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The evolution of process-based hydrologic models: Historical challenges and the collective quest for physical realism

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Abstract

The diversity in hydrologic models has historically led to great controversy on the "correct" approach to process-based hydrologic modeling, with debates centered on the adequacy of process parameterizations, data limitations and uncertainty, and computational constraints on model analysis. In this paper we revisit key modeling challenges, outlined by Freeze and Harlan nearly 50 years ago, on requirements to (1) define suitable model equations, (2) define adequate model parameters, and (3) cope with limitations in computing power. We outline the historical modeling challenges, summarize modeling advances that address these challenges, and define outstanding research needs. We illustrate how modeling advances have been made by groups using models of different type and complexity, and we argue for the need to more effectively use our diversity of modeling approaches in order to advance our collective quest for physically realistic hydrologic models.

1 Introduction

The research community exhibits great diversity in its approach to hydrologic modeling, with different models positioned at different points along a continuum of complexity. Models can be defined both in terms of process complexity, i.e., to what extent do different models explicitly represent specific processes; and spatial complexity, i.e., to what extent do different models explicitly represent details of the landscape and the lateral flow of water across model elements. Such model diversity has led to great community debates on the "correct" approach to process-based hydrologic modeling [Wood et al. 1988; Grayson et al. 1992b, 1992a; Famiglietti and Wood 1995; Reggiani et al. 1998; Beven 2002; Sivapalan et al. 2003; Maxwell and Miller 2005; Wood et al. 2011; Beven and Cloke 2012; Wood et al. 2012], with the debate centered around issues of the adequacy of process parameterizations, data limitations and uncertainty, and computational constraints on model analysis.

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This synthesis paper is an outcome of the Symposium in Honor of Eric Wood: Observations and Modeling across Scales, held June 2-3, 2016 in Princeton, New Jersey, USA. The purpose of this paper is to revisit the historical debates on process-based hydrologic modeling and ask the following question: *How can we combine different perspectives on hydrologic modeling to advance the quest for physical realism*? [Kirchner 2006; Clark et al. 2016]. Specifically, we focus attention on the three fundamental questions that were posed by Freeze and Harlan [1969] in their seminal "blueprint" for a physically-based hydrologic response model:

1. Are physically based mathematical descriptions of hydrologic processes available? Are the interrelationships between the component phenomena well enough understood? Are the developments adaptable to a simulation of the entire hydrologic cycle?
2. Is it possible to measure or estimate accurately the controlling hydrologic parameters? Are the amounts of necessary input data prohibitive?
3. Have the earlier computer limitations of storage capacity and speed of computation been overcome? Is the application of digital computers to this type of problem economically feasible?

We posit that these questions, published almost fifty years ago, are very relevant today and nicely frame the debates on process-based hydrologic modeling.

We organize the paper around the three questions posed by Freeze and Harlan, on (1) model structure; (2) model parameter values; and (3) model execution (computing). For each question we define the major research challenges, and summarize the different ways that the community has risen to meet these challenges. Our overall goals are to demonstrate how diverse hydrologic modeling approaches advance the collective quest for physically realistic hydrologic models, and to define additional research that is necessary to further advance process-based hydrologic models.

2 Model structure

2.1 Modeling challenges

The first question posed by Freeze and Harlan [1969] focuses on the adequacy of the mathematical descriptions of system of interest. Such mathematical descriptions define the structure of a model. They include both the equations used to parameterize individual processes as well as the interactions among processes and across scales.

A major research challenge is the problem of scaling, or closure [Wood et al. 1988; Blöschl and Sivapalan 1995; Reggiani et al. 2001; Beven 2006], i.e., how best to represent the influence of small-scale heterogeneities on large-scale fluxes, how best to represent interactions among processes, and the connectivity of water across the landscape. The scaling challenge is ubiquitous. For example, Mahrt [1987] demonstrates how localized areas of instability can dominate large-scale energy fluxes; Scott et al. [2008] demonstrate that transpiration from narrow riparian corridors in arid regions is much greater than the local precipitation; Seyfried et al. [2009] demonstrate that deep snow drifts produce local runoff "hotspots" that generate a disproportionate amount of the catchment runoff; Tromp-van Meerveld and McDonnell [2006a, 2006b] demonstrate that the water stored in bedrock depressions must be raised to a sufficient level in order to connect bedrock depressions and generate hillslope outflow. The community has risen to meet these scaling challenges in

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very different ways – different models use very different sets of equations to describe the large-scale manifestation of spatial heterogeneity, process interactions, and connectivity.

