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Key Points:
- We seek to increase the physical realism of hydrologic models through better way existing theory
- We seek to improve the way models are used to integrate and evaluate different process explanations
- We define a set of key issues to address that will help narrow the gap between theory and models

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Improving the theoretical underpinnings of process-based hydrologic models

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Abstract In this Commentary, we argue that it is possible to improve the physical realism of hydrologic models by making better use of existing hydrologic theory. We address the following questions: (1) what are some key elements of current hydrologic theory; (2) how can those elements best be incorporated where they may be missing in current models; and (3) how can we evaluate competing hydrologic theories across scales and locations? We propose that hydrologic science would benefit from a model-based community synthesis effort to reframe, integrate, and evaluate different explanations of hydrologic behavior, and provide a controlled avenue to find where understanding falls short.

1. Motivation

The discipline of hydrology continues to be an exciting field, with ongoing advances in field observational techniques, availability of global data products, and increasing computational power. Now, perhaps more than ever before, we are rising to the challenge of building models of everywhere [*Beven*, 2007]. Key efforts include building continental-domain hydrologic models for water security assessments [*Schewe et al*., 2014; *Mizukami et al*., 2015] and improving the representation of hydrologic processes in Earth System Models [*Clark et al*., 2015a]. These efforts require moving beyond the traditional tactics used in hydrology, such as detailed analysis and modeling of individual catchments, which makes it difficult to generalize results to large domains and other hydrologic regimes. Instead, hydrologic synthesis across space and across many elements of hydrologic theory is needed, in order to improve the physical realism and general applicability of hydrologic models, i.e., to improve hydrologic process representations across a large range of catchments [*Gupta et al*., 2014]. To this end, some have argued (somewhat optimistically) that advances in modern hydrologic modeling efforts are possible through progress on the following fundamental research challenges: identifying consistently observed behaviors across research watersheds, formulating the laws that govern macroscale hydrologic behavior, and unifying process explanations across watersheds in order to develop theory of hydrology at the catchment scale [e.g., *Dooge*, 1986; *Sivapalan*, 2005; *McDonnell et al*., 2007].

The needs of the hydrologic modeling community as articulated in this way are admittedly sizeable and potentially insurmountable. This has led others to adopt a rather pessimistic view, doubting if it is even possible to generalize hydrologic behaviors given the unique character of individual basins [*Beven*, 2000]. This raises the question, do we now, and/or will we always, lack the necessary information on climate, topography, vegetation, soils, and subsurface structure required to develop powerful and exceptionless explanations? Put differently, are the problems of underdetermination so pronounced that we cannot move beyond explanatory pluralism [*Kleinhans et al*., 2005; *Beven*, 2006a,b]? These difficulties are shared across multiple disciplines, and are described very well in Nancy Cartwright's book "How the laws of physics lie" [*Cartwright*, 1983, p. 49]:

> "Covering-law theorists tend to think that nature is well regulated; in the extreme, that there is a law to cover every case. I do not. I imagine that natural objects are much like people in societies. Their behavior is constrained by some specific laws and by a handful of general principles, but it is not determined in detail, even statistically. What happens on most occasions is dictated by no law at all [. . .]"

The purpose of this paper is to bridge these two perspectives. On the one hand, we recognize that developing a unified hydrologic theory will be incredibly useful, and, on the other hand, we also recognize that the "messy" nature of the Universe makes theory development incredibly difficult. Nevertheless, we accept that elements of hydrologic theory exist now, and it is critical to reconcile hydrologic models with existing and emerging theory. While acknowledging uncertainty, underdetermination, and the difficulty to generalize, we contend that the hydrologic community has made tremendous advances over the past few decades in our capability to explain and predict individual processes, process interactions, patterns, and scaling behavior. However, process explanations (theories) are currently scattered across research groups and not yet widely incorporated in hydrologic models. Consequently, we propose that hydrologic science would substantially benefit from a model-based synthesis effort to systematically formulate, organize, formalize, encode, and evaluate hydrologic theories, i.e., to use models as a means to summarize, integrate, and test many different, sometimes competing explanations of hydrologic behavior. The idea is that such models, along with appropriate data, would be used to synthesize current process understanding and provide a controlled avenue to find where that understanding falls short.

