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Key Points:

- Five decades of research on process-based hydrological modeling are reviewed
- Main themes are physical and mathematical consistency, rigorous numerics, and integrated models
- Research challenges discussed include model coupling, data assimilation, and subgrid variability

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Physically based modeling in catchment hydrology at 50: Survey and outlook

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Abstract Integrated, process-based numerical models in hydrology are rapidly evolving, spurred by novel theories in mathematical physics, advances in computational methods, insights from laboratory and field experiments, and the need to better understand and predict the potential impacts of population, land use, and climate change on our water resources. At the catchment scale, these simulation models are commonly based on conservation principles for surface and subsurface water flow and solute transport (e.g., the Richards, shallow water, and advection-dispersion equations), and they require robust numerical techniques for their resolution. Traditional (and still open) challenges in developing reliable and efficient models are associated with heterogeneity and variability in parameters and state variables; nonlinearities and scale effects in process dynamics; and complex or poorly known boundary conditions and initial system states. As catchment modeling enters a highly interdisciplinary era, new challenges arise from the need to maintain physical and numerical consistency in the description of multiple processes that interact over a range of scales and across different compartments of an overall system. This paper first gives an historical overview (past 50 years) of some of the key developments in physically based hydrological modeling, emphasizing how the interplay between theory, experiments, and modeling has contributed to advancing the state of the art. The second part of the paper examines some outstanding problems in integrated catchment modeling from the perspective of recent developments in mathematical and computational science.

1. Introduction

The advent of numerical modeling in hydrology coincides roughly with the birth of *Water Resources Research* (WRR). The first years of the journal document a rapid transition from electric analog and physical models to mathematical models. Early simulation studies in both subsurface [e.g., *Freeze and Witherspoon*, 1966] and surface [e.g., *Woolhiser and Liggett*, 1967] hydrology were to have a great influence on research directions in hydrology over the next half-century. To commemorate the 50th anniversary of WRR and to signal its contributions to process-based modeling in hydrology, we look back at developments in experimental, theoretical, and computational hydrology that have shaped the current state of the art in physically based catchment hydrological models (section 2), and we provide an outlook on current challenges and trends in the ongoing effort to cast these models into a rigorous and robust mathematical, physical, and numerical framework (section 3).

The roughly chronological survey allows us to trace significant advances and to mark the emergence of specialized subfields such as stochastic hydrology, parameter estimation, topographic analysis, and data assimilation. Our focus is mainly on flow processes, reflecting the traditional, central problem of rainfall-runoff partitioning in catchment hydrology, although relevant developments in solute transport will also be included. Numerical modeling of solute mass transfer and transport phenomena has been guided more by problems of soil and groundwater contamination and remediation, but in recent decades solute transport has played an increasingly prominent role in catchment hydrology, as it is essential for interpreting isotope tracer studies, for addressing travel time issues, and for incorporating geochemical and ecological phenomena in interdisciplinary models. An additional focus of the paper is on integrated surface/subsurface hydrological models (ISSHMs), as this is an area of much recent research and provides a platform for discussing developments in physically based interdisciplinary modeling, which extend beyond water flow and solute transport at the catchment scale toward multiphysics or Earth system models at much larger scales. In section 2, we review mainly WRR papers, but important contributions from other sources are also covered, especially for specialized topics and integrated, multiprocess modeling. Section 3 considers the literature from a broad range of sources and disciplines.

The models of interest are based on mass and momentum conservation principles formulated as partial differential equations (PDEs) and resolved by numerical techniques. We devote particular attention to correct representation of physical processes and their interactions, and to robust and efficient numerical techniques for space and time discretization, linearization, and coupling. Our prototype PDEs are the Richards equation (RE) for variably saturated subsurface flow, the advection-dispersion equation (ADE) for solute transport, and the Saint-Venant or shallow water equations (SWE) for overland and channel routing. The term "catchment scale" is used loosely to comprise field plots, hillslopes, and watersheds.

2. Progress Over Five Decades

This first part of the paper provides a bibliographic survey of process-based numerical modeling in hydrology over the past half-century and tracks the issues and milestones that have stimulated its progress. In the first two sections we look at very early models and at early examples of the importance of the dialogue between observation and simulation. Numerical techniques and challenges are examined in section 2.3, and developments in four important subfields are considered in section 2.4. The evolution toward integrated (e.g., surface/subsurface hydrology) and interdisciplinary (e.g., ecohydrology) models is reviewed in sections 2.5 and 2.7, respectively, while case studies that illustrate integrated or coupled phenomena are discussed in section 2.6.

2.1. Early Models

While the modeling studies in surface and subsurface hydrology published in the first five years of WRR [*Guitjens and Luthin*, 1965; *Grace and Eagleson*, 1966; *Ragan*, 1966; *Freeze and Witherspoon*, 1966, 1967, 1968; *Woolhiser and Liggett*, 1967; *Foster et al*., 1968; *Huggins and Monke*, 1968; *Onstad and Brakensiek*, 1968; *Pinder and Bredehoeft*, 1968; *Freeze*, 1969; *Hanks et al*., 1969; *Hornberger et al*., 1969; *Pinder and Jones*, 1969] not surprisingly reflect the constraints of this nascent field (e.g., simplified equations or geometrically simple domains or rudimentary discretization techniques), they also introduce procedures and raise issues that have become some of the trademarks of hydrological modeling: concern with heterogeneity, nonlinearity, and hysteresis; verification of models against analytical solutions or laboratory experiments; calibration of models against some observed response of the system; invocation of strict conservation principles; numerical discretization guided by physical features of the system being modeled; application of dimensional analysis to elucidate similarity relationships; and exploitation of the flexibility of numerical models to test hypotheses and investigate parameter sensitivities. Amidst these early studies, those of *Freeze* [1969], *Hanks et al*. [1969], and *Freeze and Banner* [1970] are also prescient on integrated saturated/unsaturated zone modeling, emphasizing physical and mathematical continuity of processes and addressing specified flux (rainfall/evaporation) and specified head (ponded water) boundary conditions that can switch type during the course of a simulation, with an air dry analog to saturation for the switching threshold during evaporation. Although these analyses were conducted with a relatively simple one-dimensional (1-D) model under homogeneous and isotropic soil conditions, the vision for a more ambitious, larger scale integrated framework is quite evident in these papers, and is conceptualized in *Freeze and Harlan* [1969].

Additional major contributions to RE-based modeling at the catchment scale were made in the early 1970s. *Freeze* [1971] presented a 3-D finite difference model with a general storage term incorporating confined and unconfined aquifer and unsaturated zone flow in a unified manner. This model was then coupled to a 1-D SWE channel flow model to demonstrate the complexity of the hydrograph separation question, the important role of subsurface flow on the runoff response of a catchment, and the influence and interplay of factors such as antecedent soil moisture conditions, rainfall, hydrogeological properties, and hillslope morphology on this response [*Freeze*, 1972a,1972b]. In a subsequent study, *Stephenson and Freeze* [1974] incorporated snowmelt processes into the runoff generation picture. The connection between the governing equations for surface (river) flow, subsurface (groundwater) flow, and solute transport was made by *Guymon* [1970] and *Guymon et al*. [1970], who drew attention in particular to the common diffusion-convection nature of the respective mass conservation equations for these domains. Early attempts at coupled hydrological models include those of *Bresler* [1973] and *Bredehoeft and Pinder* [1973] for flow and transport processes, *Pinder and Sauer* [1971] and *Konikow and Bredehoeft* [1974] for stream and aquifer dynamics, and

Smith and Woolhiser [1971] for overland flow and soil infiltration. This latter paper also discusses at length the important role of the land surface saturation or ponding status in regulating rainfall-runoff partitioning and the need for a dynamic boundary condition to properly handle this exchange. By contrast, interaction with atmospheric processes in early unconfined aquifer models was treated via infiltration and evaporation boundary conditions imposed on the free surface [*Neuman and Witherspoon*, 1970a].

Numerically, finite element techniques make their first WRR appearance in the papers of *Guymon et al*. [1970] and *Neuman and Witherspoon* [1970a,1970b, 1971] and quickly gain popularity for their greater flexibility in treating complex geometries and properties compared to finite difference schemes [*Pinder and Frind*, 1972]. Simple, computationally light, or parsimonious models have always played an important role in hydrology, and with this the use of more complex physically based models in intercomparison studies to assess the assumptions and limitations of the former class of models [*Hornberger et al*., 1970; *Mein and Larson*, 1973]. There are also early examples of coupling or conjunctive use of simplified and more rigorous models, representing different compartments of a domain or system, for instance the coupling presented in *Pikul et al*. [1974] between a 1-D RE model for vertical flow in soils and a 1-D Boussinesq model for lateral aquifer flow. This approach has been very popular in subsequent multiprocess and interdisciplinary models that integrate, either loosely (e.g., one-way passing of information) or tightly (with coupled equations and feedbacks), various submodels into a larger, comprehensive model. Finally, dedicated software tools and platforms to facilitate code building, modularization, and integration, widely used in the development of current generation open source and community models [e.g., *Wu et al*., 2014; *Clark et al*., 2015], find a progenitor of sorts in *Williams and Hann* [1972].

2.2. Lessons From Laboratory and Field Experiments

Progress in hydrological modeling has proceeded concomitantly with experimental research, the latter providing evidence for and insight into processes, mechanisms, and theories, as well as the data needed to set up and run diagnostic and predictive simulations. The strengths, successes, limitations, and failings of models vis-à-vis experiments have been and continue to be vigorously debated in the hydrological community, in defense of experimental hydrology early on [*Hewlett et al*., 1969], but soon enough calling into question modeling tenets as well [*Loague and Freeze*, 1985; *Beven*, 1989; *Grayson et al*., 1992; *Smith et al*., 1994]. No one would disagree that scientific progress requires a constant dialogue between measurement, analysis, and simulation [*Seibert and McDonnell*, 2002; *Kirchner*, 2006], or that one of the key strengths of physically based hydrological models is their ability "to assist in the analysis of data, to test hypotheses in conjunction with field studies, to improve our understanding of processes and their interactions, and to identify areas of poor understanding in our process descriptions" [*Grayson et al*., 1992]. This is the exploratory role of a mathematical model [*Larsen et al*., 2014], as important as its operational role as a forecast, prediction, and management tool.

Several of the early modeling studies mentioned in the previous section also included laboratory or field testing, with good agreement reported between measurements and model predictions [*Foster et al*., 1968; *Hanks et al*., 1969; *Freeze and Banner*, 1970; *Smith and Woolhiser*, 1971]. Additional studies along this vein include those of *Giesel et al*. [1973] for vertical flow in a homogeneous sand column including hysteresis effects, *Mein and Larson* [1973] for infiltration dynamics before and after surface ponding, *Vauclin et al*. [1979] for flow across the water table using a 2-D saturated/unsaturated zone model rather than the more limited free surface approach, *Pickens and Gillham* [1980] for 1-D unsaturated flow and solute transport under hysteretic conditions, and *Nieber and Walter* [1981] for the 2-D RE applied to a sloping soil. The seminal field studies of *Horton* [1933], *Betson and Marius* [1969], and *Dunne and Black* [1970] identified the main mechanisms of runoff generation (infiltration excess and saturation excess) and the concept of variable source areas that are very responsive to storm events. These mechanisms and responses can be routinely handled by integrated physically based models, whereas simpler or more conceptual models will often be limited to a single mechanism or will require distinct representations for different mechanisms.

As field and laboratory experiments became more elaborate, seeking to capture a wider range of natural settings and with improved measurement and monitoring capabilities, model formulations and modeling practices also adapted. The most important facet to emerge from these experimental studies is the ubiquity and high degree of spatial and temporal heterogeneity that occurs under natural field conditions. This has spurred the development of more sophisticated parameter identification procedures, stochastic approaches, and data assimilation techniques that are surveyed in the following sections. Other advances, such as novel theories and models that deal specifically with the problems of preferential flow (through soil macropores and geological fractures, for instance), unstable flow (fingering), averaging and scaling porous media properties, and complex reactive transport phenomena, are briefly reviewed here. Mathematical and computational aspects of these theories and models will be discussed in more detail in section 3.

There is abundant evidence, through both experimental and simulation studies, for the influence of spatio-temporal variability in parameters (including inputs and boundary conditions) on hydrological responses over a range of scales [*Morin and Benyamini*, 1977; *Wilson et al.*, 1979; *Binley et al.*, 1989a; *Julien and Moglen*, 1990; *Woolhiser et al.*, 1996; *Scanlon et al.*, 1999; *Western et al.*, 1999; *Zehe and Blöschl*, 2004; *Fiori and Russo*, 2007; *Didszun and Uhlenbrook*, 2008]. Techniques for averaging or interpolating model parameters such as hydraulic conductivity locally (e.g., between grid cells or elements in a numerical discretization) are presented by *Appel* [1976], *Haverkamp and Vauclin* [1979], *Warrick* [1991], and *Zaidel and Russo* [1992]. At the hillslope and catchment scales, the notion of equivalent parameter values has been investigated [*El-Kadi and Brutsaert*, 1985; *Binley et al.*, 1989b; *Wildenschild and Jensen*, 1999; *Brooks et al.*, 2004], and upscaling, similarity, filtering, and other approaches have been introduced to extrapolate information from local measurements or estimates and to render consistent the measurement and modeling scales [*Warrick et al.*, 1977; *Peck et al.*, 1977; *Beckie*, 1996; *Renard and de Marsily*, 1997; *Efendiev et al.*, 2000; *Cushman et al.*, 2002; *Neuweiler and Cirpka*, 2005].