The different solutions to the scaling/closure problem can be distinguished by the extent to which the effort is focused on developing new large-scale flux parameterizations or numerically integrating the small-scale heterogeneities across space. Such differences are perhaps best illustrated by considering the different approaches used to simulate the transmission of water through catchments. In bucket-style rainfall-runoff models – at the simplest end of the complexity continuum – the large-scale transmission of water is often defined as a linear (or near-linear) function of water storage [e.g., see the synthesis in Clark et al. 2008]. Such large-scale closure relations implicitly represent the small-scale heterogeneity of flow paths, including the localized areas of high conductivity (e.g., macropores) that dominate the large-scale response [Beven and Germann 1982; McDonnell 1990]. By contrast, the more complex 3D variably saturated flow models typically use small-scale closure relations [Maxwell and Miller 2005; Rigon et al. 2006], where unsaturated hydraulic conductivity is defined as a highly non-linear function of soil moisture [e.g., Van Genuchten 1980]. These 3D models compute large-scale fluxes by spatially integrating the small-scale heterogeneities [Maxwell and Kollet 2008; Kollet et al. 2010]. These differences in solutions to the scaling problem are not mutually exclusive, and both sets of solutions can occur in the same model.

When viewed in this way, the different solutions to the scaling/closure problem are readily shared among different modeling groups that employ very different modeling approaches. To explain this perspective, consider the inequality that describes ideal relationships between the model resolution and the length scale of resolved and unresolved processes [Wood et al. 1988]

$$l \ll D \ll L \tag{1}$$

where l is the length scale of the rapidly varying hydrologic response, L is the length scale of the slowly varying quantities, and D is the length scale of the model element (note the assumption that the spatial scale of processes below the grid resolution is clearly separated from the spatial scale of processes above the model resolution; a condition that is rarely achieved in practice [Fan and Bras 1995]). Critically, equation (1) requires that processes below the length scale of the model element must be represented implicitly (e.g., through large-scale flux parameterizations) and processes above the length scale of the model element must be represented explicitly (e.g., through numerical integration over spatially distributed model elements).

The move of large-domain hydrologic and land models towards "hyper" resolution [Wood et al. 2011], e.g., 1-km or 100m, emphasizes the need for general parameterizations of hydrological processes at this scale. However, this is still an unsolved problem: we do not have firm evidence that the structure and parameter values of our element-scale equations correspond to hydrologic reality at those scales. One of the most important causes of this difficulty is the spatial heterogeneity in the initial and boundary conditions, and in the material properties of the medium. This heterogeneity occurs at multiple spatial scales, and has multiple physical causes [Seyfried and Wilcox 1995]. The multiple scales of heterogeneity are manifest as multiple dominant processes [Grayson and Blöschl 2001], and also as processes without a well-defined spatial scale (e.g. preferential flow in the snowpack, on the land surface, in the subsurface). These problems cannot be solved solely by numerical integration across space. The next section summarizes recent in developing large-scale flux parameterizations, and in effectively resolving dominant processes.

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2.2 Modeling solutions

The common challenge of developing large-scale flux parameterizations has been addressed in a number of ways. One class of methods is statistical-dynamical flux parameterizations, where large-scale fluxes are defined based on probability distributions of sub-grid or sub-element model state variables. For example, area-average infiltration can be parameterized based on probability distributions of water table depth [Beven and Kirkby 1979; Sivapalan et al. 1987] or on probability distributions of soil moisture [Moore and Clarke 1981; Wood et al. 1992]. Similar statistical-dynamical approaches are used to parameterize the impact of frozen soils on area-average infiltration [Koren et al. 1999] and the impact of spatial variability of snow on area-average energy fluxes [Luce et al. 1999; Liston 2004; Clark et al. 2011a]. Another class of methods is scale-dependent parameterizations, where new flux parameterizations are defined directly at the scale of interest. Examples of this class of methods include the empirically derived storage-discharge relationships described earlier [Ambroise et al. 1996; Clark et al. 2008; Fenicia et al. 2011; Brauer et al. 2014]. Similarly, large-scale stability corrections, used in computations of land-atmosphere energy fluxes, implicitly represent the impact of local pockets of instability on large-scale fluxes [Mahrt 1987]. There is a strong need to synthesize, evaluate, and compare these large-scale parameterizations, in order to improve the physical realism of hydrologic models [Clark et al. 2011b; Clark et al. 2015b; Clark et al. 2016].