The central thesis of this paper is as follows: it is possible to increase the physical realism and general applicability of hydrologic models by making better use of the elements of hydrologic theory that exist now. To this end, we explore the following three questions:

1. What are the key elements of current hydrologic theory? This requires research to reconcile consistently observed behavior in research watersheds with explanations of hydrologic processes, process interactions, and scaling behavior, and includes algorithmic implementations of explanations as encoded in models.
2. How should we incorporate the elements of existing hydrologic theory in models? This requires developing multiple parameterizations and numerical approximations of process explanations of a given theory, within a common modeling framework, implemented as falsifiable (testable) hypotheses. In this context, a community-based hydrologic modeling endeavor is needed, one like those implemented successfully in the atmospheric science and land-atmosphere interactions communities [*Lawrence et al*., 2011; *Hurrell et al*., 2013].
3. How should we evaluate competing hydrologic theories across scales and locations (while explicitly recognizing uncertainty)? To address this question, we argue that research is needed to design and implement a suite of diagnostic metrics to evaluate model hypotheses (using incomplete and inexact information), and to test the utility of models for prediction/extrapolation.

In addressing these questions, we follow a Popperian approach for discovery and learning via formulation of testable (falsifiable) hypotheses [*Popper*, 1959]. As highlighted in Figure 1, we adopt the modeler's perspective with a focus on the iterative refinement of models and theory via systematic testing of multiple hypotheses. Our main contribution is to define a key set of research challenges, and methods for addressing them, in order to improve the link between theory, models, and data.

A key facet of our approach is that we seek to improve the theoretical underpinnings of process-based hydrologic models, regardless of their complexity and intended purpose. We consider models of varying process complexity (i.e., models with a different number of processes explicitly represented), as well as models of different spatial complexity (i.e., spatially explicit models with different degrees of spatial discretization and connectivity, and spatially implicit lumped hydrologic models). Our primary considerations include both the underlying theories used to explain hydrologic behavior and how

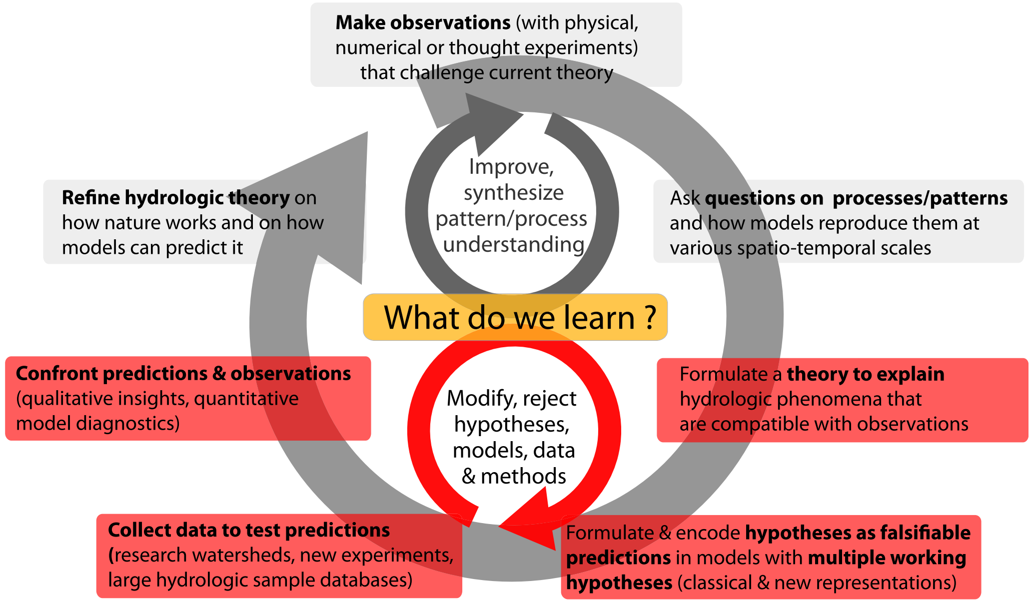

Figure 1. A theoretically grounded approach to hydrologic model development, following the scientific method as defined by *Popper* [1959]. This graphic is inspired by *Garland* [2015].

