states and are often not even approximately uniform. Although there are ways of dealing with their variability – either explicitly through distributed (deterministic) models or implicitly through upscaling methods – it is not a straightforward exercise. Additional assumptions need to be made about the variability, both in space and time and, often most importantly, about the nature and locations of the flow paths, but much of this information may be "unknowable" in practice (Savenije, 2001). One is then far removed from the fundamental equations and on the "thin ice" of models for a particular application. This is also one of the reasons why models generally need to be calibrated to the particular site of interest (Freeze and Harlan, 1969).

There are two classical paradoxes in hydrology – dispersion in the subsurface tends to deviate from Fick's law (Levy and Berkowitz, 2003), and runoff events mainly contain old (pre-event) water (Kirchner, 2003). Both paradoxes are related to small-scale equations not being applicable at the larger hydrological scale because of media heterogeneities (*see* **Chapter 13, Pattern, Process and Function: Elements of a Unified Theory of Hydrology at the Catchment Scale, Volume 1**, **Chapter 152, Modeling Solute Transport Phenomena, Volume 4**).

The issues of heterogeneity relate to the empirical flux laws but not to the balance equations as the latter are valid at any scale. Issues of heterogeneity also arise in specifying initial and boundary conditions from measurements. Notwithstanding these problems, point scale equations along with continuum mechanics are an essential basis for hydrology (*see* **Chapter 5, Fundamental Hydrologic Equations, Volume 1**) both for understanding system dynamics and for making quantitative predictions.

HYDROLOGICAL MEASUREMENTS – WHY SIZE MATTERS

With the exception of the laboratory case, experiments are not repeatable under exactly the same boundary and initial conditions in hydrology; it is nature that does the experiments (Dunne, 1998; Zehe and Blöschl, 2004). Because of this, observations generally depend on the climatic and hydrological context. From the 1960s, there have been numerous national and international programs, initially on experimental catchments, to examine similarities and differences across different climatic and hydrological conditions (*see* **Chapter 121, Intersite Comparisons of Rainfall-runoff Processes, Volume 3**, **Chapter 203, A Guide to International Hydrologic Science Programs, Volume 5**). These programmes have provided valuable insights but generalizing the findings beyond the areas of interest has always been difficult (*see* **Chapter 133, Rainfall-runoff Modeling of Ungauged Catchments, Volume 3**). Each aquifer, catchment, and river reach – in fact each episode – seems to have particularities that cannot be specified in full detail. Because of this, in addition to going into process detail for a single site (which has been the traditional approach), contrasting different catchments and different aquifers based on what has been termed *comparative hydrology* has recently been singled out as an important avenue to progress in hydrology (*see* **Chapter 3, Hydrologic Concepts of Variability and Scale, Volume 1**, **Chapter 121, Intersite Comparisons of Rainfall-runoff Processes, Volume 3**), with the eventual goal of a common method for assessing and quantifying hydrological similarity.

A key to the progress in the natural sciences is the ability to measure variables to an accuracy that is useful and at the scales one is interested in. This is another challenge in hydrology as, in many instances, the processes of interest are of a scale that is not directly amenable to the measurement techniques available (Klemeš, 1983). Most measurements are collected by point samples, while processes occur over catchments, aquifers, and landscapes. In the time domain, one is often more interested in (temporal) averages (e.g. sediment and nutrient loads) than in the snapshots as can be obtained in dedicated experiments (*see* **Chapter 92, Water Quality Monitoring, Volume 3**). Because of this, much of hydrology is constrained by measurement techniques (*see* **Chapter 122, Rainfall-runoff Modeling: Introduction, Volume 3**). This is particularly the case for spatial distributions which are more difficult to sample than time series (Grayson and Blöschl, 2000), especially for hydrological dynamics that take place beneath the ground surface.