Statistical-dynamic flux parameterizations rely on the assumption that the model scale D is large compared to the length- or time-scale of the heterogeneity of hydrological response l. In other words, the size of a model element is large compared to the scale-of-fluctuation [Rodríguez‐Iturbe 1986] or the integral-scale [Dagan 1994] of the underlying process. In that case, univariate probability density functions can be used that, when spatially, temporally or probabilistically integrated, result in small variance representative parameters at the scale of the model elements that do not depend on the model state (called full closure). However, if l and D are comparable in scale, this becomes problematic. Here, much can be learned from the upscaling research that has been done in stochastic subsurface hydrology to derive representative hydraulic conductivities at the scale of model blocks [see Sánchez-Vila et al. 1996 for a review]. These approaches can be distinguished into two main categories [Bierkens and Van der Gaast 1998]: direct upscaling, whereby the spatial statistics, i.e. mean and spatial covariance, of the block-scale hydraulic conductivity are directly derived from integrating the small scale spatial statistics, and indirect upscaling where the hydraulic conductivity is first stochastically simulated or interpolated at the smallest scale and then upscaled by non-linear averaging. Direct methods work best for heterogeneity that can be described by multi-Gaussian random functions. However, numerical integration across space may be necessary if the heterogeneity is more organized or of larger complexity. It is important to notice however, that full closure is often not possible, resulting in representative parameterizations that change with the model state.

The challenge of effectively resolving dominant processes has also been attacked in different ways. While one tactic is to simply discretize the domain into the highest resolution grid that modern computers allow (the numerical integration across space described above) [Freeze and Harlan 1969; Maxwell et al. 2015], this approach constrains capabilities to extensively experiment with alternative model configurations and to characterize model uncertainty [Beven and Cloke 2012; Wood et al. 2012]. Hence, for practical reasons, the challenge of spatial integration is commonly met using concepts of hydrologic similarity, often implemented at multiple levels of granularity within the same model. At a fine level of granularity, Wang and Leuning [1998] make separate stomatal conductance calculations on sunlit and shaded leaves to improve scaling from the leaf to the

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canopy. Similarly, Swenson and Lawrence [2012] make separate energy balance calculations over snow covered and snow free terrain to improve estimates of large-scale energy fluxes. At the system scale many models spatially integrate across discrete landscape types to capture the large-scale manifestation of small-scale heterogeneity [e.g., Flügel 1995; Tague and Band 2004]. For example, Newman et al. [2014] spatially integrate across a small number of discrete landscape types in order to reproduce the local runoff "hotspots" described by Seyfried et al. [2009]. More recently, Chaney et al. [2016a] demonstrate that the use of spatially interacting hydrologic response units can reduce computational cost of a fully distributed hydrologic model by three orders of magnitude without appreciable losses in information. Like the large-scale flux parameterizations, there is a strong need to rigorously compare different approaches to explicitly resolve dominant processes.

An interesting twist is the interplay between explicitly representing small-scale processes and avoiding or reducing redundant calculations across large model domains. For example, in the push for hillslope-resolving models across large geographical domains, one approach is to use the concept of representative hillslopes [Troch et al. 2003; Hazenberg et al. 2015; Ajami et al. 2016]. The representative hillslope has a length dimension much smaller than the length scale of the model element, and the hillslope is discretized into columns along an axis perpendicular to the stream in order to explicitly resolve lateral flow processes. The hydrologic and energy fluxes from this single hillslope, or averaged across local hillslopes of different types, are then considered representative of the model element as a whole. This approach spatially integrates both along a hillslope and among hillslopes. Such multi-scale approaches show considerable promise and will likely be increasingly used to represent how small-scale heterogeneities, interactions among processes and the connectivity of water across the landscape affects large-scale behavior.