process explanations are represented in models. We accept that different models answer different questions; but argue that all process-based models should be as deeply rooted as feasible in the available hydrologic theory. The purpose of the model defines the simplifications of the theory that the modeler is willing to tolerate. By considering a broad range of process-based models, our desired outcome is to encourage more widespread adoption and scrutiny of hydrologic theory as part of model development.

The remainder of this paper is organized as follows. In section 2, we define what we mean by hypotheses, laws, and theories, and place typical pragmatic approaches to hydrologic model development in the context of discovery and learning. In section 3, we discuss exemplary areas in hydrology where the community has made progress in understanding hydrologic processes and developing mathematical representations of the process understanding. Our intent is to demonstrate how current hydrologic theory can be used to improve the scientific rigor of hydrologic models. In section 4, we briefly discuss how current hydrologic theories can be incorporated within a modeling framework, and in section 5, we discuss how theories can be tested and refined. We close with concluding remarks in section 6.

2. The Gap Between Theory and Models

Theory means different things to different people. To some, theory defines a concept that is unproven—a guess, or an educated guess—rather than a systematized understanding with explanatory power [*Corneliussen*, 2015]. To others, theory is an antonym of application, where efforts may be described as "very theoretical" even in the absence of explanation. More precise definitions are available in recent papers in hydrology. For example, *Sivapalan* [2005] defines theory as "*the set of ideas or concepts that is best able to describe or explain the system of interest, the catchment, its presence in the landscape, its behavior, and its function in relation to other systems*." Similarly, *Ehret et al.* [2014] define theory as the

> "Explanation of some aspect of the natural world, established by following the scientific method and confirmed by observation and experiment (empirical evidence). A theory has explanatory and predictive power; its strength is related to the parsimony of its principles, the diversity of phenomena it can explain and the quality of its falsifiable predictions [. . .]"

A theory is distinct from a scientific law—laws predict phenomena (e.g., Fourier's Law, Fick's Law, Ohm's Law, or even Darcy's Law, all of which are used in hydrologic models), but do not explain why phenomena occur. A theory is also distinct from a hypothesis, which is a falsifiable statement (usually a quantifiable corollary under specific conditions) used to test a given theory (Figure 1).

For us, hydrologic theories are the stories that we tell to explain observed hydrologic processes. In this simple and general definition, we permit theories of varying strength (i.e., of varying explanatory and predictive power), we permit theories that explain and predict only a subset of hydrologic processes (i.e., the theories need not be comprehensive), and we do not require that theories be accepted as an accurate explanation by a broad cross section of the scientific community. In this sense, we define hydrologic theory as our explanations of individual processes, process interactions, patterns, and scaling behavior. Our definition of theory is deliberately permissive—we all strive for theories that are strong, unified, and well accepted, but at this stage, we do not impose such restrictions so that we can focus on testing, refining, and reconciling the widest set of theories that already exist.