Over the years, hydrologists have developed ways of dealing with the space–time variability and the scale incompatibility of measurements in various ways. The most efficient methods have been ways of aggregating the variability by prudent measurements. The classical examples are measurements of runoff from catchments that aggregate the within-catchment variability and pumping tests of aquifer transmissivities that aggregate the subsurface hydraulic variability within the depression cone (Anderson, 1997). More elaborate measurements require either laboratory analyses with typical sample sizes of 1 dm^3, although tracer experiments and irrigation/flume experiments can deal with somewhat larger scales of tens of meters. Because of this, the sampling design in terms of the space and time scales is critically important for capturing the natural variability in a representative way in addition to ensuring the accuracy of the instruments (*see* **Chapter 6, Principles of Hydrological Measurements, Volume 1**). In long-term monitoring, where networks are operated by national hydrographic services, space and time scales are usually large, while in dedicated field experiments organized by groups of scientists, space and time scales tend to be small, although, recently, a number of large-scale field experiments have been undertaken (*see* **Chapter 203, A Guide to International Hydrologic Science Programs, Volume 5**). In the latter, remote sensing methods play an important role as they are able to sample at finer spatial scales and wider areas than has been traditionally possible in hydrology (*see* **Chapter 47, Sensor Principles and Remote Sensing Techniques, Volume 2**). With recent advances in monitoring techniques from small-scale computer tomography to large-scale remote sensing methods as well as better logistics (*see* **Chapter 6, Principles of Hydrological Measurements, Volume 1**), measurements are increasingly able to capture wider scale ranges, but a scale problem remains for which statistical (nonprocess-based) and deterministic (process-based) upscaling methods have been developed (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**, **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**).

THE STATISTICAL APPROACH – STATISTICS, SELF SIMILARITY, AND UP/DOWNSCALING

There are two types of approaches to representing hydrologic systems, statistical, and deterministic. In both of them, data play an important role and both of them have their merits. The statistical approach is warranted if random variability (i.e. variability we are unable to interpret/predict in detail) prevails (*see* **Chapter 7, Methods of Analyzing Variability, Volume 1**; **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**; **Chapter 10, Concepts of Hydrologic Modeling, Volume 1**; and **Chapter 125, Rainfall-runoff Modeling for Flood Frequency Estimation, Volume 3**). It represents the bulk information (frequency, distribution, dependence) not the details (spatial and temporal occurrence, dynamics). In the statistical approach it is not usually possible to take causal processes into account, which renders the extrapolation potential more limited than that of the deterministic approach, but extrapolation may not be needed for the application at hand and it is the main method used in many applied hydrologic problems. On the other hand, the statistical approach may be able to deal with systems that are too complex to be dealt with in a deterministic way.

A range of statistical techniques for representing variability are in use in hydrology. Typical steps in a sequential analysis of statistical variability are (i) looking at the data, (ii) analyzing the statistical distribution of the data, (iii) analyzing the first and second order moments (including an analysis of statistical dependence), and (iv) analyzing the data by more elaborate methods such as series expansion (*see* **Chapter 7, Methods of Analyzing Variability, Volume 1**). In these steps increasingly more complex descriptions are introduced. The second moments (variance and correlation coefficients) are of particular importance in hydrology as they are a measure of spread and hence variability of a variable. The classical example is the representation of the spread of a plume of concentration by the second moments. In a temporal (and spatial) context, the second moments can be used to represent the continuity of correlated time series (and correlated random fields) through correlation functions or variograms. In the time domain, the correlations can be used for stream flow forecasting (time series analysis), in the space domain for spatial estimation using geostatistical methods (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**). Series expansions go a step further by representing the variable of interest by a sum of deterministic functions of random variables. To the latter type of methods belong spectral analysis, wavelet analysis, principal component analysis, and empirical orthogonal functions. Their main value in hydrology lies in the reduction of the dimensionality of the system to assist in identifying the main controls if the patterns are not apparent in large data sets (*see* **Chapter 7, Methods of Analyzing Variability, Volume 1**).