A key challenge is to isolate and scrutinize competing modeling approaches to represent scaling and heterogeneity. Peters-Lidard et al. (this issue) proposes the idea that the approximations in our models can be treated as hypotheses that can be tested in an information-based framework. Such advances in model evaluation methods will be critical in order to accelerate advances in process-based hydrologic models.

3 Model parameters

3.1 Modeling challenges

The second question posed by Freeze and Harlan [1969] focuses on the availability of data to define system properties (model parameter values).

A key part of this modeling challenge revolves around the availability and quality of spatial information on model parameters. For some model parameters, spatial information simply does not exist. Examples of missing parameters include those that define the temporal decay of snow albedo and the recession characteristics of shallow aquifers. In such situations process-based hydrologic and land models often treat these uncertain parameters as physical constants, adopting hard-coded parameters that are selected based on order-of-magnitude considerations or on limited experimental data [Mendoza et al. 2015; Cuntz et al. 2016]. For other parameters the available spatial information is limited to broad landscape characteristics; e.g., the parameters controlling carbon assimilation and stomatal conductance are typically tied to vegetation type [Bonan et al. 2011; Niu et al. 2011], or the available soil maps impose the same hydraulic properties over large areas [Miller and White 1998]. Such ill-defined information on vegetation and soils greatly underestimates the tremendous spatial heterogeneity that occurs in nature. Finally, when

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spatial information does exist it may have limited spatial representativeness and relevance – for example, the information on hydraulic conductivity from soil pits may only have weak relations with the transmission of water throughout catchments [Beven 1989]. Such limitations notwithstanding, the challenge, really, is to make the most of the information we do have, and generate new information where we can (e.g., new observations), in order to improve estimates of the spatial variations in the storage and transmission properties of the landscape, including the scale dependence of these properties and their transferability across spatio-temporal scales [Klemeš 1986; Samaniego et al. 2010; Melsen et al. 2016]. The next section summarizes how the hydrologic modeling community is rising to this challenge.

3.2 Modeling solutions

The solutions to improve information on model parameters are general and can be applied across multiple models of different type and complexity. We see three specific paths forward. First, there are numerous opportunities to improve information on geophysical properties, including estimates of vegetation structure [Simard et al. 2011], soil depth [Pelletier et al. 2016], soil properties [Chaney et al. 2016b], bedrock depth and permeability [Fan et al. 2015] and the physical characteristics of rivers [Gleason and Smith 2014]. Second, it is possible to improve the way that geophysical information is used to estimate model parameters. For example, the Multi-scale Parameter Regionalization (MPR) approach of Samaniego et al. [2010] focuses attention squarely on the transfer functions that relate geophysical attributes to model parameters – Samaniego et al. apply transfer functions at the finest spatial scale of the geophysical data (e.g., the soil polygons) and then apply parameter-dependent operators to upscale the fine-scale model parameters to the resolution of the model. The parameter estimation in MPR is hence centered on the coefficients in the transfer functions used to relate geophysical attributes to model parameters, maximizing the information extracted from the geophysical data. Much research has focused on pedotransfer functions to relate soil properties to soil parameters [e.g., Schaap et al. 2001], and there has been limited work to relate geophysical attributes to other model parameters such as those controlling the impact of soil moisture on saturated areas [Balsamo et al. 2011]. Third, there is considerable scope to improve the way that multivariate data is used to constrain model parameter values. A key path forward is to identify different signatures from the data that can be used to improve parameter values in different parts of the model [Gupta et al. 2008; Yilmaz et al. 2008; Pokhrel et al. 2012; Vrugt and Sadegh 2013; Rakovec et al. 2015]. Together, focused effort on improving geophysical information, improving the links between geophysical information and model parameters, and better constraining model parameters, will go a long way to improve parameter values across multiple models.

A very different solution is stochastic modeling. Stochastic modeling accepts that controlling parameters are impossible to measure or estimate, and instead generates synthetic model parameter fields using probability distributions with assumed length scales. For example, Maxwell and Kollet [2008] use spatially correlated random fields of saturated hydraulic conductivity to define the fine-scale spatial structure of their model domain, and evaluate the impact of this fine-scale structure on hillslope runoff. These approaches thus derive from the indirect upscaling methods (numerical integration across space) developed in stochastic subsurface hydrology. Similar approaches were used by Kollet et al. [2010] in their proof-of-concept study illustrating the spatial integration of fine-scale 3D variably saturated flow simulations. The downside of such stochastic simulation approaches is that multiple realizations are necessary to separate the signals from the

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Discussions

imposed random variability, making such approaches computationally challenging for fine-scale simulations over large geographical domains [Fatichi et al. 2016].