The presence and roles of preferential flow and fingering in porous media flow and transport dynamics have drawn much attention, owing to the significant measurement and modeling challenges raised by these phenomena [*Duguid and Lee*, 1977; *Mosley*, 1979; *Beven and Germann*, 1982; *Glass et al.*, 1989; *McDonnell*, 1990; *Mulholland et al.*, 1990; *Pearce*, 1990; *Scanlon et al.*, 1997; *Wilcox et al.*, 1997; *Ritsema et al.*, 1998; *Zhou et al.*, 2002; *Beven and Germann*, 2013]. Two-domain models (and related mobile-immobile, dual-porosity, dual-permeability, and bicontinuum conceptualizations) are by now commonly used to deal with fractured media in groundwater hydrology and with macropore flow in catchment hydrology [*Germann and Beven*, 1985; *Sudicky*, 1989; *Gerke and van Genuchten*, 1993; *Zurmühl and Durner*, 1996; *Jørgensen et al.*, 1998; *Laine-Kaulio et al.*, 2014]. The two-domain paradigm has also proven useful in solute transport modeling when reaction kinetics and other nonideal or nonequilibrium mass transfer phenomena needs to be accounted for [*Cameron and Klute*, 1977; *Nkedi-Kizza et al.*, 1983; *Gillham et al.*, 1984; *Brusseau*, 1994; *Gallo et al.*, 1996; *Harvey and Gorelick*, 2000]. Various theories and models to explain and predict the occurrence of unstable flow in unsaturated media have been posited over the years, with the most recent ones favoring saturation or pressure overshoot as a prerequisite mechanism for fingering [*Diment et al.*, 1982; *Eliassi and Glass*, 2001; *Cueto-Felgueroso and Juanes*, 2009; *DiCarlo*, 2013].

The many well-established experimental hillslope and catchment sites throughout the world are founts of valuable data for a wide range of modeling studies. In many cases these sites continue to be monitored and are able to exploit the latest advances in sensor technology (ground-based instruments and networks as well as airborne and satellite platforms) to measure parameters, state variables, and fluxes at improved resolutions and accuracies. Well-documented laboratory and field sites include the Las Cruces trench site [*Hills et al.*, 1991; *Wierenga et al.*, 1991; *Oliveira et al.*, 2006], the Tarrawarra experimental catchment [*Western et al.*, 1999], the macrodispersion experiment (MADE) site [*Harvey and Gorelick*, 2000; *Fiori et al.*, 2013], and the Panola Mountain research watershed [*Freer et al.*, 2002; *Tromp-van Meerveld and McDonnell*, 2006]. Several other experimental studies are described in detail in various journal special issues focused on specific topics (e.g., understanding process dynamics at aquifer-surface water interfaces [*Krause et al.*, 2014]). There are also a number of recent natural and laboratory experiments that have a highly interdisciplinary focus and are assembling extensive data sets on water, energy, and nutrient fluxes across soil/land surface/plant/atmosphere interfaces. Examples include the network of critical zone observatories established in the U.S. [*Anderson et al.*, 2008], the TERENO network of experimental catchments in Germany [*Zacharias et al.*, 2011], the Landscape Evolution Observatory (LEO) at the Biosphere 2 facility near Tucson in Arizona [*Niu et al.*, 2014c], and the Chicken Creek artificial catchment near Cottbus in Germany [*Hofer et al.*, 2012].

2.3. Computational Advances

The numerical techniques used in process-based hydrological modeling typically originate in the mathematics and computation literature and are adapted and further developed for groundwater and surface water applications, often in symbiosis with other engineering and geoscience fields that deal with porous media, coupled and multiphase systems, scale issues, etc. (e.g., petroleum reservoir simulation, nuclear waste disposal, CO_2 sequestration) [*Aziz and Settari*, 1979; *Chavent and Jaffré*, 1986; *Larsson*, 1992; *Pruess et al.*, 2004; *Neerdael and Finsterle*, 2010; *Nordbotten and Celia*, 2011]. As mentioned in section 2.1, finite element techniques quickly established a foothold in hydrological modeling, and this approach has continued to evolve. Subsequent studies have explored particular aspects of finite element methods such as Galerkin-based formulations, different element types and shapes, a variety of basis function classes, coordinate transformations, the handling of sharp fronts, and specialized methods for steady state problems [*Gray and Pinder*, 1976; *Pickens and Lennox*, 1976; *Frind and Verge*, 1978; *Hayhoe*, 1978; *Narasimhan et al.*, 1978; *Frind and Matanga*, 1985]. Other spatial discretization approaches have been proposed that can offer appealing accuracy, efficiency, or ease of implementation advantages under certain conditions (e.g., steady state analyses, large-scale applications). These include integrated finite difference, finite difference with nonorthogonal grids, finite volume, mixed finite element, analytic element, and cellular automata methods [*Narasimhan and Witherspoon*, 1976; *Strack*, 1976; *Putti et al.*, 1990; *Beckie et al.*, 1993; *Eymard et al.*, 1999; *Manzini and Ferraris*, 2004; *Mendicino et al.*, 2006; *Kees et al.*, 2008; *Putti and Sartoretto*, 2009; *An et al.*, 2010; *Mazzia et al.*, 2011]. Traditional finite difference techniques, simple to implement but not so amenable to the geometric complexities of two- and three-dimensional spaces, are instead the most common discretization along the time axis. Other temporal discretization approaches that have been proposed over the years include finite elements, the Laplace transform technique, and spectral methods [*Gray and Pinder*, 1974; *Cheng and Ou*, 1989; *Dunbar and Woodbury*, 1989; *Sudicky*, 1989; *Gambolati*, 1993].

Numerical modeling of Richards' equation faces additional challenges connected to the strong nonlinearity of this equation that arises from the pressure dependence in the soil moisture and hydraulic conductivity parameters. Accuracy and mass conservation can be improved by using alternative formulations of RE or by applying appropriate primary variable transformations [*Celia et al.*, 1990; *Kirkland et al.*, 1992; *Rathfelder and Abriola*, 1994; *Pan and Wierenga*, 1995; *Diersch and Perrochet*, 1999; *Williams et al.*, 2000]. Solving RE requires that the equation be linearized, and Newton-based iterative schemes, including less accurate approximations such as the Picard method, are commonly used for this purpose [*Brutsaert*, 1971; *Huyakorn et al.*, 1984; *Paniconi and Putti*, 1994; *Gustafsson and Söderlind*, 1997; *Casulli and Zanolli*, 2010; *Lott et al.*, 2012], although noniterative approaches have also been proposed [*Paniconi et al.*, 1991; *Kavetski et al.*, 2002; *Ross*, 2003; *Crevoisier et al.*, 2009]. The convergence behavior of an iterative scheme at each time step of the RE solution can be advantageously used to adapt the step size during the simulation, while noniterative schemes can rely on local truncation error estimates to dynamically control the step size [*D'Haese et al.*, 2007]. However, more sophisticated time stepping approaches and other specialized techniques are needed to ensure overall robustness and efficiency of RE solvers, in particular for difficult problems such as dry soil infiltration and highly heterogeneous media [*Hills et al.*, 1989; *Ross*, 1990a; *Harter and Yeh*, 1993; *Forsyth et al.*, 1995; *Pan et al.*, 1996; *Miller et al.*, 1998; *Jones and Woodward*, 2001].

Solving the advection-dispersion equation is also very challenging. Two problems in particular have drawn attention over the years: accurate calculation of groundwater velocities (computed by the flow solver, but needed by the ADE solver) and dealing with advection versus dispersion dominated solute transport processes. The former problem can be dealt with by using higher order and mixed hybrid finite element techniques, control volume approximations, and velocity reconstruction methods [*Yeh*, 1981; *Chiang et al.*, 1989; *Cordes and Kinzelbach*, 1992; *Durlofsky*, 1994; *Mosé et al.*, 1994; *Putti and Cordes*, 1998; *Cordes and Putti*, 2001; *Kees et al.*, 2008], while methods such as upstream weighting (or upwinding), Eulerian-Lagrangian discretization, high order Godunov-type finite volumes as naturally extended by discontinuous Galerkin approaches, and time-splitting have been proposed for accurately resolving the very different numerical behaviors of the advective and dispersive components of ADE [*Sun and Yeh*, 1983; *Cheng et al.*, 1984; *Thomson et al.*, 1984; *Healy and Russell*, 1993; *Perrochet and Bérod*, 1993; *Zhang et al.*, 1993; *Bellin et al.*, 1994; *Mazzia et al.*, 2000; *Saaltink et al.*, 2004; *Rivière*, 2008]. Adding chemical reactions and other mass transfer phenomena to a solute transport model introduces additional numerical difficulties arising from time scale differences between mass transfer and transport dynamics and the complexity of exchanges between multiple species and phases [*Rubin*, 1983; *Valocchi and Malmstead*, 1992; *Miller et al.*, 2013].

For both flow and transport models, numerical discretization in space and time (and linearization if required) reduces the original governing PDEs into a sparse algebraic system of equations. Highly robust and efficient preconditioned Krylov-based methods have evolved to be the most widely used schemes for solving such systems, although other techniques such as strongly implicit, alternating direction implicit, and multigrid procedures have also been proposed [*Trescott and Larson*, 1977; *Gambolati et al*., 1986; *McKeon and Chu*, 1987; *Hill*, 1990; *Larabi and De Smedt*, 1994]. Boundary and initial conditions can greatly influence both the numerical performance of a model and the hydrological responses obtained. The general types of boundary conditions and how to implement them are described in detail in many of the previously cited papers that present complete numerical flow or transport models. A good exposition for a 3-D variably saturated finite element flow model is provided, for example, by *Huyakorn et al*. [1986]. A handful of other studies have examined specific aspects related to boundary and initial conditions, such as the treatment of boundary conditions for flux- versus volume-averaged concentration formulations in ADE models [*Parker and van Genuchten*, 1984], the effects of spin-up initialization for a large-scale integrated hydrologic model [*Ajami et al*., 2014], and the impact on hillslope infiltration when a surface boundary condition becomes no-flow at the end of a rainfall event [*Jackson*, 1992]. Land surface boundary conditions are particularly critical for integrated surface/subsurface hydrological models and will be further discussed in section 2.5.

In addition to improving existing numerical techniques to make water flow and solute transport models more accurate and robust (iterative solvers, hybrid schemes, velocity reconstruction methods, etc), novel approaches are emerging that promise significant gains in computational efficiency and in the ability to account for data and model uncertainty. Computational efficiency is critical as ISSHMs are increasingly applied at larger scales, at finer grid resolutions, or in an ensemble context (i.e., hundreds or thousands of simulations that systematically sample a parameter space—e.g., saturated hydraulic conductivity—or a range of scenarios—e.g., climate change). The idea behind adaptive gridding [*O'Neill*, 1981; *Gottardi and Venutelli*, 1992; *Trangenstein*, 2002; *Esfandiar et al*., 2015] is simple and very appealing in practice—the computational mesh is locally refined where numerical error is likely to be highest (for instance at an infiltration front)—but for complex 2-D or 3-D simulations these local areas can shift very rapidly in space and time. Model reduction techniques [*Morel-Seytoux and Daly*, 1975; *Vermeulen et al*., 2005; *Siade et al*., 2010; *Pasetto et al*., 2011, 2013b; *Leube et al*., 2012; *Li et al*., 2012] seek to project the discretized equations of a numerical model into a subspace of much lower dimensionality (reduced order), but here as well further research is needed to render the techniques applicable to complex simulations that involve highly nonlinear dynamics.