The presence of patterns or organized variability is not always considered a favorable property in statistical analyses. They can involve nonstationarity, outliers, non-Gaussian (non-normal) behavior, and thresholds, which are all characteristics commonly encountered in hydrological data but not compatible with the usual statistical methods (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**). This is particularly an issue when extreme values (floods, precipitation extremes, low flows, extreme concentrations) are analyzed by statistical methods (*see* **Chapter 37, Rainfall Trend Analysis:**

Return Period, Volume 1; **Chapter 125, Rainfall-runoff Modeling for Flood Frequency Estimation, Volume 3**). Analyses of extremes are of particular relevance in applied hydrology and water resources management. On the other hand, organization tends to produce striking similarities across scales. Little wiggles look like big ones, statistically, and short ones like long ones. The remarkable thing is that whatever hydrologic variable is examined, it more often than not turns out that there exists similarity to the same variable examined at a different scale, at least over a certain range of scales. This is termed *self similar or fractal behavior* (*see* **Chapter 8, Fractals and Similarity Approaches in Hydrology, Volume 1**) and is related to the more general observation, that there is variability at all scales with the strength of variability (e.g. quantified in terms of the second moment) increasing with scale. In the past decades, statistical fractals have been widely used in many branches of hydrology, as they are appealing because of three main reasons. First, they deal with the presence of variability over a wide range of scales, which is consistent with observations. Second, this type of behavior can be related, at least qualitatively, to the dynamic behavior of nonlinear systems, which is an interesting paradigm for hydrological processes. Third, and perhaps most important for practical applications, fractal concepts lead to parsimonious descriptions of rainfall, landscapes, drainage networks, geologic media, and so on. This means that the statistical models only involve a few parameters and these can be estimated more robustly than the more numerous parameters of traditional concepts. Some of the fractal methods are based on the first and second moments (*see* **Chapter 7, Methods of Analyzing Variability, Volume 1**) but others involve more complex descriptions.

Statistical methods, including fractal concepts, can be used efficiently to address the scale incompatibility of hydrological processes, measurements, and predictions. They lend themselves to transferring information between various scales, for example, between point scale measurements and catchment scale prediction; or large-scale model output and small-scale predictions. These methods are termed *upscaling and downscaling methods* (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**). The first generic task of upscaling/downscaling is to derive the statistics of a variable at one scale from the statistics of the same (or another) variable at another scale. Methods range in complexity from regressions between the variables at different scales to upscaling theory of stochastic hydrogeology (*see* **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**). The second generic task is to generate spatial patterns (or time series) given the statistical characteristics of the variable one means to represent. This can be either through interpolation between a number of samples or, alternatively, various disaggregation methods where one is interested in obtaining a number of realizations of the variable of interest that all exhibit the same statistics as the data. Some of these methods focus on the second moments by making use of correlation functions or variograms (*see* **Chapter 7, Methods of Analyzing Variability, Volume 1**, **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**).

A range of statistical methods are available for upscaling point rainfall to catchments, for disaggregating rainfall in time, for downscaling the output of global circulation models to the scale of catchments, to relate the flood characteristics of catchments of different sizes, to transfer soil moisture across scales both in a catchment and climate modeling context, and for characterizing and generating subsurface media (*see* **Chapter 9, Statistical Upscaling and Downscaling in Hydrology, Volume 1**). One of the more general observations used in many of the statistical upscaling methods is that aggregation makes processes appear smoother, so variability decreases with aggregation area.

The statistical upscaling/downscaling approach does not attempt to represent the processes in full detail but rather relies on (lumped) summary descriptions of variability. Similar to other statistical methods, this has the benefit of robustness but at the expense of limited extrapolation potential. Alternative upscaling methods exist that involve equations of the underlying process dynamics in various branches of hydrology including dynamic hydrologic models (*see* **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**), land–atmosphere interactions (*see* **Chapter 29, Atmospheric Boundary-Layer Climates and Interactions with the Land Surface, Volume 1**), soil water flow (*see* **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**), and stochastic subsurface hydrology (*see* **Chapter 147, Characterization of Porous and Fractured Media, Volume 4**, **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**).