A remaining challenge, that seems to be difficult to solve, is to parameterize the deeper subsurface at regional to continental scales in order to support large-domain groundwater modeling [Bierkens 2015; Clark et al. 2015a]. Methods such as MPR [Samaniego et al. 2010] will not help here because MPR relies on large-extent high-resolution auxiliary information that is available for the surface and shallow sub-surface (topography, soils, land cover), but not for the deeper subsurface. Also, stochastic methods are of limited use, as they will not capture the large structural variability in the formations and layers that dominate continental domains. Recent attempts to parameterize the sub-surface are a good first step. These include maps of global permeability and porosity for upper 50 m of the world's aquifers [Gleeson et al. 2014], global regolith thickness [Pelletier et al. 2016] and global thickness of the upper aquifers [De Graaf et al. 2015; Fan et al. 2015; Fan 2015]. However, these datasets have been globally extrapolated from locally established empirical relationships between subsurface properties and surface lithology [Hartmann and Moosdorf 2012], soil maps and surface topography on the other hand. None of these approaches resolve the multi-layer structure of aquifers and aquitards. As a consequence, they provide a useful guide the interaction between groundwater and evaporation, but have limited use for resolving true hydrogeological challenges such as assessing global groundwater depletion, groundwater age and land subsidence related to groundwater pumping. Concerted efforts are needed to compile a global hydrogeological multilayer model based on national geological maps and archives and local- and regional scale groundwater modelling studies, providing the rich information on the subsurface that already exists for soils.

4 Model execution (computing)

4.1 Modeling challenges

In their final question Freeze and Harlan [1969] ask if the computer limitations of storage capacity and speed of computation have been overcome, and if their blueprint for process-based hydrologic modeling is now economically feasible. Interestingly, we have made substantial (and economically feasible) advances in computing, yet we have also pushed beyond what they could envision with model resolution and process complexity. As a result computing remains, ironically, a present-day challenge, and we still routinely push available computing resources to their limit [Kollet et al. 2010; Wood et al. 2011]. We still struggle with tradeoffs among process complexity, spatial complexity, domain size, ensemble size, the time period of the model simulation. We also still struggle to run our most complex models for a large number of model configurations, for example, experimenting with different model parameter sets, different process parameterizations, and different spatial architectures. To answer Freeze and Harlan's question: The computing limitations have not been overcome.

The challenge is as follows: As we push our models to the limit in terms of process complexity, spatial complexity, and domain size, the computational expense of these complex configurations may permit only a single deterministic simulation for a short time period [e.g., Maxwell et al. 2015; Fatichi et al. 2016]. Such preferences for complexity and large-domain simulations arguably sacrifice opportunities for model analysis, model improvement, and uncertainty characterization. The end result is that our model complex models may struggle with physical realism – computational limitations mean that it is

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Discussions

difficult to identify and resolve problems in our most complex models; hence more complex models may not have as much physical realism as computationally frugal alternatives.