Data assimilation is a powerful methodology that allows model simulations and observation data to be integrated in a dynamically consistent manner, producing better estimates or predictions of a state variable of interest (e.g., stream discharge or groundwater levels) than either of these sources of information (models and data) used on their own [*Kitanidis and Bras*, 1980; *McLaughlin*, 1995, 2002]. Early applications of data assimilation in hydrology focused on integrating remote sensing data into large-scale land surface models, on demonstrating the potential for soil moisture profile retrieval with a 1-D Richards equation, and on assessing simple assimilation schemes in ISSHMs [*Houser et al*., 1998; *Hoeben and Troch*, 2000; *Paniconi et al*., 2003a]. The ensemble Kalman filter (EnKF) [*Evensen*, 2003] and the particle filter [*Smith and Gelfand*, 1992] are the most commonly used data assimilation techniques in hydrological modeling [*Reichle et al*., 2002; *Chen and Zhang*, 2006; *Weerts and El Serafy*, 2006; *Camporese et al*., 2009; *Ng et al*., 2009; *Pauwels and De Lannoy*, 2009; *Hendricks Franssen et al*., 2011; *Pasetto et al*., 2012; *Ridler et al*., 2014]. The ensemble framework used in these assimilation methods to compute the statistical quantities of interest allows EnKF and particle filters to be applied not only for updating model states but also for uncertainty estimation, model performance diagnostics, parameter estimation, and sensor failure analysis [*Van Geer et al*., 1991; *Moradkhani et al*., 2005; *Goegebeur and Pauwels*, 2007; *Liu and Gupta*, 2007; *Hendricks Franssen and Kinzelbach*, 2008; *Sun et al*., 2009; *Trudel et al*., 2014; *Pasetto et al*., 2015]. Advanced computational methods for hydrological modeling, including reduced order modeling and data assimilation, will be further discussed in section 3.

2.4. Other Developments

Table 1 highlights important advances made in the development of physically based models [e.g., *Narasimhan and Witherspoon*, 1976; *Celia et al*., 1990; *Gerke and van Genuchten*, 1993], but also in areas that are highly relevant to hydrological modeling but that have evolved into major fields of their own: characterizing the highly nonlinear constitutive relations in unsaturated media [e.g., *Mualem*, 1976; *Clapp and Hornberger*, 1978]; parameter estimation and model calibration methods [e.g., *Yeh*, 1986; *Gupta et al*., 1998]; catchment and flow path delineation from topographic data [e.g., *Band*, 1986; *Tarboton*, 1997]; and stochastic

Table 1. Ranking by Citation of the WRR Papers Referenced in This Survey[a]

Authors	Year	Title	Number of Times Cited[b]
Mualem	**1976**	**A new model for predicting the hydraulic conductivity of unsaturated porous media**	**1824**
Beven and Germann	1982	Macropores and water flow in soils	950
Gelhar and Axness	**1983**	**Three-dimensional stochastic analysis of macrodispersion in aquifers**	**936**
Clapp and Hornberger	**1978**	**Empirical equations for some soil hydraulic properties**	**871**
Sudicky	**1986**	**A natural gradient experiment on solute transport in a sand aquifer: Spatial variability of hydraulic conductivity and its role in the dispersion process**	**638**
Tarboton	**1997**	**A new method for the determination of flow directions and upslope areas in grid digital elevation models**	**636**
Gelhar et al.	**1992**	**A critical review of data on field-scale dispersion in aquifers**	**624**
Yeh	**1986**	**Review of parameter identification procedures in groundwater hydrology: The inverse problem**	**551**
Carsel and Parrish	**1988**	**Developing joint probability distributions of soil water retention characteristics**	**544**
Freeze	**1975**	**A stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media**	**530**
Celia et al.	1990	A general mass-conservative numerical solution for the unsaturated flow equation	494
Gupta et al.	**1998**	**Toward improved calibration of hydrologic models: Multiple and noncommensurable measures of information**	**494**
Howard	**1994**	**A detachment-limited model of drainage basin evolution**	**449**
Dunne and Black	1970	Partial area contributions to storm runoff in a small New England watershed	445
Carrera and Neuman	**1986**	**Estimation of aquifer parameters under transient and steady state conditions: 1. Maximum likelihood method incorporating prior information**	**418**
Gerke and van Genuchten	1993	A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media	362
Bencala and Walters	1983	Simulation of solute transport in a mountain pool-and-riffle stream: A transient storage model	347
Mackay et al.	1986	A natural gradient experiment on solute transport in a sand aquifer: 1. Approach and overview of plume movement	344
O'Loughlin	**1986**	**Prediction of surface saturation zones in natural catchments by topographic analysis**	**327**
Band	**1986**	**Topographic partition of watersheds with digital elevation models**	**311**
Mein and Larson	1973	Modeling infiltration during a steady rain	309
Zhang and Montgomery	**1994**	**Digital elevation model grid size, landscape representation, and hydrologic simulations**	**309**
Harvey and Bencala	1993	The effect of streambed topography on surface-subsurface water exchange in mountain catchments	305
. . .			
Woolhiser and Liggett	1967	Unsteady, one-dimensional flow over a plane—The rising hydrograph	232
. . .			
Narasimhan and Witherspoon	1976	An integrated finite difference method for analyzing fluid flow in porous media	221
. . .			
Freeze and Witherspoon	1967	Theoretical analysis of regional groundwater flow: 2. Effect of water-table configuration and subsurface permeability variation	209
Freeze	1971	Three-dimensional, transient, saturated-unsaturated flow in a groundwater basin	205
Pinder and Jones	1969	Determination of the ground-water component of peak discharge from the chemistry of total runoff	203

[a]The bold entries pertain to the subfields discussed in section 2.4. The breaks in the sequence ("..." in the first column) extend the list to the 200 citations level with papers dealing specifically with physically based modeling.
[b]Values as of 3 May 2015 from the WRR website link for each paper.

hydrology [e.g., *Gelhar and Axness*, 1983; *Gelhar et al.*, 1992]. Some of the milestone developments in these subfields will be reviewed in this section.

The solution of the Richards equation for flow in variably saturated porous media requires stipulation of the relationship between soil moisture and pressure head and between relative hydraulic conductivity and pressure head. The derivation of suitable soil hydraulic characteristics has thus received much attention, ranging from seminal early studies based on fitting mathematical functions to experimental data, to later more foundational studies that seek links to soil texture, pore structure, and other soil properties, to very recent approaches that incorporate adsorptive water retention and film conductivity under dry soil conditions [*Brooks and Corey*, 1964; *Verma and Brutsaert*, 1970; *Mualem*, 1976; *Clapp and Hornberger*, 1978; *van Genuchten and Nielsen*, 1985; *Carsel and Parrish*, 1988; *Russo*, 1988; *Tyler and Wheatcraft*, 1990; *Kosugi*, 1994; *Perrier et al.*, 1996; *Peters*, 2013]. Simplified forms of the hydraulic functions, for instance exponential relationships, can be useful for obtaining analytical solutions to RE [*Broadbridge and White*, 1988; *Pullan*, 1990; *Srivastava and Yeh*, 1991; *Basha*, 1994]. The most commonly used soil characteristic equations have also been extended to bimodal or multimodal pore size distributions for use in dual-permeability models of joint matrix and preferential flow [*Mohanty et al.*, 1997; *Köhne et al.*, 2002]. Finally, a number of studies have also parameterized capillary hysteresis in the hydraulic functions and have reported favorable comparisons against laboratory data [*Mualem*, 1974; *Hoa et al.*, 1977; *Kool and Parker*, 1987]. Despite its importance, hysteresis is not represented in many ISSHMs, in part because of insufficient experimental data and in part because it acts at a scale too small to be considered in most ISSHM applications.

Model calibration and parameter estimation are crucial to any hydrological modeling endeavor, owing to the difficulties in measuring adequately and accurately system properties and state variables that can be highly variable in space and time and in the uncertainties inherent in any model representation of physical processes. There has been continuous and steady progress in model calibration techniques (and more generally inverse methods) over the past five decades, with the most advanced techniques often developed and tested first for simple (e.g., lumped empirical) models, to be subsequently adapted to more complex distributed and physically based models [e.g., *Neuman*, 1973; *Cooley*, 1977; *Gupta and Sorooshian*, 1983; *Kitanidis and Vomvoris*, 1983; *Kuczera*, 1983; *Sorooshian and Gupta*, 1983; *Sorooshian et al*., 1983; *Carrera and Neuman*, 1986; *Yeh*, 1986; *McLaughlin and Townley*, 1996; *Gupta et al*., 1998; *Senarath et al*., 2000]. For subsurface applications the target parameter is most often the saturated hydraulic conductivity, although there are also examples of parameter estimation for the unsaturated soil hydraulic characteristics [*Kool and Parker*, 1988; *Russo*, 1988; *Mishra and Parker*, 1989]. For PDE-based numerical models the main challenges to robust calibration and estimation regard computational cost, nonunique solutions (ill-posedness), and multiple possible objectives and variables [e.g., *Anderman and Hill*, 1999; *Keating et al*., 2010]. Discharge at a catchment outlet is by far the most widely used response variable for calibrating and validating hydrological models. With an increasing availability of observation data for multiple variables and the increasing number and complexity of processes represented in integrated physically based models, it becomes imperative to conduct sensitivity analyses and to assess model performance against multiresponse data [e.g., *Clark et al*., 2011b; *Brunner et al*., 2012; *Rakovec et al*., 2014]. Response variables should include both integrated measures (e.g., outlet flow rate and solute concentration, total system water storage and solute mass, and total groundwater recharge) and distributed responses (e.g., soil moisture, mass concentration, and exchange fluxes at different points along a sensor network).

Drainage networks can be extracted from topographic or terrain data as represented by a digital elevation model (DEM), with the aid of geographic information systems and other spatial analysis tools. These catchment partitioning algorithms also provide a representation of surface flow paths and a computation of upslope drainage areas. The most widely used procedures are based on uniformly gridded terrain data [*Band*, 1986; *Fairfield and Leymarie*, 1991; *Dawes and Short*, 1994; *Tarboton*, 1997; *Orlandini et al*., 2003; *Orlandini and Moretti*, 2009; *Pelletier*, 2013; *Orlandini et al*., 2014], but other DEM representations such as contour data (vector-based approaches) or triangular irregular networks (TINs) have also been used [*Goodrich et al*., 1991; *Moore and Grayson*, 1991; *Moretti and Orlandini*, 2008]. Overland flow models based on irregular surface grids (vector or TIN) can offer computational advantages (greater efficiency) over uniform grid models. DEM-based criteria for delineating hillslope/valley transitions and overland flow/channel flow regimes have also been developed [*Montgomery and Dietrich*, 1989; *Montgomery and Foufoula-Georgiou*, 1993; *Howard*, 1994; *Orlandini et al*., 2011], as well as algorithms that extend the basic procedures to lake-dominated landscapes [*Mackay and Band*, 1998], tidal channel networks [*Fagherazzi et al*., 1999], and valley bottoms and riparian areas [*Gallant and Dowling*, 2003]. The ready availability of DEM-processed data has facilitated the discretization and parameterization of physically based surface and subsurface models at the catchment scale [*Paniconi and Wood*, 1993; *Julien et al*., 1995], and it has spurred the development of distributed-parameter models based on topographic indices, wetness parameters, and other indicators or predictors of a catchment's saturation response to rainfall events [*O'Loughlin*, 1986; *Barling et al*., 1994]. These distributed models, to some degree inspired by or extensions of the widely used TOPMODEL [*Beven and Kirkby*, 1979], fill a niche in being more sophisticated than lumped parameter models but more parsimonious and computationally efficient than numerical PDE-based models. Notwithstanding the great conveniece of DEM-derived catchment discretizations, there are also important problems related to the representation of topography in hydrological modeling. Subgrid topographic variability effects and changes in attributes (watershed size, width functions, slope-area relationships, curvature, stream channel features) when discretizing a catchment at different DEM resolutions result in significant differences in simulated responses (outlet discharge, water table depths, saturation patterns, etc) [*Wolock and Price*, 1994; *Zhang and Montgomery*, 1994; *Walker and Willgoose*, 1999; *Choi et al*., 2007; *Sulis et al*., 2011b]. Additional challenges are discussed in section 3.2.

Early stochastic approaches in hydrology, whereby key model parameters such as saturated hydraulic conductivity and porosity are represented by probability distributions and sampled through a Monte Carlo procedure, were introduced to examine the impacts of spatial variability on hydrological response and to deal with the difficulties of capturing this response using equivalent (uniform) parameterizations [e.g., *Freeze*, 1975; *Smith and Hebbert*, 1979]. Subsequent developments include analyses based on stochastic differential equations solved by perturbation and other methods, representation of model inputs (e.g., rainfall) as random variables, and generation of random fields for model parameters [*Bakr et al*., 1978; *Freeze*, 1980; *Mantoglou and Wilson*, 1982; *Tompson et al*., 1989]. Various theories, models, and field and laboratory experiments have been described that address specific issues of flow and transport behavior in heterogeneous systems, in the mass transport case focused predominantly on the problem of scale dependence in the dispersivity coefficients and more generally on non-Fickian dispersion phenomena [*Schwartz*, 1977; *Pickens and Grisak*, 1981a,1981b; *Dagan*, 1982; *Gelhar and Axness*, 1983; *Sudicky*, 1986; *Neuman*, 1990; *Gelhar et al*., 1992; *Engesgaard et al*., 1996]. More recently fractional PDEs have been proposed to address anomalous dispersion in solute transport for surface and subsurface applications [*Benson et al*., 2000; *Cushman and Ginn*, 2000; *Zhang et al*., 2005; *Deng et al*., 2006].