THE DETERMINISTIC APPROACH – MODEL CONCEPTS AND WHY UPSCALING AND DOWNSCALING IS NEEDED

The alternative to the statistical approach is the deterministic approach, which, likewise, has numerous merits. Deterministic relationships can be formulated in a causal way by making use of the fundamental equations and hence can be used for examining "what happens if" questions in a more reliable way than is typically possible with statistical methods. The downside, however, is that the processes may easily become too complex, so care needs to be taken to limit the models to those processes that are tractable and/or for which sufficient data are available. In terms of their application, there are two main uses of deterministic models – explanatory models for furthering our understanding of a particular system and predictive models for producing estimates of some future or changed state. In both instances, there exists a range of model types, from lumped to spatially distributed, from low dimensional to high dimensional involving many parameters. The simplest ones are based on input–output relationships of the area of interest, the intermediate ones on some degree of understanding (conceptual models), and the most complex ones are based on the fundamental equations discussed earlier (*see* **Chapter 10, Concepts of Hydrologic Modeling, Volume 1**; **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**; and **Chapter 134, Downward Approach to Hydrological Model Development, Volume 3**).

Model conceptualization and building usually follows a set number of steps including collecting and examining data and other evidence, assessing which processes may be important for the problem at hand, designing a scheme of the most important process dynamics in the modeler's mind, designing a mathematical model to represent these concepts, calibrating the model by using the data of the region, and testing the model by a separate data set of the same region. If the testing satisfies the modeler's expectations, then the model is ready for use, otherwise one or more of the steps need to be repeated (*see* **Chapter 10, Concepts of Hydrologic Modeling, Volume 1**; **Chapter 122, Rainfall-runoff Modeling: Introduction, Volume 3**; and **Chapter 155, Numerical Models of Groundwater Flow and Transport, Volume 4**). An important component of the model building process and model application is the assessment of the model and data uncertainty to create confidence in the reliability of the model and model predictions (*see* **Chapter 10, Concepts of Hydrologic Modeling, Volume 1**, **Chapter 79, Assessing Uncertainty Propagation Through Physically based Models of Soil Water Flow and Solute Transport, Volume 2**).

In many subdisciplines of hydrology, spatially distributed deterministic models are currently used in a routine way both for addressing practical water resources issues and for more theoretical analyses. The tremendous computing power that is available today facilitates the application of high-resolution models and there exists sophisticated software, particularly for subsurface hydrology and open channel flow. While the usefulness of these models is undisputed, there does remain significant uncertainty with the predictions for several reasons including data limitations and the model formulation (*see* **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**, **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**, Grayson *et al.*, 1992). Specifically, the scale issues discussed earlier in the context of fundamental hydrological equations play an important role here, as the empirical flux laws used in these models are indeed point scale equations (Beven, 1989). Awareness of these issues has triggered research into upscaling methods that are able to deal with unknown (small scale) spatial variability in the context of deterministic models. Much of the recent interest started in the 1970s with the early work of A. Freeze and L. Gelhar on aggregating the groundwater flow equation, based on a stochastic approach (*see* **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**), and picked up additional momentum in the 1980s when it was realized that the spatial heterogeneity of the land surface is important for atmospheric models (Gelhar *et al.*, 1977; Eagleson, 1986; Shuttleworth, 1988; **Chapter 32, Models of Global and Regional Climate, Volume 1**, **Chapter 177, The Role of Large-Scale Field Experiments in Water and Energy Balance Studies, Volume 5**). Those branches of hydrology where the basic equations are known with some degree of confidence (e.g. groundwater flow and transport) have had significant progress, but in other areas such as catchment hydrology and hill slope hydrology progress has been slower (Blöschl, 2001). The upscaling methods are either based on volume averaging or ensemble averaging (i.e. averaging all possible realizations on the same location) of the underlying equations. The aggregation methods tend to work very well if (i) the scale of the natural variability to be averaged (such as grains) is small as compared to the scale of the variability to be explicitly represented (such as geologic formations), and (ii) if the small-scale variability is random and does not exhibit organized patterns. Hydrologic variability tends to exhibit organized patterns such as preferential flow and variability tends to occur at all scales, so the upscaling methods have not been used as widely in practice as would be merited by their theoretical underpinnings. The variability within each grid cell of distributed models is hence dealt with in a number of alternative ways including the effective parameter method and statistical schemes for representing this variability (*see* **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**). The most sophisticated methods of dealing with these scale issues have been developed in subsurface hydrology (*see* **Chapter 66, Soil Water Flow at Different Spatial Scales, Volume 2**; **Chapter 147, Characterization of Porous and Fractured Media, Volume 4**; and **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**), and to a lesser degree in land–atmosphere interactions (*see* **Chapter 29, Atmospheric Boundary-Layer Climates and Interactions with the Land Surface, Volume 1**), although promising research is underway in catchment hydrology as well (*see* **Chapter 11, Upscaling and Downscaling – Dynamic Models, Volume 1**).