To expand on what we mean by theory, we provide some examples of general process explanations. First, consider snowmelt. Snowmelt is driven by the net fluxes of solar and long wave radiation, sensible and latent heat, the heat advected by precipitation, and the diffusion of heat throughout the snow-soil system [*Clark et al.*, 2015c, equation (11)]. This general understanding of snowmelt energetics is well established and incorporated into process-based models [*Slater et al.*, 2001; *Etchevers et al.*, 2004]. A common algorithmic simplification is that snowmelt can be parameterized as a function of air temperature [*Hock*, 2003], which could be put in "law" form as "snow melts faster on warm days" or "the amount of snow that melts each day varies linearly with air temperature." This temperature-index approach to snow modeling has some relationship with energy balance theory. For example, several components of the energy balance, including sensible heat flux and incident longwave radiation (which dominates the energy balance in many settings [*Ohmura*, 2001]), are explicit functions of air temperature. However, generalizing using temperature-index snow models is limited because strong spatial variations in temperature-melt relationships make it difficult to extrapolate the model parameters across space. Moreover, these simplifications are likely to fail for extreme events or under climate change where the correlation between air temperature and snow-atmosphere energy fluxes is nonstationary [*Huss et al.*, 2009]. Similar issues may arise for other physical processes—for example, parameterizing potential evapotranspiration as an empirical function of air temperature, i.e., neglecting energy balance theory, can exaggerate the hydrologic sensitivity to climate change [*Milly and Dunne*, 2011; *Sheffield et al.*, 2012; *Roderick et al.*, 2014].

More generally, consider explanations (theory) for a suite of interacting hydrologic processes. For example, with theory encoded in a model, we can (to some extent) explain and predict the area-average infiltration due to spatial variability in water table depth [*Beven and Kirkby*, 1979], spatial variability in soil moisture [*Moore and Clarke*, 1981; *Wood et al.*, 1992], or spatial variability in hydraulic conductivity [*Hawkins and Cundy*, 1987]. We have critiques and comparisons of these process theories [*Beven*, 1997; *Clark and Gedney*, 2008; *Clark et al.*, 2008]. Similarly, we can explain and predict area-average transpiration related to spatial variability in vegetation phenology [*Koster and Suarez*, 1992; *Liang et al.*, 1994; *Bonan et al.*, 2002] or related to spatial variability in plant-available water [*Famiglietti and Wood*, 1994; *Koster et al.*, 2000]. We can also explain and predict nonlinear recession behavior based on spatial heterogeneity in hydraulic conductivity [*Clark et al.*, 2009; *Harman et al.*, 2009] or nonlinearity in runoff generation associated with thresholds, hydrologic connectivity, and hydrologic hotspots [*Tromp-van Meerveld and McDonnell*, 2006; *Lehmann et al.*, 2007; *Seyfried et al.*, 2009; *Zehe and Sivapalan*, 2009; *Jencso and McGlynn*, 2011]. The point of highlighting these example research areas is that many process explanations already exist; the issue is that many important process explanations are not widely implemented as falsifiable hypotheses. Most commonly, the explanations (theory) for a particular behavior (formulated as a law rather than a hypothesis) are accepted within a given model and applied outside of the basins where the theory may have originally been developed and tested. This represents a missed opportunity to generalize and further test the same theory in different basins.

The gap between theory and models becomes evident when we consider that, in practice, a pragmatic rather than a process-based approach to hydrologic model development is generally followed. The pragmatic approach uses spatial discretizations, process parameterizations, and time stepping schemes borrowed from other extant models (e.g., reliance on the 1-D moisture-based form of Richards' equation in land models [*Clark et al.*, 2015a]). The pragmatic approach is often quite effective in generating predictions—multiple processes can lead to similar behavior, and hence multiple processes can be represented by the same law [*McDonnell*, 2013]; however, this often comes at the expense of poor explanatory power and poor parameter transferability. The process-based approach, by contrast, is the classical approach described in recent textbooks and papers [*Beven*, 2012; *Gupta et al*., 2012]: to first develop a conceptual representation of our understanding of how the world works based on inductive reasoning from observations, i.e., the theories we use to explain hydrologic behavior, and then encode algorithmic simplifications of our conceptualizations in a numerical model. Only a handful of hydrologic studies have followed the process-based approach to hydrologic models, by encoding theories as testable hypotheses in order to challenge and refine our understanding of hydrologic behavior [*Freer et al*., 2004; *Lehmann et al*., 2007; *McMillan et al*., 2012; *Euser et al*., 2013; *Fenicia et al*., 2014].