2.5. Integrated Surface/Subsurface Hydrological Models

In an early paper on numerical modeling in variably saturated porous media, *Cooley* [1971] commented on the need for a "unified approach to the study of subsurface water flow above and below the water table, because from a fluid dynamic point of view the water table is an artificial boundary." The research communities for groundwater aquifers and for soil zone processes were at the time quite separate, and each had its own modeling approaches. Today, three-dimensional, distributed-parameter numerical models for solving combined formulations of the Richards and groundwater flow equations (as well as the equations for solute transport) are commonplace, and it is the land surface that may be regarded as an analogous boundary (or interface), in this case between the specializations and models of subsurface hydrology, surface hydrology, and atmospheric science/hydrometeorology. An update of the above quote that reflects this shift could be that of *Levine and Salvucci* [1999]: "By treating conditions at the boundaries between groundwater, the vadose zone, and the atmospheric boundary layer as fixed quantities, potentially important feedbacks are ignored. [. . .] The interaction of surface, vadose zone, and groundwater fluxes should therefore be considered in models of watershed-scale hydrologic processes." These modeling shifts respond to needs for greater process understanding, but are also contingent on numerical and computational advances that make it possible to resolve ever more complex systems. In addition, current research in integrated surface/subsurface modeling is also driven by water resource management imperatives [*Winter et al*., 1998]. The management context can add further levels of coupling to a physically based hydrological model, such as optimization and decision analysis techniques [*Gorelick*, 1983; *Cheng et al*., 2009; *Kollat et al*., 2011], but these will not be dealt with in this survey.

Quantitative analysis of the interactions between surface and subsurface waters has a long history in the hydrological literature [e.g., *Theis*, 1941]. Early modeling studies, in addition to those cited in section 2.1, include: *Winter* [1978, 1983], who used 3-D subsurface modeling and appropriate boundary conditions to investigate aquifer and vadose zone interactions with a lake; *Govindaraju and Kavvas* [1991], who coupled overland, channel, and 2-D surface models to assess variable source area dynamics at the hillslope scale; *Nield et al*. [1994], who performed very detailed simulations of the interactions between groundwater and surface water bodies in a vertical section; *Pohll et al*. [1996], who estimated potential infiltration and deep groundwater recharge fluxes from ponded nuclear subsidence craters; *Singh and Bhallamudi* [1998], who examined numerical aspects of an integrated model of 1-D overland flow and 2-D subsurface flow; and *Reggiani et al*. [2000], who introduced the representative elementary watershed concept for deriving catchment-scale conservation equations for integrated hydrologic flows based on the averaging approach of *Hassanizadeh and Gray* [1979]. The current generation of ISSHMs generally features a comprehensive treatment of subsurface (3-D saturated and unsaturated media) and surface (1-D or 2-D overland and channel) flow with two-way coupling between the two domains.

While the groundwater flow and Richards equations are quite standard for the subsurface, the approaches for surface flow are more varied and often consist of some approximation (e.g., kinematic or diffusion wave) of the shallow water equations [*Li et al*., 1975; *Morris and Woolhiser*, 1980; *Viera*, 1983; *Ponce*, 1986; *Govindaraju et al*., 1988; *Ponce*, 1990; *Westerink and Gray*, 1991; *Gottardi and Venutelli*, 1993; *Richardson and Julien*, 1994; *Orlandini and Rosso*, 1996; *Bajracharya and Barry*, 1997; *Heng et al*., 2009], with either a rill flow (1-D) or sheet flow (2-D) paradigm adopted for overland flow [*Zhang and Cundy*, 1989; *Abrahams and Parsons*, 1990; *Hairsine and Rose*, 1992a,1992b; *Abrahams et al*., 1994; *Myers*, 2002; *Howes et al*., 2006]. Both rill and sheet flow approaches need to be more carefully studied in conjunction with ISSHMs, as the spatial averaging to distribute a ponding head over a DEM cell can have important accuracy implications, for instance in nonlinear phenomena such as infiltration-runoff partitioning. Over a longer term, local processes of erosion and sedimentation will determine rill formation and shape, and models based on channel initiation mechanisms [*Perron et al*., 2008; *Smith*, 2010] can be coupled to ISSHMs to capture these processes. Scaling relationships between channel characteristics and discharge are commonly used to parameterize the hydraulic geometry relations in SWE models [*Leopold and Maddock*, 1953; *Orlandini and Rosso*, 1998; *Singh et al*., 2003; *Dodov and Foufoula-Georgiou*, 2004].

Current ISSHMs include InHM [*VanderKwaak and Loague*, 2001; *Smerdon et al*., 2007; *Mirus et al*., 2011], CATHY [*Bixio et al*., 2002; *Camporese et al*., 2010], tRIBS [*Ivanov et al*., 2004], MODHMS [*Panday and Huyakorn*, 2004; *Phi et al*., 2013], HydroGeoSphere [*Jones et al*., 2006, 2008; *Brunner and Simmons*, 2012], ParFlow [*Kollet and Maxwell*, 2006], GEOtop [*Rigon et al*., 2006; *Endrizzi et al*., 2014], PIHM [*Qu and Duffy*, 2007; *Kumar et al*., 2009], IRENE [*Spanoudaki et al*., 2009], Cast3M [*Weill et al*., 2009], PAWS [*Shen and Phanikumar*, 2010], OpenGeoSys [*Delfs et al*., 2012; *Kolditz et al*., 2012], GSFLOW [*Huntington and Niswonger*, 2012], and MIKE SHE [*Hansen et al*., 2013]. Some of these models also extend the surface/subsurface coupling to solute transport (HydroGeoSphere, Cast3M, and CATHY) [*Jones et al*., 2006; *Weill et al*., 2009, 2011; *Mügler et al*., 2011], erosion and sediment transport (tRIBS) [*Kim et al*., 2013], and thermomechanical processes (OpenGeoSys) [*Kolditz et al*., 2012]. The key differences between these various models, aside from the equations and dimensionality used to represent overland and channel flow as mentioned above, will lie in the coupling approaches that are used (e.g., simultaneous versus iterative versus sequential solution of the surface and subsurface equations; first-order exchange term versus boundary condition switching to resolve the fluxes across the surface/subsurface interface). Since each of these models has its own raison d'être and development history, there will of course be many other differences between them, including how the terrain is represented (gridded or TIN, continuous or staggered landscape), the numerical schemes for spatiotemporal discretization and linearization, the diversity and complexity of boundary conditions, and so on. Several classification schemes for integrated surface/subsurface hydrological models have been proposed, and various studies have assessed the different approaches that are used for coupling and resolution of these numerical models [*Morita and Yen*, 2002; *Gunduz and Aral*, 2005; *Kampf and Burges*, 2007; *Dawson*, 2008; *Furman*, 2008; *Ebel et al*., 2009; *Park et al*., 2009; *Dagès et al*., 2012; *Fiorentini et al*., 2015]. When ISSHMs are extended to solute transport, careful attention to coupling strategies and numerical solution techniques is also needed for the flow and transport system in the case where solute concentrations can alter the flow field, as for instance via fluid density variations in saline environments, of which seawater intrusion in coastal aquifers is a classic example [*Voss and Souza*, 1987; *Herbert et al*., 1988; *Oldenburg and Pruess*, 1995; *Putti and Paniconi*, 1995; *Simmons et al*., 2001; *Diersch and Kolditz*, 2002; *Mazzia and Putti*, 2005; *Povich et al*., 2013].

Capturing the full complexity of surface/subsurface interactions is critical in ISSHMs, since the exchanges across the land surface (rainfall and evaporation) [*Camporese et al*., 2010; *Abati and Callari*, 2014; *Liggett et al*., 2014], with a river or stream network (including seepage faces) [*Cooley*, 1983; *Rulon et al*., 1985], and at the bottom or interior of the domain (including tile drains) [*Fipps and Skaggs*, 1989; *MacQuarrie and Sudicky*, 1996; *Rozemeijer et al*., 2010; *Hansen et al*., 2013] can be fundamental determinants of the internal flow and transport dynamics of the system and can cause significant numerical difficulties. The role and handling of the evaporation boundary condition in ISSHMs has not received much attention compared to the treatment of infiltration processes, in part perhaps because of the preeminence of the rainfall-runoff partitioning problem in hydrological modeling. There is a very strong feedback between evaporation and near-surface soil moisture [e.g., *Schmugge et al*., 1980; *Bernard et al*., 1981], and, analogous to what occurs at the instance of ponding during a rainfall event, there is a transition from atmosphere-controlled (stage-one) to soil-limited (stage-two) evaporation as the soil dries. This can be handled via the land surface boundary condition in an ISSHM [e.g., *Camporese et al*., 2014b], but the precise nature of the transition process (gradual versus threshold, for instance) [*Brutsaert and Chen*, 1995; *Salvucci*, 1997] and the importance of factors such as subgrid-scale surface roughness [*Albertson and Parlange*, 1999] will affect how evaporation is parameterized in these models, and requires further study.

Model intercomparison is an important means for assessing the performance and establishing the numerical and physical limitations of competing models. While early studies often focused on comparing very different modeling approaches (e.g., lumped or conceptual versus distributed or physically based) [*Sloan and Moore*, 1984; *Troch et al*., 1993; *Michaud and Sorooshian*, 1994; *Refsgaard and Knudsen*, 1996], more recent efforts have focused on models belonging to a common class and on the establishment of benchmark problems [*Scanlon et al*., 2002b; *Paniconi et al*., 2003b; *Woods et al*., 2003; *Sulis et al*., 2010; *Maxwell et al*., 2014]. Benchmarking is essential for establishing a standard set of test cases and for bringing together the modeling community to directly and openly assess competing formulations, parameterizations, and algorithms [*Smith et al.*, 2004; *Sebben et al.*, 2013]. An early example of a benchmark problem in subsurface hydrology is the Borden sand aquifer in southern Ontario [*Sykes et al.*, 1982; *Mackay et al.*, 1986], which has been used extensively in solute transport investigations and is one of the test cases selected for the Phase 2 ISSHM intercomparison study [*Kollet et al.*, 2015]. This intercomparison effort for physically based, integrated, catchment-scale hydrological models follows similar initiatives in subsurface reactive transport, radionuclide migration, carbon sequestration, land data assimilation, and land surface modeling [*Larsson*, 1992; *Henderson-Sellers et al.*, 1995; *Boone et al.*, 2004; *Pruess et al.*, 2004; *Xia et al.*, 2012; *Steefel et al.*, 2015].

2.6. Case Studies With Physically Based Models

Where formal benchmark test cases and model intercomparison exercises are useful for assessing model capabilities and limitations, any modeling case study based on scenario (synthetic) simulations or on field and laboratory experiments can fulfill a model's exploratory, hypothesis testing role. We illustrate this role via four examples connected to perennially important modeling issues: boundary conditions (hypotheses concerning the impact of processes at and across the soil/bedrock interface); grid resolution (exploring climate change impacts in large-scale applications), unsaturated zone complexities (exploring solute transport mechanisms and controls), and hydrograph separation (hypotheses concerning flow pathways and travel times).

A soil layer on sloping bedrock is a common conceptualization in hydrological modeling at the hillslope and subcatchment scales. At these small scales morphology, vegetation, and climate can all be quite accurately represented, whereas pedology and geology are much more difficult to characterize. Thus further approximations are often introduced regarding the prevailing directions of flow, the degree of impermeability of the soil-bedrock interface, the presence of layers and other inhomogeneities in the soil and aquifer, the influence of the unsaturated zone, and so on. This allows for simplified, even analytical, models to be derived, based for instance on the widely used kinematic wave and Boussinesq equations for groundwater flow in unconfined aquifers [*Guitjens and Luthin*, 1965; *Beven*, 1981; *Smith and Hebbert*, 1983; *Zecharias and Brutsaert*, 1988a,b; *Troch et al.*, 2003; *Chapman*, 2005; *Troch et al.*, 2013]. In physically based integrated modeling there is greater flexibility in how the bottom boundary of a hillslope or catchment is represented, as well as any interface to an underlying bedrock aquifer or other type of layered heterogeneity, and there are tailored numerical schemes for leaky-aquifer systems and groundwater recharge calculation [e.g., *Sahuquillo*, 1983; *Cheng and Ou*, 1989; *Sanford*, 2002; *Scanlon et al.*, 2002a] that can be used without simplifying the model physics. Certainly at larger scales the impermeable bedrock paradigm needs to be relaxed as deeper groundwater flows can contribute significantly to streamflow [e.g., *Frisbee et al.*, 2011]. Moreover field and modeling experiments over a range of scales suggest strongly that the way bottom boundaries, bedrock interfaces, and other layers are treated (impermeable versus leaky or fractured, smooth versus nonuniform with microtopographic relief features, etc) will have a large impact on hydrological response (pressure head distributions, lateral flow connectivity, capillary barrier effects, groundwater recharge and discharge, timing and magnitude of outflow hydrograph peaks, etc) [*Ross*, 1990b; *Montgomery et al.*, 1997, 2002; *Buttle and McDonald*, 2002; *Freer et al.*, 2002; *Uchida et al.*, 2002, 2003; *Katsuyama et al.*, 2005; *Tromp-van Meerveld and McDonnell*, 2006; *Ebel et al.*, 2008; *Broda et al.*, 2011].