LINKING IT ALL TOGETHER – FEEDBACKS AND ELEMENTS OF A THEORY

Over the past decades there has been a trend in the hydrological sciences for a more comprehensive representation of hydrological processes, moving from an isolated description of one particular component of the hydrologic cycle to integrating hydrology with biogeochemical processes (KNAW, 2005). To a large degree, this is reflected in the many articles of this encyclopedia that deal with process links. This trend has been triggered both by the increase in computing power and a realization that feedbacks in the hydrological cycle may be more important than traditionally acknowledged, particularly for climate impacts. Changes in development paradigms in society seem to have played a major role also **Chapter 203, A Guide to International Hydrologic Science Programs, Volume 5**; Falkenmark, 1991). Feedbacks are manifold and occur at many scales, and they involve a range of other disciplines. In the feedback between the water and energy balances at the land surface, soil moisture plays a crucial role. At longer time scales, there exist feedbacks between hydrology and landscape evolution and feedbacks between hydrology and soil formation (*see* **Chapter 4, Organization and Process, Volume 1**). Feedbacks between hydrological water dynamics and biological processes occur at many scales and in many ways, for example, in subsurface flow and transport through microbial activity (*see* **Chapter 105, Microbial Transport in the Subsurface, Volume 3**), in soil formation (Jenny, 1980), in the vegetation dynamics at the land–atmosphere interface (*see* **Chapter 12, Co-evolution of Climate, Soil and Vegetation, Volume 1**) and in erosion processes (*see* **Chapter 80, Erosion and Sediment Transport by Water on Hillslopes, Volume 2**), and through biofilm and macrophyte dynamics in open channel flow and transport (e.g. Battin and Sengschmitt, 1999; Stephan and Gutknecht, 2002). One avenue to address feedbacks has been to link the various processes by coupled models (Bronstert *et al.*, 2005). The strength of this avenue is that the experience with models for each of the processes to be coupled is usually available, but model complexity may limit the practical applicability. The other avenue has been to make the feedbacks themselves a focus of theoretical, quantitative research and this seems to be an emerging area of hydrology, particularly the interactions of vegetation, land surface hydrology and climate (*see* **Chapter 12, Co-evolution of Climate, Soil and Vegetation, Volume 1**). Through transpiration and photosynthesis, the vegetation links the energy, water, and biogeochemical cycles. A number of strategies have been put forward to explain the functioning of vegetation dynamics such as those based on ecological optimality hypotheses (Eagleson, 1998; **Chapter 12, Co-evolution of Climate, Soil and Vegetation, Volume 1**).