The pragmatic modeling approach most often applied in practice tends to sever the link between the models and the body of theory, thereby impeding continued refinement of our process understanding. Specifically, the pragmatic approach focuses attention on a model's predictive competence rather than its explanatory power. This limits our ability to generalize about hydrologic behaviors, leading to model "tuning" for particular basins, giving the impression that every basin is unique [*Beven*, 2000; *McDonnell et al*., 2007]. If we cannot trust these models to generalize across observed space now, how can we trust them to predict historically unseen conditions? There is, at present, only a thin theoretical foundation to support applying models in new settings. Even worse, when models fail in new settings, it is difficult to know which body of theory requires updating, particularly when it is faster and easier to update the parameters and move on with the immediate task at hand—generating predictions.

3. Toward a Model-Based Synthesis of Hydrologic Theory

We now return to the primary concern of this paper: to reconcile hydrologic models with existing hydrologic theory. The first question is then "what theory"? Do the elements of hydrologic theory already exist, or is theory something that the hydrologic research community has yet to discover? Much of the relevant literature—e.g., *Searching for the Holy Grail of scientific hydrology* [*Beven*, 2006b]—concludes that our quest for explanations and model parameterizations of large-scale fluxes has not yet been successful. Although we agree with this, we recognize that hydrological research has produced many process explanations and model parameterizations that can be much better exploited in models than has been done to date. Therefore, we propose to first synthesize and test existing hydrological knowledge in models, before identifying what knowledge is crucially missing.

Key questions that need to be addressed are:

1. What existing hydrologic theories are included in models and what aspects of theory are ignored or not well assimilated?
2. What are the most important aspects of hydrologic theory that are not yet incorporated in models?
3. In what parts of extant models do existing theories have the most (and the least) explanatory power?

The first issue at hand is therefore to identify some useful elements of existing hydrologic theory. We consider advances in both the explanatory and predictive capabilities of models in three main areas: (a) developing ways for the structure of the landscape to be better represented in the structure of models; (b) advancing understanding of how small-scale processes combine to produce large-scale fluxes (emergent behavior) and the development of ways to parameterize this effect in models; and (c) advancing understanding of how the principles of optimality (or ecological and landscape evolution) can be used to make macroscopic predictions at the scale of interest. The following subsections expand on these topics.

3.1. Reflecting the Structure of the Landscape in the Structure of Models

The modeling community has pursued multiple methods to reflect the structure of the landscape in hydrologic models. An interesting example is Keith Beven's "alternative blueprint" [*Beven*, 2002], which provides a substitute for the Freeze-Harlan blueprint for physics-based hydrologic modeling [*Freeze and Harlan*, 1969]. Beven's idea is that the structure of hydrologic models should reflect the structure of the landscape (e.g., topography, vegetation, soils, geology), and he emphasizes the need to extensively experiment with different model structures and parameter sets in order to identify an ensemble of "behavioral" hydrologic models [*Beven*, 2002]. However, applications of this alternative blueprint typically use models of lower state dimension, i.e., models with extensive lumping of physical processes and of the physical landscape, which can obscure the connection between the model structure and the landscape structure [although see *Peters et al.*, 2003; *Rinaldo et al.*, 2006; *Fenicia et al.*, 2014]. The key question here is as follows: to what extent do models reflect our explanations of landscape controls on the space-time variability in hydrologic states and fluxes?