4.2 Modeling solutions

There are several solutions to these computational challenges, all of which are now being advanced by leading process-based hydrologic modeling groups. The first solution, and the most obvious, is to exploit advances in massively parallel computation (e.g., exa-scale computing) and advances in numerical solution methods [Kollet et al. 2010; Wood et al. 2011; Paniconi and Putti 2015; Fatichi et al. 2016]. This solution is often implemented by running a complex model for the finest grid resolution possible over the domain of interest [e.g., Maxwell et al. 2015]. A second solution to the computing challenge is to identify model configurations that avoid redundant calculations while still capturing dominant processes. This can be accomplished using the concept of hydrologic similarity, i.e., recognizing that there is no need to repeat calculations for areas of the landscape with very similar forcing and geophysical properties [e.g., Flügel 1995; Tague and Band 2004]. As noted earlier, recent applications of hydrologic similarity methods have shown that it is possible to reduce run times by two to three orders of magnitude, without any loss in information content [Newman et al. 2014; Chaney et al. 2016a]. Also, hydrologic similarity concepts can be effectively applied using multi-scale methods in order to resolve the dominant spatial gradients that drive flow; for example, using representative hillslopes in order to explicitly resolve lateral flow processes [Troch et al. 2003; Berne et al. 2005; Hazenberg et al. 2015; Ajami et al. 2016]. A third solution to the computing challenge, especially the concern that the computational cost of complex models sacrifices opportunities for analysis, is to focus on improving model analysis methods. Analysis of complex models is possible by developing surrogate models, i.e., models that emulate the behavior of complex models and run very quickly [Razavi et al. 2012]. Analysis of complex models is also possible through computationally frugal model analysis methods that require a fewer number of model simulations [Rakovec et al. 2014; Hill et al. 2015]. A way to support these type of methods is to use quasi-scale invariant parameterizations (e.g., MPR) to estimate transfer function parameters at coarser resolutions instead of using a high-resolution model setting. Since parameters obtained with the MPR technique are transferable across scales without significant performance loss, models can be applied at higher spatial resolutions as shown by Kumar et al 2013. This alternative would lead to computationally efficient large-scale hydrologic predictions and allows performing parameter estimation over large domains.

In short, solving computing challenges will require judiciously combining emerging computing capabilities, advanced numerical methods, justifiable model simplifications, and extensive use of computationally frugal model analysis methods.

5 Summary and next steps

In this paper we review key advances in process-based hydrologic models. We start with the seminal blueprint for a process-based hydrologic model, where Freeze and Harlan [1969] pose a series of questions that highlight the following three challenges: (1) reasonable mathematical descriptions of hydrologic processes; (2) sufficient information on model parameters; and (3) limitations in computing. We summarize the different ways that the community has risen to meet each of these challenges, emphasizing how diverse hydrologic modeling approaches are advancing our collective quest for physically realistic models.

In our view the challenges posed by Freeze and Harlan remain relevant today, and nicely frame the needs for future research. Specifically,

1. There is still considerable scope to improve mathematical descriptions of hydrologic processes. A major research challenge is the scaling/closure problem, i.e., to represent how large-scale fluxes are shaped by small-scale heterogeneities, interactions among processes, and the connectivity of water across the landscape. While the community has made progress in this challenge, through statistical-dynamical models, stochastic upscaling theory, scale-appropriate flux parameterizations, and spatial integration across discrete landscape types, much work is still required both to develop new closure schemes and to systematically compare existing modeling approaches.

2. There is also considerable scope to improve information on model parameter values and their associated uncertainties. Advances in parameter estimation will require focused effort on improving the available geophysical information (e.g., through improved observations), improving the links between geophysical information and model parameters, and more effective use of multivariate data to constrain model parameter values.

3. There is also a strong need to more effectively use the available computing resources. We argue here that in addition to exploiting advances in massively parallel computation and numerical solution methods, we can also make much more effective use of the available computing through more efficient/agile models (e.g., use of hydrologic similarity concepts). More effective use of available computing resources increase capabilities for model analysis and uncertainty characterization, shining the light toward further model improvements.

Stepping back, we see that the questions posed by Freeze and Harlan [1969] are indeed very challenging, and that the community has risen to hydrologic modeling challenges in diverse and productive ways. The community has made noteworthy advances in improving mathematical descriptions of hydrologic processes, in parameter estimation, and in identifying justifiable model simplifications that make more effective use of available computing resources. Many of these modeling advances are general, and can be applied across multiple models of different type and complexity. Looking forward, we argue that it is important to take a unified perspective, deliberately departing from previous debates on the "correct" approach to hydrologic modeling, and more effectively use the diversity of modeling tools in order to advance our collective quest for physically realistic hydrologic models.

The key challenge is perhaps best posed recently by Eric F. Wood: "*What modeling experiments need to be performed to resolve the "scale" question and what is the trade-off among model complexity, the physical basis for land parameterizations and observational data for estimating model parameters?*" [Wood 2012]. This issue stimulates and organizes our research activities. We need to continually (and collectively) refocus on this challenge in order to accelerate advances in process-based hydrologic models.

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Discussions

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