ISSHM applications in the literature are mainly aimed at the field, hillslope, and small catchment scales, although there are an increasing number of studies over larger regions ($O(10^3)$ km^2 and higher), even up to the continental scale [*Lemieux et al.*, 2008]. Climate change impact assessment is a typical case of large-scale ISSHM application (e.g., HydroGeoSphere [*Goderniaux et al.*, 2009]; MIKE SHE [*van Roosmalen et al.*, 2009]; ParFlow [*Ferguson and Maxwell*, 2010]; CATHY [*Sulis et al.*, 2011a, 2012]; GSFLOW [*Huntington and Niswonger*, 2012]; PAWS [*Niu et al.*, 2014d]). The hydrological model can either be coupled to an atmospheric model [*Maxwell et al.*, 2011], or be driven by forcing data (precipitation, temperature, etc) derived from regional climate models (RCMs) or general circulation models (GCMs), generally based on Intergovernmental Panel on Climate Change emissions scenarios. Additional input and observation data (evapotranspiration, watershed storage changes, etc) can be obtained from satellites. Since RCMs and GCMs operate at much coarser resolutions than ISSHMs, dynamical or statistical downscaling procedures are generally used to adapt the atmospheric data to the hydrological model grid. Numerical challenges associated with hydrological simulations over very large domains, in addition to obvious computational efficiency issues, include subgrid variability (for topography as mentioned previously, but also for other processes and controls) and mesh skewness and aspect ratio (distortion and imbalance between vertical and horizontal discretizations). Computational efficiency can be addressed by code parallelization, recognized even in early hydrological modeling studies [e.g., *Meyer et al*., 1989] and recently assessed for coupled surface/subsurface models [*Kollet et al*., 2010; *Hwang et al*., 2014; *De Maet et al*., 2015]. For a catchment size of $O(10^3)$ km^2 at $O(10^0-10^1)$ m DEM resolution and $O(10^{-2}-10^{-1})$ m vertical discretization, the numerical grid will have $O(10^9-10^{10})$ cells or degrees of freedom and could only be simulated on massively parallel architectures with highly efficient scaling.

Many very detailed field and modeling case studies of solute transport in unsaturated media have been conducted over the years. This wealth of information bears re-examination as ISSHMs increasingly consider not only flow but also mass transport and transfer phenomena, and since exchanges of water and solutes across the land surface interface will often occur under unsaturated conditions. The numerous issues and challenges addressed in these case studies involve dispersion, hysteresis, anisotropy, air entrapment, fractionation, dry soil phenomena, advanced theories of mixing, and treatment of boundary conditions and surface/subsurface coupling terms. *Butters et al*. [1989] and *Russo et al*. [1989a, 1989b] examined hysteresis effects and the mobile-immobile conceptualization for a bromide tracer experiment conducted in a loamy sand field. *McCord et al*. [1991] investigated the hypothesis of a variable, state-dependent anisotropy in hydraulic conductivity for layered, hysteretic soils. *Wilson and Gelhar* [1981] conducted a perturbation model analysis of solute dispersion and showed that spatial variations in moisture content affect solute plume spreading even without dispersive mixing, and that the rates of solute displacement are typically much smaller than the rates of moisture displacement. *De Smedt and Wierenga* [1984] found that larger dispersion coefficients are needed for unsaturated compared to equivalent (comparable pore water velocities) saturated flow experiments, and that a mobile-immobile model provided a better description of solute breakthrough curves than the standard, single-domain ADE model. For the tritium and bromide tracer experiments at the Las Cruces trench site in a semiarid area of southern New Mexico, standard models gave good prediction of wetting front movement during infiltration but poor prediction of point soil water content and tracer transport [*Hills et al*., 1991; *Wierenga et al*., 1991]. In their synthesis of more than 300 solute transport experiments from the literature, *Haggerty et al*. [2004] concluded that the estimated mass transfer timescale is better correlated to residence time than to pore water velocity and that mobile-immobile models yield reasonable predictions. *Russo et al*. [1998] conducted 3-D experiments and numerical simulations of reactive and passive tracers with consideration also of the roles of atmospheric boundary conditions and water uptake by plant roots. They found that velocity fluctuations enhance lateral solute mixing and slow down longitudinal spreading. Finally, *Havis et al*. [1992] explored solute mixing processes across the surface/subsurface interface under infiltration-runoff partitioning.

Simulation models that allow particle tracking or that provide probabilistic frameworks for computing travel time distributions and flow pathways make it theoretically possible to partition streamflow hydrograph contributions into overland runoff, shallow subsurface flow, and deep groundwater discharge (base flow), although in practice the distinctions may still be difficult to make, because of continual mixing between surface and subsurface waters (e.g., reinfiltration of overland flow) and the dynamic interaction between seepage faces, variable source areas, and the catchment outlet. Nonetheless the problems of travel time estimation, flow path characterization, and hydrograph separation are important ones and are connected to the equally complex problem of discerning preevent (old) and event (new) water contributions to storm runoff and streamflow response. These issues were raised in several early simulation and field studies [*Pinder and Jones*, 1969; *Freeze*, 1972a,1972b; *Hewlett*, 1974; *Pilgrim*, 1976; *Abdul and Gillham*, 1984; *Pearce et al*., 1986; *McDonnell*, 1990], and have been addressed more recently with coupled flow/transport and stochastic models that exploit new theoretical developments, together with experimental studies and other analyses [*Crane and Blunt*, 1999; *McGuire et al*., 2005; *Jones et al*., 2006; *Botter et al*., 2008; *Fiori et al*., 2009; *Botter et al*., 2010; *Park et al*., 2011; *Rinaldo et al*., 2011; *Benettin et al*., 2013; *Partington et al*., 2013].

2.7. Interdisciplinary Models

In this section we go beyond integrated surface/subsurface and flow/transport hydrological models toward models that represent also the interactions between soil, biota, open water, cryosphere, and atmosphere and that can simulate diverse stores and fluxes (water, energy, carbon, CO_2 and other gases, nutrients and other solutes) across a variety of interfaces [*Newman et al*., 2006; *Paola et al*., 2006]. Research in water resources is by its very nature an interdisciplinary endeavor [*Freeze*, 1990], but recent trends extend beyond water resources, connecting hydrology to ecology, meteorology, geochemistry, soil physics, and other disciplines. The case for interdisciplinary research to expand the reach of hydrological science was made early on by *Post et al*. [1998], calling in particular for ecohydrological studies on paired catchments. An important function of interdisciplinary models is the characterization of the spatiotemporal distributions, pathways, and residence times of water and other constituents over a range of scales [*Lin et al*., 2006]. In implementing ecohydrological and Earth system models, challenges arise in maintaining consistency of representation and parameterization amongst submodels, considering also that many of these submodels are not strictly based on mass and momentum conservation principles. There is a tendency to a plug-in approach that allows for rapid inclusion of many disparate process modules. As more processes are integrated, there is inevitable dilution of the overall model's PDE conservation equation basis, with a tendency to think directly in a discretized mode leading to latent pitfalls in terms of, for example, scale representation and overall consistency in formulation.

It will be important to conduct sensitivity and uncertainty analyses for these interdisciplinary models, as they introduce new parameters and feedback channels that will impact individual state variables and overall model responses. Equally important will be model testing and validation via benchmarking as described earlier. Finally, prominence should be given also to mathematically sound model development and analysis. An example of an ecohydrological feedback hypothesis that has been much studied is that groundwater depth and the dynamics of the vegetation layer condition interactions between soil water and atmospheric water content and strongly influence local weather patterns [*Maxwell et al*., 2007; *Juang et al*., 2007; *Maxwell and Kollet*, 2008; *Siqueira et al*., 2009; *de Arellano et al*., 2012; *Gentine et al*., 2013]. In a numerical modeling study incorporating detailed vegetation dynamics, it has been shown that the buffering effects of plant behavior, via for example hydraulic redistribution, are fundamental to correctly capture the full soil-plant-atmosphere feedback cycle and that the vegetation layer impacts cloud formation and rainfall predisposition [*Manoli et al*., 2014; *Bonetti et al*., 2015]. Accurate modeling of vegetation dynamics is fundamental to capturing these effects that can influence both hydrological and climatic simulations; incorrect averaging or parameterization may not produce the appropriate behavior.

The modeling of soil-plant interactions has been a longstanding topic in hydrological research, with early models of root water uptake presented by *Feddes et al*. [1974], *Federer* [1979], and *Molz* [1981] and successfully tested against field data. The role of vegetation in hydrology involves also evapotranspiration, which can be a dominant component in a catchment's water balance. Important dynamics between vegetation, soil, water, and atmosphere therefore occur at both the single plant scale and the field (or catchment) scale. At the catchment scale the spatial distribution of vegetation will to some degree be driven by patterns of water availability [*Thompson et al*., 2011], which are in turn determined by climate and the morphological, geological, and hydraulic properties of the catchment and soils. The most common formulation for root water uptake, still used in current models, is a sink term that incorporates a root density distribution term into Richards' equation. A three-dimensional variant of the root water uptake scheme was introduced and tested in simulations of transient soil water flow around an almond tree by *Vrugt et al*. [2001]. A review of common root water uptake schemes is provided by *Jarvis* [2011]. A simpler approach, albeit applicable only to shallow-rooted vegetation, involves a single threshold parameter that controls the boundary condition switching in an RE-based model between atmosphere-controlled and soil/plant-limited evapotranspiration [*Camporese et al*., 2014b].

More advanced schemes for vegetation-soil-atmosphere interaction include the approach implemented in CATHY by *Manoli et al*. [2014] that accounts for whole plant transpiration and leaf-level photosynthesis in addition to root water uptake, the soil-plant root model of *Mendel et al*. [2002] that includes effects of hydraulic lift (i.e., the transport of water from moist into drier soil layers through plant root systems), and the scheme introduced by *Kroener et al*. [2014] that includes a nonequilibrium relation between water content and water potential in the rhizosphere for handling water flow in both the soil and mucilage. In a computational study, *Schröder et al*. [2009] use grid refinement around the roots to accurately resolve soil-root water interactions. In a different approach to the scaling issue in soil-plant interactions, *Siqueira et al*. [2008] propose an RE-based model that couples radial water movement toward rootlets (millimeter scale, diurnal cycle) to a vertical flow component (meter scale, interstorm timescale). *Ivanov et al*. [2008] couple a model of plant physiology to tRIBS and examine water-energy-vegetation linkages at time scales from hourly to interannual for a semiarid environment. At a larger spatial scale, *Marani et al*. [2006] couple an RE model and a plant water uptake scheme to investigate ecological, hydrological, and morphological interactions in a wetland environment. Several studies have examined the impact of vegetation on overland and channel flows, including *Hammer and Kadlec* [1986] who use a 1-D model of groundwater-stream interaction, *Katul et al*. [2011] who incorporate a flow resistance factor for submerged vegetation into the Saint-Venant equation for flood routing, and *Kim et al*. [2012] who use tRIBS to assess the roles of terrain slope, bed roughness, and other factors on the interactions between submerged vegetation and overland flow.

Important examples of surface-subsurface hydrological and ecological interactions occur at the local scale between river and aquifer and between channel and hillslope and include phenomena in hyporheic zones and lowland catchments [*Cardenas*, 2015]. Surface-subsurface interactions in these environments have implications for riparian ecology (including the health of aquatic habitats) and river restoration efforts. The processes involve not just water flow but also solute transport (including nutrients) and heat transfer. Early studies with physically based models at the river reach scale were aimed at representing pool-and-riffle sequences typical of mountain streams and headwater catchments and at examining the role of streambed topography [*Bencala and Walters*, 1983; *Harvey and Bencala*, 1993; *Springer et al*., 1999; *Saenger et al*., 2005; *Loheide and Gorelick*, 2007; *Cardenas and Gooseff*, 2008]. The stream components of these coupled models are innovative in that they necessarily differ conceptually from open channel models. Additional studies in riparian and lowland environments have examined: links in runoff dynamics from landscape elements to the channel network and the relative contributions of hillslope and riparian zones to streamflow response [*McGlynn and McDonnell*, 2003; *Jencso et al*., 2009]; hydrological connectivity across the hillslope/riparian/channel continuum, threshold runoff responses, groundwater ridging, and hysteretic behavior in catchment storage-discharge relationships [*Bates et al*., 2000; *McGuire and McDonnell*, 2010; *Mahmood and Vivoni*, 2011; *Weill et al*., 2013; *Camporese et al*., 2014a; *Pierini et al*., 2014]; impacts of land clearance (removal of deep-rooted vegetation) in the hyporheic zone on the state of connection between an aquifer and a river [*Banks et al*., 2011]; and flood formation, propagation, and inundation dynamics with a coupled 2-D SWE and saturated groundwater model [*Viero et al*., 2014].