To develop and test theories that relate landscape properties to hydrologic behavior, we propose that the following tasks should be systematically dealt with:

a. Investigate how available theories can enable information on geomorphology, topography, vegetation, soils, and geology to be better used for defining model structure/parameters in different landscapes [*Samaniego et al.*, 2010; *Schaefli et al.*, 2014; *Zehe et al.*, 2014].
b. Investigate the challenges in model-landscape mapping when hydrologic models are the basis for water quality and stream ecosystem models. Typical challenges include how to incorporate representations of the dynamics of surface flow connectivity between sediment sources and the stream channel [*Bracken et al.*, 2015], the distinct thermal and biogeochemical signatures associated with different flow paths and network topology [*Kurylyk et al.*, 2014; *Leach and Moore*, 2015], as well as the behaviors of in-stream algae, invertebrates and fish [*Power et al.*, 1995; *Ceola et al.*, 2014];
c. Develop approaches for model-landscape mapping that can be applied in models of varying complexity, and account for landscape heterogeneity; and
d. Investigate to what extent it is possible, with typically available information, to discriminate among competing models to define alternative model structures in different landscapes [*Jakeman and Hornberger*, 1993; *Gupta and Nearing*, 2014].

These issues dig into to the heart of different philosophical approaches to hydrologic modeling [*Harman and Troch*, 2014], especially the extent to which the details of the landscape are included in models, and the extent to which modelers pursue the quest for explanation versus prediction. For example, does the lumping of processes and the landscape in spatially lumped models limit the extent to which the structure of the landscape can be reflected in the structure of models? Put differently, is the structure of the landscape actually better reflected in spatially explicit models, where the higher granularity of process representations and the higher granularity of the landscape discretization enable examination of how geomorphology and spatial variability in topography, vegetation, soils, and geology affect the space-time variability in hydrologic states and fluxes? To what extent are spatially explicit models limited by the available data? Are models with detailed spatial representations extensible to other watersheds that are very different from where they were developed? Focused attention on these issues will help with the model implementation and testing of theories that map patterns to processes [*Sivapalan*, 2005; *McDonnell et al.*, 2007], and will help improve how the details of the landscape are represented in models [*Wigmosta et al.*, 1994; *Beven and Freer*, 2001; *Bonan et al.*, 2002; *Tague and Band*, 2004; *Vivoni et al.*, 2005; *Clark et al.*, 2015b].

3.2. Scale-Emergent Behavior

A key challenge in hydrologic model development is to explain and predict how small-scale processes combine to affect large-scale fluxes [*Reggiani et al.*, 1998; *Reggiani et al.*, 1999; *Beven* 2006b; *McDonnell et al.*, 2007; *Troch et al.*, 2009]. This typically involves (a) formulating conservation equations for physically meaningful control volumes within the model domain and (b) parameterizing fluxes at the boundaries of model control volumes in a way that represents the impact of subgrid-scale heterogeneities on grid-average fluxes. A major model development challenge is parameterizing grid-average fluxes, termed the "closure problem" [*Reggiani et al.*, 1998, 1999; *Reggiani and Schellekens*, 2003; *Beven*, 2006b]. Solutions to the closure problem have proved to be rather difficult [*Zehe et al.*, 2006; *Harman and Sivapalan*, 2009].

To synthesize current hydrologic theory and modeling approaches, and to advance scale-appropriate flux parameterizations, the following tasks should receive immediate attention:

a. Identify which theories can explain and predict the impacts of structural and process heterogeneity on large-scale fluxes.
b. Investigate the relative advantages of the different methods used to represent how small-scale process interactions affect large-scale behavior.