This line of research focusing on feedbacks may assist in addressing a certain tendency of fragmentation of the subdisciplines in hydrology with papers "digging the same hole deeper" prevailing over comprehensive views as pointed out by some analysts (Burges, 1998). Although diversity of approach has great advantages and has probably been one of the strengths of the hydrological sciences, it is also important to stimulate a process of seeing how one picture fits with another. Hydrologists are now actively thinking about what may be the elements of a theory of hydrological sciences (*see* **Chapter 13, Pattern, Process and Function: Elements of a Unified Theory of Hydrology at the Catchment Scale, Volume 1**). Most hydrologists would probably agree that theories for some hydrologic processes exist – a linear theory of the rainfall runoff relationship (Dooge, 1973), a theory of infiltration (e.g. Smith *et al.*, 2002), a theory of stochastic hydrogeology (*see* **Chapter 154, Stochastic Modeling of Flow and Transport in Porous and Fractured Media, Volume 4**), but a comprehensive hydrologic theory in its own right is still lacking. It is important that a theory is different from a model in many respects – a theory would have to apply to a variety of circumstances, for example, a range of climates, geological settings, and a range of scales. Similar to a model, one would expect it to be predictive and it must be falsifiable. From a theory one would expect that it has been so thoroughly tested and developed that we know there is indeed some range of phenomena for which they give correct predictions *every time*. With current hydrologic models this does not seem to be the case. These theories would always remain part of our understanding of hydrology, even when new findings take us beyond them in certain ways. The theory would not be invalidated, but rather extended, by new findings. Clearly, the status of a theory is more than that of a model.

There may be still some way until a formulation of this theory becomes viable, but there is value in speculating about elements that may assist in putting it together (*see* **Chapter 13, Pattern, Process and Function: Elements of a Unified Theory of Hydrology at the Catchment Scale, Volume 1**). A new theory may involve an increased focus on interactions and feedbacks between different processes such as those involving vegetation, as this would entail a broadening of the scientific perspectives. To address the generalization issue, a theory may use comparative hydrology (*see* **Chapter 3, Hydrologic Concepts of Variability and Scale, Volume 1**) to develop a common method for assessing and quantifying hydrological similarity through comparisons between catchments in different hydrologic regimes. The theory would have to be valid for all these regimes. Patterns of hydrological response should perhaps be given particular attention to isolate the processes that have led to them, to reconcile the catchment functioning with the observations, and for testing hypotheses about process interactions and feedbacks. The level of complexity of a theory will clearly be an important consideration. An elegant, parsimonious theory may be favored over a more complex one provided it captures the essential complexity as suggested by the Occam's razor principle (Sivapalan *et al.*, 2003). In this respect, characteristic scales and scaling concepts (Skøien *et al.*, 2003) that focus on the order of magnitudes (similar to fluid dynamics) may assist. In a broader Earth Science context one may wonder where the place is of hydrology in the realms of physics and biology (Sivapalan, 2003). Harte (2002) noted: "Physicists seek simplicity in universal laws. Ecologists revel in complex interdependencies. A sustainable future for our planet will probably require a look at life from both sides". In a similar vein it is likely that hydrology will have to adopt some of the more complex and less universal concepts ecology is rich in, in addition to the traditional quest for physical concepts. For a hydrological theory to become influential, it will likely have to combine elements from both physics and ecology.

Acknowledgments

I would like to thank the many individuals who have shaped my own evolving ideas on hydrology over the years, in particular, Murugesu Sivapalan, Rodger Grayson, and Dieter Gutknecht. I owe much to all of them. I am indebted to Murugesu Sivapalan who contributed to this article through numerous discussions and to Alfred Paul Blaschke, Uwe Haberlandt, Ralf Merz, Dan Moore, Kurt Roth, Jan Szolgay, David Tarboton, Andrew Western, and Ross Woods for offering advice and many constructive criticisms, which have helped to substantially improve the article. Funding from the Austrian Academy of Sciences Project HÖ 18 is gratefully acknowledged.

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