We end this section with a brief mention of other processes, beyond vegetation and root water uptake described above, that have been integrated into hydrological models and ISSHMs, such as large-scale land surface and energy balance dynamics, CO_2 fluxes, and snow processes. As with hydrological modeling, the nature of spatial variability over a range of scales plays an important role in controlling the responses from ecohydrological and other interdisciplinary models. From an experimental standpoint, the complexity of the problem can be perceived from a series of field studies conducted at the Reynolds Creek watershed in Idaho, where *Seyfried and Wilcox* [1995] examine the influence of factors such as shrub cover, soil depth to bedrock, snow drifting, soil freezing, wind, and elevation, each acting at a different characteristic scale, on infiltration, runoff, streamflow, groundwater recharge, snowfall distribution, and other responses. Water exchanges across the land surface are strongly dependent on temperature, in particular for evapotranspiration, and thermal effects can influence subsurface water movement. The full complexity of exchange processes between the soil and the atmosphere is however still far from being understood, but, as discussed in *Bonetti et al*. [2015], needs to be captured correctly in ISSHMs.

Early (pre-ISSHM) examples of coupled subsurface water-heat transport and subsurface-atmosphere modeling include *Milly* [1982, 1984] at the soil column scale (1-D RE-based model) and *York et al*. [2002] and *Maxwell and Miller* [2005] at scales commensurate with regional climate modeling. Coupling of ISSHMs with land surface models that include energy balance and various ecohydrological processes (e.g., carbon exchanges) are described for the ParFlow [*Kollet and Maxwell*, 2008; *Rihani et al*., 2010; *Rahman et al*., 2014], PAWS [*Shen et al*., 2013], and CATHY [*Niu et al*., 2014a, 2014b] models. *Šimůnek and Suarez* [1993, 1994] present a detailed model for water movement, CO_2 transport and production, heat flow, and equilibrium and kinetic hydrogeochemical processes in soils that includes also root uptake of water and CO_2. *Camporese et al*. [2006] extend an ISSHM to include peatland deformation (swelling and shrinking of peat soils) by introducing a constitutive relationship whereby porosity varies with moisture content. *Clark et al*. [2011a] provide a detailed review of snow modeling approaches and the factors that influence the spatial variability of snow water equivalent at the hillslope and catchment scales. Several studies have used integrated numerical models to investigate ecohydrological phenomena in tidal environments, including solute exchanges and the spatial patterns of salt marsh vegetation and sediments [*Ursino et al*., 2004; *Wilson and Gardner*, 2006; *Moffett et al*., 2012]. In *Ivanov et al*. [2010] the tRIBS model with vegetation is applied at the hillslope scale to explore the homogenizing effect of vegetation dynamics on soil moisture distribution.

3. Current Challenges

In parallel to the development of hydrology as a science [*Eagleson*, 1991], the past 50 years has seen tremendous scientific advances in the fields of physics-based modeling and applied mathematics. The advent of modern functional analysis, introduced to the applied community by the work of *Courant and Hilbert* [1962] in the U.S. and by *Lions and Magenes* [1960] in Europe, led to the development and subsequently application of variational techniques to the solution of PDEs, thereby paving the way to modern numerical analysis and computation. This has enabled a more thorough understanding of the intricacies of numerical discretization methods as well as the development of sound mathematical models yielding a much improved and robust description of the physical behavior of a system. In our view, an important challenge in hydrological science is to incorporate these mathematical modeling advances within the context of the complex and incompletely known structures that typify hydrological systems. This is congruent with the research trends of recent years, as described in the previous section, that see an increased number of interdisciplinary modeling efforts engaged in the difficult attempt to cast the early empirism of hydrological science into a more rigorous and robust framework.

In this section, we discuss the potential contributions that advanced mathematical and computational methods can make to resolving some of the outstanding problems in physically based hydrological modeling. We first examine process representation in integrated models (section 3.1), followed by novel approaches for surface PDEs, numerical discretization, and subgrid resolution (section 3.2), and finally simulation techniques for improved model performance (section 3.3).

The section will focus on comprehensive integrated catchment models since these encompass most of the open problems to be addressed.

3.1. Process Representation in Integrated Catchment Modeling

In the past decade a more comprehensive approach to physically based modeling of catchment dynamics has emerged, as seen for instance in the number of ISSHMs introduced by an expanding community of researchers pursuing the visionary ideas of *Freeze and Harlan* [1969] expressed almost half a century ago (see section 2.5). Rapid growth in computing power as well as the development of more efficient and accurate numerical techniques have been driving forces behind this effort. A fundamental requirement of these recent approaches is the use of modern, fast, accurate, and scalable numerical methods to simulate the different processes acting at proper characteristic scales. The coupling of such diverse processes is still not well understood, but the growing trends to use innovative mathematical and numerical techniques and to intercompare and benchmark different codes [e.g., *Sulis et al*., 2010; *Maxwell et al*., 2014] have led to a better understanding of underlying processes and of any given model's range of applicability.

3.1.1. Surface-Subsurface Flow Modeling

The most common approach to coupling surface and subsurface flow dynamics is based on the numerical solution of the system formed by the three-dimensional Richards equation for saturated-unsaturated flow in groundwater and a simplified form of the two-dimensional depth-integrated shallow water equations for modeling water flow at the terrain surface:

$$S_s S_w(\psi)\frac{\partial \psi}{\partial t}+\phi\frac{\partial S_w(\psi)}{\partial t}=\nabla\cdot[\boldsymbol{K_s}k_r(\psi)\nabla(\psi+z)]+q_s(x,t)+q_e(x,t)/m \quad (1)$$

$$\frac{\partial h}{\partial t}=\nabla\cdot(\boldsymbol{v}h)+q_e(x,t)+q_r(x,t) \quad (2)$$

where S_s is the specific storage coefficient [L^{-1}], $S_w(\psi)$ is the saturation function [-], ψ is the pressure head [L], ϕ is the porosity [-], $\boldsymbol{K_s}$ is the saturated hydraulic conductivity tensor [LT^{-1}], $k_r(\psi)$ is the relative permeability function [-], z is the vertical coordinate [L] (positive upward), q_s is a general source/sink term [T^{-1}], q_e represents exchange fluxes between the surface and subsurface components [LT^{-1}], m is the thickness of the surface-subsurface flux exchange zone, h is the surface water table depth [L], $\boldsymbol{v}$ is the water velocity vector [LT^{-1}], and q_r(x,t) is a source/sink term [LT^{-1}]. Note that the SWE system is often represented only by the mass continuity equation (or incompressibility condition) and that the full momentum equations are generally approximated using Manning's approach relating water velocity to terrain slope and water table depth:

$$v_x = \frac{\sqrt{S_x}}{n} h^{2/3} \text{ and } v_y = \frac{\sqrt{S_y}}{n} h^{2/3}$$

where S_x and S_y [L] are the friction slopes, typically identified by the components of the terrain gradient, and n [TL$^{-1/3}$] is Manning's coefficient. The exchange fluxes are calculated so as to enforce continuity of the subsurface and surface fluxes and to match surface water table with subsurface pressure head while neglecting momentum conservation. More details of this approach will be discussed below when we examine model coupling.

3.1.2. Surface-Subsurface Transport Modeling

In contrast to flow modeling, there has been comparatively less research on surface/subsurface solute transport. A simple and commonly employed methodology for physically based catchment-scale transport modeling [*Sudicky et al.*, 2008] consists in using the velocities calculated from the flow simulator to define an advective field transporting the solute mass. Besides the classical limitation due to the difficulty of detailing varying scale spatial heterogeneities, this approach neglects the complex interactions between the surface and subsurface components. An attempt to describe such complex interactions was proposed by *Weill et al.* [2011] using a time-splitting approach to capture the different time scales characterizing the coupled phenomenon. This is however an open field of research, and a comprehensive theoretical framework embracing the physical mechanisms acting at the surface/groundwater interface is still beyond reach.

Denoting with *c(x,t)* the solute concentration [-] (assuming normalized concentration) on both the surface and subsurface domains, the mass balance for the solute is given by the classical advection-dispersion equation:

$$\phi \frac{\partial S_w c}{\partial t} = \nabla \cdot [\boldsymbol{D}(\boldsymbol{v}) \nabla c - \boldsymbol{v} c] + q_{cs}(x,t) \quad (3)$$

where $\boldsymbol{v}$ is the fluid velocity field as calculated by the flow model and q_{cs} is the volumetric exchange flux between the surface and subsurface components [T^{-1}]. The previous equation contains variables that need to be adapted to the different domains. Thus, S_w and ϕ indicate water saturation and soil porosity, respectively, if transport occurs in the subsurface domain. They assume a unit value if transport is defined on the surface domain. The velocity $\boldsymbol{v}$ is a 3-D vector that embodies a locally 2-D field defined (projected) on the terrain surface when solving SWE. In the porous domain, $\boldsymbol{v}$ is the 3-D water phase Darcy velocity as evaluated by the RE solver. The dispersion coefficient $\boldsymbol{D}(\boldsymbol{v})$ represents mechanical dispersion due to tortuosity within the porous medium or due to turbulence in the surface component. In this latter case it is often modeled via eddy diffusion. Molecular diffusion is usually modeled by a spheric tensor that can be added directly to the dispersion coefficient.

Equation (3) is well-posed if the velocity field is globally and locally conservative [*Klausen and Russell*, 2005], i.e., the divergence theorem must hold for every subdomain. In practice, this last statement implies the intuitive conditions that at the boundary of any subset fully contained in the model domain the flux $q(x) = \boldsymbol{v}(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x})$, $\boldsymbol{n}(\boldsymbol{x})$ being the external unit vector normal to the subdomain boundary, must be continuous at any point $\boldsymbol{x}$. Velocity fields that satisfy this property are called conservative and have been the focus of numerous studies [e.g., *Chavent and Roberts*, 1991; *Cordes and Kinzelbach*, 1992, 1996; *Mosé et al.*, 1994; *Putti and Cordes*, 1998; *Cordes and Putti*, 2001]. It should be noted that the conservation property is not an accuracy condition in the sense that numerical convergence is independent of this property. However, it is nowadays recognized that this is a necessary condition for obtaining small mass balance errors in any transport model using the velocity field as driving mechanism. In our context, it is thus of fundamental importance that the flow solver enforce the conservation condition on the elements used in the numerical discretization, or in other words that the numerical discretization scheme be locally conservative. This property is realized by control-volume based methods such as finite volumes (including multipoint flux approximations [*Aavatsmark et al.*, 1998; *Aavatsmark*, 2002]) and mixed finite elements, but not by classical finite elements [*Putti and Sartoretto*, 2009]. To overcome this problem, a promising general method to postprocess the nonconservative finite element velocity field has been proposed by *Kees et al.* [2008] on the basis of a-posteriori error estimators developed by *Larson and Niklasson* [2004]. This method, based on a local variation of the computed velocities, assumed to be constant in each element, that enforces flux conservation across element faces, has been recently tested by *Povich et al.* [2013] in the context of coupled salt water flow and transport modeling and by *Beirão da Veiga et al.* [2014b] in the context of mimetic finite differences.

The conservation property must be imposed also at the interface between the surface and subsurface domains by appropriate coupling conditions. *Weill et al.* [2011] assert that the total flux from the surface domain must equilibrate Cauchy boundary conditions in the subsurface components. *Ebel et al.* [2007] and *Sudicky et al.* [2008] do not impose any constraint on the flow field and just assume continuity of the discrete fluxes as given by the flow solver. It is important to recognize that the phenomena governing solute exchange between surface and subsurface components are still largely unknown at the scales of interest in catchment simulation. Mechanisms such as solute dilution/concentration at the surface due to evapotranspiration and root water uptake interact with the movement of contaminants during infiltration and routing processes, adding complexity and uncertainty to the mathematical development of coupled models. While increasing efficiency and flexibility in novel numerical approaches, combined with continual advances in computing technology, allow the simulation of coupled phenomena at unprecedented scales, there is still a fundamental gap in process understanding and modeling. There is thus a need for more detailed theoretical and experimental studies to address the modeling of coupling phenomena acting at different scales, starting with reevaluation and model-based reinterpretation of past experimental studies as noted in section 2.6.

3.1.3. Model Coupling

The coupling of different physical phenomena in hydrology and other domains has received much attention in the past few years [*Gaston et al.*, 2012]. A multiphysics system comprises multiple processes, governed by different principles, that act simultaneously [*Keyes et al.*, 2011]. A further classification distinguishes between processes that take place within the same spatial domain and processes that communicate across an idealized interface (or a narrow buffer zone). In the case of hydrological modeling of water flow in a catchment, two important phenomena can be distinguished: surface routing and subsurface seepage. These are governed by the same physical principles, namely conservation of mass, momentum, and energy, but different simplifications and averages are needed to come up with well-posed and solvable mathematical models. The multiphysics aspect arises from the fact that surface flow is active on an essentially two-dimensional Euclidean surface modeling the terrain, generally represented by a DEM, while subsurface seepage occurs in a three-dimensional domain. The coupling between the two processes must then account for the exchanges of fluxes of mass, momentum, and energy across the idealized interface constituted by the DEM. This is only a rough description of the multiphysics couplings and feedbacks that occur in a hydrological basin. In fact, with reference only to the hydrological water cycle, accurate modeling cannot neglect, for example, the interactions between soil and atmosphere as mediated by vegetation (see section 2.7). One of the fundamental conclusions of *Keyes et al.* [2011] is that modeling the coupling between different phenomena requires the development of sound mathematical and numerical tools. It is crucial that modeling and experimental advances be described by well-posed mathematical equations and that the numerical approaches that are used for their practical solution be consistent and convergent. Addressing these problems via interdisciplinary studies involving physics, hydrology, and applied mathematics is an important future challenge.

Coupling between surface and subsurface water flow was initially studied by *Beavers and Joseph* [1967] and later refined by *Saffman* [1971] within the context of small-scale porous media applications, such as grain filters in the chemical industry and fuel cells. The original model of *Beavers and Joseph* [1967] arises from an experimental study in which water moves on top of a filtrating porous bed. In this situation the surface flow is governed by Navier-Stokes equations, possibly simplified by neglecting the temporal and convective terms (the so-called Stokes model), and filtration is governed by Darcy's law. The fundamental observation, supported by experimental outcomes, is that while Stokes velocity and pressure effectively correspond to their respective fluid quantities, the Darcy velocity and pressure, being defined in the porous domain, are spatial averages over a representative volume. As a result, at the interface the tangential component of the surface water velocity $\boldsymbol{v}_t = (v_x, v_y)$ cannot be the same as the tangential component of Darcy's velocity $\boldsymbol{q}_t = (q_x, q_y)$. Starting from this observation, *Beavers and Joseph* [1967] propose the following interface condition:

$$\frac{\partial \boldsymbol{v}_t}{\partial z} = \frac{\alpha_{BJ}}{\sqrt{Tr(K)}} (\boldsymbol{v}_t - \boldsymbol{q}_t)$$

where z is the vertical coordinate, α_{BJ} is an empirical coefficient, and *Tr(K)* is the trace of the saturated hydraulic conductivity tensor, i.e., the sum of its diagonal components. *Saffman* [1971] assumed the surface flow tangential velocity to be proportional to the shear stress, thus leading to the possibility of neglecting $\boldsymbol{q}_t$ in the above equation. The same result was obtained also by *Dagan* [1979] and used to derive validity and generalizations of Darcy's law. In practice, the so-called Beavers-Joseph or Beavers-Joseph-Saffman

(BJS) condition postulates the existence of a velocity jump at the interface, with magnitude controlled by the coefficient α_{BJ}. The BJS condition was later justified mathematically via homogenization theory by *Jäger and Mikelic* [2000] and *Jäger et al*. [2001], who also derived a jump relationship between the pressures of the surface and subsurface fluids. *Discacciati et al*. [2002] and *Miglio et al*. [2003] extended these considerations to a 3-D domain suggesting the following set of interface conditions:

$$\boldsymbol{v} \cdot \boldsymbol{n} = \boldsymbol{q} \cdot \boldsymbol{n}$$

$$\frac{\partial \boldsymbol{v}_t}{\partial z} + \nabla_{xy} v_z = \frac{\alpha_{BJ}\sqrt{3}}{\sqrt{Tr(K)}}(\boldsymbol{v}_t - \boldsymbol{q}_t)$$

$$h = \psi$$

The first equation imposes flux balance. The second equation is a 3-D extension of the BJS condition imposing momentum continuity. The last condition states that the surface water table depth must be equal to the porous medium pressure head. *Discacciati et al*. [2002] and *Miglio et al*. [2003] also defined a domain decomposition algorithm that iterates between distinct surface and subsurface domain solvers, and they showed the well-posedness of both the mathematical and numerical schemes together with the convergence of the domain decomposition approach. While generally assumed valid, the BJS condition postulates knowledge of the full 3-D velocities in both the surface and subsurface domains at the interface. In the case of a 2-D depth-averaged SWE the flux and momentum balance conditions above must be transformed into a flux exchange mechanism, an approach that is usually implemented via the proper definition of source terms. Extensions have been recently proposed by *Dobberschütz* [2015] who derived a generalized form of the BJS condition taking into account a possibly nonplanar geometry of the interface. A comprehensive review of this problem is presented in *Ehrhardt* [2012].

At the scale of interest for catchment flow dynamics, the fundamental notion that is most often employed is that of continuity of water pressure and fluxes at the surface/groundwater interface, while the BJS momentum balance condition is generally neglected. The specific implementations of these conditions are manifold, and three main coupling strategies can be identified, with all other methods proposed in the literature being variations of these. The first mechanism [*VanderKwaak and Loague*, 2001; *Panday and Huyakorn*, 2004; *Sudicky et al*., 2008; *Brunner and Simmons*, 2012] is based on the concept of conductance or first-order flux exchange, already mentioned by *Freeze and Harlan* [1969], by which the flux exchange term is considered proportional to the difference in pressure head at the interface between the surface and subsurface domains. The constant of proportionality is a conductance, and postulates the existence of a surface layer where water exchange between the surface and porous medium domains are localized. The nonlinear system of equations obtained after time discretization couples the surface and subsurface components via the linear flux exchange condition. Pressure and flux continuity at the interface is then enforced. A more complex variant of this approach is presented by *Weill et al*. [2009], who rewrite the surface routing equations in a format similar to RE. This equation is then activated on a surface layer, assumed of finite depth, and the equations solved simultaneously. The resulting discretization can be thought of as imposing an infinite conductance in an artifical layer. Note that the conductance parameter can be viewed as a Lagrange multiplier enforcing the pressure continuity constraint at the surface/subsurface interface. These approaches are attractive for their simplicity and allow a fully coupled numerical solution of the two systems. However, they have the drawback that the size or even the existence of the exchange layer cannot be verified experimentally and thus the value of the relevant parameters can only be calibrated indirectly. *Bixio et al*. [2002] and *Camporese et al*. [2010] use an algorithm similar to the domain decomposition method proposed by *Discacciati et al*. [2002], aided by a time-splitting mechanism making careful use of explicit (for surface routing) and implicit (for subsurface flow) time discretizations. By this approach, the solution of the surface routing problem yields boundary conditions for the RE solver. In turn, the solution to RE yields flux contributions to the SWE. These water exchange contributions are evaluated so that mass conservation is enforced. Complex nonlinear and time-varying boundary conditions are then defined to allow for the accurate simulation of surface water and soil-limited infiltration and evaporation regimes. In the third coupling strategy [*Kollet and Maxwell*, 2006], simplified shallow water equations provide the value of the flux for the Neumann boundary conditions imposed on the RE solver at the surface/subsurface interface. The numerical solution is then obtained by setting up a system of equations coupling the surface and subsurface modules via the boundary terms, enforcing at the same time the pressure continuity condition. This yields a fully coupled system of nonlinear equations that is solved simultaneously by a Newton method. A variant of this approach was analyzed numerically by *Dawson* [2006] in the framework of local discontinuous Galerkin methods. The algorithm proposed solves the surface and subsurface components separately to allow for different time stepping adaptation in view of the different time scales that characterize the different processes, analogous to the time discretization approach used in *Camporese et al*. [2010].

3.2. Novel Approaches for Surface PDEs, Numerical Discretization, and Subgrid Resolution

3.2.1. PDEs on Surfaces and Topography Approximation

Surface flow modeling is largely based on simplifications of the shallow water equations [*Gottardi and Venutelli*, 1993; *Santillana and Dawson*, 2009]. The SWE hypothesis asserts that the water wavelength is much larger than the wave height. This allows a dimensionality reduction by evaluating appropriate averaged velocities and water depth defined on the surface where the flow occurs, i.e., right at the surface/subsurface interface defined by the DEM. While this approach is well-established for flat terrain, e.g., ocean modeling, or for the surface of the Earth in atmospheric modeling, how to properly define the averaged quantities when the bottom is a complex surface, such as a catchment topography, is an unresolved issue. It is typical of any surface routing model to assume that the averaging operation is performed along a vertical path, leading to the well-known condition of hydrostatic pressure distribution along this direction. However, when defined on a curved topography, averaging cannot operate along the vertical and the above hydrostatic condition can be approximated along the direction normal to the bottom surface. Moreover, if the topography displays important curvatures, the averaging must be performed along a path that is orthogonal to the 3-D velocity vector at any point of the fluid domain, the so-called cross-flow integration path [*Bouchout and Westdickenberg*, 2004]. This definition is implicit, since the velocity vector is an unknown of the problem, and effectively prevents the achievement of an explicit dimensionality reduction. A few attempts have been made to make this argument rigorous [*Boutounet et al*., 2008], but more studies are needed to achieve a sound theory of shallow water flow over curved domains [*Pavlov et al*., 2011].

The last observation is connected to another important field of study, namely DEM analysis and definition. Starting from elevation data that, given current laser-based and radar-based technologies, can be obtained at unprecedented spatial resolutions, the key and yet not fully resolved question is how to define a mathematical model for the terrain surface and related hydrological quantities. The work of *Tarboton et al*. [1988] and successively the minimum energy reinterpretation of *Rinaldo et al*. [1992] suggest a fractal nature of digital elevation models at the scales of interest. However, how to deal with such a geometrical structure in surface routing simulators is not evident at all. Although network-based models, as developed, for example, by *Orlandini and Rosso* [1998], naturally inherit any fractal geometry of the underlying drainage network, they do not take into consideration the full geometrical structure of elevation data and consequent 3-D curvature effects. We believe this to be an exciting and promising area of multidisciplinary study where advanced mathematical techniques drawn from the field of differential geometry come into play. An example of this is the recent work of *Orlandini et al*. [2014], where collaboration between hydrologists and mathematicians has led to sound developments in the field of drainage network analysis of a 3-D surface. More effort needs to be devoted to this area of research to increase the fidelity of the DEMs extracted from observations and to assess the approximation errors arising from the numerical discretization of the PDEs defined on the terrain surface, following the steps delineated by *Dziuk and Elliott* [2013].

3.2.2. Numerical Discretization Methods

The past few decades have seen important developments in the evolution and analysis of discretization methods for differential equations. While the field of numerical ordinary differential equations has matured, culminating with the publication of a number of high quality numerical software libraries [e.g., *Hindmarsh et al*., 2005], the field of numerical PDEs is still under active development. Recent studies of discretization methods for PDEs have focused not only on the convergence behavior of the schemes but also on the reproduction at the discrete level of properties known to be valid at the continuous level. For example, the study of monotonicity properties of standard discretizations for elliptic equations that first appeared in *Brezzi et al*. [1989], where monotonicity for mixed finite element methods was analyzed, followed by *Forsyth* [1991], where discrete maximum principle conditions for standard linear Galerkin methods were introduced, has evolved passing through the work of *Putti and Cordes* [1998], who studied conditions under which physically coherent fluxes can be evaluated (the positive transmissibility condition). More recent analyses by *Bertolazzi and Manzini* [2005], *Younes et al*. [2006], and *Mazzia* [2008] have shed light on this problem and on the fact that there is an intrinsic relationship between geometry of the computational grid and the monotonicity properties of the discretization schemes.

A related issue with immediate implications for hydrological modeling is that of locally conservative numerical discretizations [e.g., *Klausen and Russell*, 2005], a property that is of fundamental importance for obtaining conservative discrete velocity fields [*Putti and Sartoretto*, 2009]. The fundamental concept that has led to these analyses is that the convergence behavior of a scheme cannot be tested in real world applications since grid refinement is impractical. Hence the numerical and physical soundness of a simulation must be supported by indirect physical or analytical evidence that needs to be collected at a fixed (unrefined) grid scale. The most recent developments in this area have led to the construction of the mimetic finite difference method and the closely related virtual element method [*Brezzi et al*., 2005, 2007; *Beirão da Veiga et al*., 2014a]. As the names imply, these methods mimic the physical and mathematical properties of the governing equations by a hierarchical use of Stokes theorem and integration by parts to arrive at discretizations that maintain these properties at the discrete level. The main advantage for hydrological applications is that mimetic/virtual methods can be defined on very general (3-D) cell shapes. The power of this characteristic has seen only limited application, but its potential for handling geometrically complex heterogeneities (for example) should be explored, especially in combination with multiscale techniques.

3.2.3. Upscaling, Subgrid Resolution, and Multiscale Modeling

Subgrid resolution tries to incorporate into the simulation algorithm the small-scale physical features of a phenomenon that cannot be resolved at grid sizes typical of catchment-scale simulations. Subgrid resolution and multiscale discretization methods are intimately related: either subgrid processes are summarized by ad hoc simplified mathematical models whose solution can be obtained in practical terms by closed-form functions, or the subgrid problem must be solved numerically. In both cases the information at the small scale needs to be transferred to the computational domain (nodes or edges). While widely used in atmospheric and ocean modeling through the well-established large eddy simulation approach [*Meneveau and Katz*, 2000; *Albertson et al*., 2001] and in shallow water modeling to handle bottom geometrical irregularities [*Defina*, 2000], subgrid resolution procedures are less rigorously developed in physically based distributed catchment models (they are used for instance in some compartment or bucket-based hydrological models). Subgrid resolution is critical for model implementation at a workable DEM or grid cell size. This can be efficiently obtained via multiscale simulation [*Efendiev et al*., 2000; *Efendiev and Hou*, 2009], using either finite element or finite volume schemes [*Chen et al*., 2003; *He and Ren*, 2005] to mathematically and numerically extrapolate the needed subgrid information on the course grid.

On the other hand, a purely numerical approach is not sufficient to thoroughly define the coarse scale behavior of nonlinear processes such as infiltration (or more generally unsaturated water flow) and coupling of surface and subsurface components. In this case upscaling of both model parameters and model equations is necessary [*Cushman et al*., 2002]. Tools developed for these purposes, based mainly on volume averaging methods [*Whitaker*, 1999] or homogenization theory [*Hornung*, 1997], are difficult to extend to catchment simulation. In these cases simpler numerical approaches, for example, simultaneous calibration of model parameters at different scales and linking the multiscale processes via empirical functional relationships [*Samaniego et al*., 2010; *Kumar et al*., 2013], have been introduced to define upscaled parameterizations, with the upscaled process described as an analog of the fine grid process. Future research in this area is needed to develop more rigourous upscaling techniques with the aim of finding both regionalized model equations and model parameters starting from the fine scale contributions. To do this one has to first find the homogenized models at the appropriate scales of appearance of the single processes and then proceed in a hierarchical way to the larger scales. To better illustrate this idea, consider the example of water infiltration at the soil surface. It is a very local phenomenon and homogenized models are needed even at subhillslope scale. On the other hand, at the larger scale, if one looks for example at streamflow formation, the important characteristics are surface-subsurface water partitioning and the consequent resident times of the different components. Addressing the concurrent simulation of all these processes may require the coupling of different models, i.e., a multiphysics approach as described in section 3.1. Important developments of these methodologies will include the use of model reduction to increase the efficiency of computations [*Efendiev et al*., 2012].

An important example where subgrid resolution methods can be useful is that of preferential flow, a phenomenon that is ubiquitous in porous media environments and that acts at a scale that cannot be represented in reasonably sized grids. We distinguish two types of preferential flow mechanism. The first is related to the hypothesis, supported by experimental evidence, of the existence of fast flow paths in the subsurface [e.g., *Hopp and McDonnell*, 2009; *James et al*., 2010]. The possibilities for taking into account this type of preferential flow are manifold. One obvious option is to model this pipe flow directly, but this is not appealing because of the impossibility, with the current state of the art in geophysical techniques, of collecting sufficient and reliable measurements to characterize the flow geometry and mechanisms. An alternative is the two-domain paradigm discussed in section 2.2, with some lumped subgrid modeling approach to identify appropriate parameterizations. The second type of preferential flow mechanism, instability or fingering, is related to infiltration processes from the surface. Accuracy in modeling this contribution is fundamental to prediction of rainfall-runoff partitioning. Subgrid models are being considered for this mechanism as well, based for example on dynamic capillary curves [*Nieber et al*., 2005] or on equations other than RE [*Cueto-Fulgueroso and Juanes*, 2008; *DiCarlo*, 2010, 2013], together with the important question of identifying equivalent or upscaled infiltration fluxes from local infiltration models. This last question is more related to averaging or homogenization techniques described earlier than to parameterization, but nonetheless it is an important issue that should be addressed in the future to improve on the ability of models to simulate preferential flow processes.

A question that is often asked is what are the most important processes that need to be represented in physically based models, but this is an ill-posed question, as the issue of representation is not independent of the scale at which the process is modeled [*Bierkens et al*., 2014]. Hence a relationship between process modeling and discretization must exist. This very general issue is common to all hydrological problems. All the above methods can and should be used to systematically investigate the relationship between measurement scale (spatial and temporal) and model resolution, both in terms of geometry, i.e., grid size and large scale heterogeneities, and physics, i.e., process description. From a purely numerical point of view, classical upscaling methods are necessary to describe phenomena that cannot be represented at the employed mesh size. Larger scale heterogeneities can be represented as long as sufficient data are available. Understanding the fine balance between process description, model resolution, and the amount of observation data is an important topic that should be studied with the aid of ISSHMs. New-generation physically based lumped models, possibly based on stochastic approaches [*Benettin et al*., 2013], may also play a key role in homogenization frameworks that seek to balance process uncertainty and model detail, and may provide an important theoretical foundation for subgrid resolution modeling. Data assimilation methods, discussed further below, are able to quantify model mismatch against observations, and are thus an ideal platform to guide the assessment not only of the quality of the available data but also of the representativeness of the model processes (for instance with respect to missing or poorly described components).

3.3. Simulation Techniques for Improved Model Performance

3.3.1. Scientific Computing and Parallelization

The field of scientific computing and parallelization is progressing rapidly in conjunction with emerging large-scale computing innovations. The most critical kernel of any scientific solver is the efficient solution of the large sparse systems of linear algebraic equations arising from the numerical discretization of PDEs. Preconditioned Krylov-based methods are usually the solvers of choice for these systems [*Bergamaschi and Putti*, 1999; *Bergamaschi et al*., 2006]. A recent review of Krylov methods with particular reference to water resources applications is presented in *Miller et al*. [2013]. The crucial component for the efficient and robust application of this class of methods is the definition of appropriate preconditioners that render the problem tractable. Unfortunately, in most cases, efficient preconditioning is problem-dependent and general-purpose software is suboptimal in many applications. In addition, preconditioning is often a purely sequential process and its parallelization is not trivial. Recent trends in problem-dependent preconditioning involve the use of approximate inverses of the system matrix coupled with controlled fill-in and algebraic multilevel approaches [*Janna et al*., 2015]. A review of these specialized methods is found in *Ferronato* [2012].

Efficient linear system solvers play a fundamental role also in the solution of nonlinear systems arising from the numerical discretization of the relevant PDEs. Globalized inexact Newton-like methods are the standard approaches used in this case. Inexactness comes into play by requiring that Krylov-based iteration be stopped at increasingly small residuals. The rationale for this is the observation that the Newton direction at the beginning of the nonlinear phase is far from being accurate, and the scheme converges as long as this residual is a descent direction for the functional form associated with the nonlinear system. Thus using a constant tolerance for exiting the linear solution phase is useless and leads to oversolving. These methods have now become standard use and a number of software packages provide efficient implementations.

Research in this field should concentrate on seeking to improve the convergence characteristics of Newton methods without the use of costly globalization techniques. Recent methods for Richards' equation have been proposed by *Casulli and Zanolli* [2010] that exploit the typical behavior of the soil hydraulic functions to define two nested iterations that guarantee quadratic convergence of a Newton-like method. Improvements to Picard iteration schemes, which avoid using derivatives of the nonlinear functions (e.g., in the RE hydraulic functions) that often are responsible for the ill-conditioning of the Jacobian matrix, should also be pursued. Along this line, the recent work on Anderson acceleration [*Walker and Ni*, 2011; *Lott et al.*, 2012] seems promising. Finally, more research on preconditioners better suited to the nonlinear iteration case [e.g., *Bergamaschi et al.*, 2006, 2013] is also needed.

3.3.2. Reduced Order Modeling

Reduced order models (ROMs) are low-dimensional surrogate models used to replace the full system model so as to reduce the computational cost of parametric simulations needed, for example, in inverse problem or data assimilation applications. ROMs are based on an off-line procedure that develops the surrogate model, followed by an on-line procedure where the ROM is repeatedly employed. Recent research in this field has been spurred by advances in proper orthogonal decomposition and reduced basis finite element methods [*Kunisch and Volkwein*, 2001; *Vermeulen et al.*, 2004; *Grepl and Patera*, 2005; *Bui-Thanh et al.*, 2008; *Quarteroni et al.*, 2011; *Manzoni*, 2014]. Both approaches are based on the Galerkin projection of the full system model onto a space generated by a small set of significant full model solutions (snapshots). The main idea is that the description of the solution as a linear combination of the basis functions of the space generated by the snapshots is highly accurate notwithstanding its low dimensionality. The main question is how to determine the optimal and parameter-independent snapshot set. The applicability of these methods is currently limited to problems where repeated simulations are needed, mainly optimization problems [e.g., *Siade et al.*, 2012] and Monte Carlo simulation [e.g., *Pasetto et al.*, 2011, 2013a], but their use is evolving also toward the solution of linear and nonlinear systems [*Jang*, 2013]. Although the effectiveness of ROM for highly nonlinear problems is still to be proved, we believe this to be a very exciting field of research with great potential in inverse problems and any stochastic application where an ensemble of realizations needs to be built.

3.3.3. Uncertainty Quantification and Data Assimilation

Flow and transport processes in catchment simulations are characterized by incomplete knowledge about physical processes and model parameterization. Quantification of these uncertainties is a fundamental step for a better understanding of simulation outputs and for more reliable forecasts. The classical calibration phase seeks to determine the set of parameters that minimize some measure of the discrepancy between observation and model results. This is well known to be a highly ill-posed problem mostly due to incomplete process understanding and to the limited accuracy and representativeness of field measurements. Recent attempts to resolve these issues have looked to data assimilation techniques and stochastic filtering theory. These methods have gained popularity since the introduction of Monte Carlo-based approaches such as the ensemble Kalman filter [*Evensen*, 2003]. Ensemble data assimilation techniques are highly appealing in the context of physically based hydrological simulation as they can address simultaneously questions of both parameter identification and real-time uncertainty quantification. However, the procedures are very computationally intensive owing to the construction of the ensemble of model realizations needed to propagate in time the statistical properties of the joint probability density functions (pdf) of modeled system states and observations.

The reliability and applicability of data assimilation methods can be improved by means of more accurate approximation of the (random) functions belonging to the probability space of the posterior pdf. This statement can be exemplified by looking at well-known differences between EnKF and particle filters [*Pasetto et al.*, 2012]. Kalman-based filters such as EnKF share the important limitation of using only the first and second moments to approximate the posterior joint pdf, thus effectively employing a Gaussian hypothesis that is not always warranted. On the other hand, filters that are not restricted by the Gaussian assumption, such as particle filters, do not use explicit information on the covariance function of the joint pdf, thus requiring large ensemble dimensions to effectively approximate the posterior probability space. Two research questions related to these issues that need to be addressed are: i. finding more accurate approximations of the functions in probability space; and ii. improving the computational efficiency in the construction of the ensemble replicates. This field can greatly benefit from the application of the ROM approach described above not only for the construction of the ensemble members but also in the development of efficient time-updates of the covariance matrices needed in data assimilation processes [e.g., *Pham et al*., 1998; *Kitanidis*, 2015].

4. Conclusions

This paper has surveyed five decades of research on physically based numerical models in hydrology, examining the interplay between theoretical, computational, and experimental advances and providing an outlook on current issues and future challenges in several areas of model development and validation. The review has been centered on the main themes of consistent physical and mathematical representation of processes and parameters, robust and efficient numerical algorithms, and integrated and interdisciplinary models. We have examined how researchers have dealt with perennial issues of heterogeneity, nonlinearity, and scale through the years, and have followed key developments and trends toward more complex models (higher dimensioned equations, coupled systems, comprehensive boundary conditions, multiple processes, larger scales, etc). A recent example that encapsulates this trend is hyper-resolution hydrological modeling [*Wood et al*., 2011; *Beven and Cloke*, 2012; *Bierkens et al*., 2014; *Mascaro et al*., 2015], featuring large-scale simulations predicated on fully distributed, physically based descriptions of groundwater, soil, vegetation, and atmosphere dynamics, eventually to be used in combination with atmospheric circulation modeling as substitutes for current highly parameterized land surface models at the continental scale. This and other developments in integrated, high-resolution, multiphysics modeling will require research progress on several fronts connected to the main themes of the paper: improving numerical schemes for nonlinear equations, exchange fluxes, adaptive grids, and curved surfaces; adopting model performance-enhancing techniques such as code parallelization, model reduction, and data assimilation; harmonizing the roles of complex versus simpler (low-dimensional, reduced order, parsimonious) physically based models; establishing correct coupling procedures for surface/subsurface models; dealing with subgrid variability and multiscale processes; and intensifying model intercomparison and benchmarking efforts based on multiresponse data sets from experimental hillslopes and watersheds.

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