In addressing these tasks, we recognize that emergent behavior has been represented in many different ways in many different models, providing an existing theoretical backbone to hydrologic models. The main approaches are (a) spatial integration of the small-scale equations [*Maxwell and Kollet*, 2008; *Kollet et al*., 2010]; (b) development of "scale-appropriate" flux parameterizations, such as subgrid probability distributions [*Beven and Kirkby*, 1979; *Moore and Clarke*, 1981; *Liang et al*., 1996; *Koren et al*., 1999; *Luce et al*., 1999], and new (upscaled) model equations [*Mahrt*, 1987; *Essery et al*., 2008], including empirically derived storage-discharge relationships [*Ambroise et al*., 1996; *Clark et al*., 2008; *Fenicia et al*., 2011]; (c) representing the role of thresholds and connectivity in defining larger-scale responses (e.g., the need to fulfill depression storage as in wetlands and bedrock topography) [*Freer et al*., 2002; *Tromp-van Meerveld and McDonnell*, 2006; *Clark et al*., 2009; *Jencso et al*., 2009; *Zehe and Sivapalan*, 2009; *Spence et al*., 2010; *Shook et al*., 2013]; and (d) formulation of macroscopic principles acting at the scale of interest [*Rodríguez-Iturbe et al*., 1992; *Caylor et al*., 2009; *Schymanski et al*., 2009a; *Schymanski et al*., 2010]. These modeling approaches are not mutually exclusive, indicating the lack of a unifying theory in hydrology [*Sivapalan*, 2005]. Most models include some mix of methods to parameterize the impact of subgrid-scale heterogeneities on large-scale fluxes, and it is necessary to synthesize, evaluate, and compare these methods, and most particularly the theory that they encode, in order to improve explanations of hydrologic processes and improve the physical realism of hydrologic model structures.

3.3. Optimality-Emergent Behavior

The idea of self-optimization of biological systems is closely related to the theory of evolution and natural selection [*Sutherland*, 2005]. In ecohydrology and geomorphology, optimality principles have been applied to explain various observed patterns and predict responses of natural systems to external forcing based on the idea that the most probable landscape evolution pathway is that toward effective dissipation of energy gradients or that natural selection favors plants with optimal use of the available resources [*Rodríguez-Iturbe et al*., 1992; *Rigon et al*., 1993; *Eagleson*, 2002; *Schymanski et al*., 2008; *Schymanski et al*., 2009a; *Zehe et al*., 2013; *Bonan et al*., 2014; *Schymanski et al*., 2015]. In contrast to predicting large-scale behavior emerging from small-scale processes, optimality seeks to predict emergent behavior stemming from self-organization following a macroscopic extremum principle, such as maximization of net carbon profit for vegetation or maximization of energy dissipation or entropy production for both physical and biological systems. The appeal of such extremum principles is that they reduce the number of unknowns in a system, which facilitates generalization, testing, and falsification [*Schymanski et al*., 2009b; *Schaefli et al*., 2011]. At the same time, optimality theory can inspire new questions about underlying processes.

Canopy photosynthesis, for example, is commonly modeled using a mechanistic photosynthesis model, representing the canopy either as one or two big leaves or layers of foliage, each of which has their own biochemical properties [*de Pury and Farquhar*, 1997]. The photosynthetic parameters for each leaf or foliage layer are generally assigned empirically or through calibration. In contrast, *Schymanski et al*. [2007] used a similar mechanistic photosynthesis model, but predicted the number of foliage layers and the photosynthetic capacity in each layer based on the hypotheses that these are optimal for achieving the maximal net carbon profit for the given observed water use. They found that the resulting leaf area index and canopy photosynthesis rates were consistent with observations in a tropical savanna during the wet season, but greatly overestimated during the dry season. This inspired the question if water use and foliage maintenance during the dry season has a different set of costs associated with it than during the wet season, and led to successful development of optimality-based models of the root system [*Schymanski et al*., 2008] and an integrated model including canopy, roots and the water balance [*Schymanski et al*., 2009a]. In each of these studies, optimality helped predicting system properties that were commonly parameterized empirically, illustrating its capacity to generate falsifiable predictions.

An optimality-based model and a detailed mechanistic model may result in similar macroscopic predictions, for example, about vegetation water use in the different environments, but the latter would need more detailed input information and yield more detailed predictions about surviving plant types in a given environment. One could expect that optimal resource use might generally act to reduce spatial variance in soil moisture by enhanced evapotranspiration (ET) in wet systems and more conservative ET in dry systems. From a more mechanistic point of view, high moisture systems should generally consist of plants that have less conservative water use strategies and water transport systems (think Coastal Redwoods), because light competition will more commonly limit individual survival [*Ambrose et al*., 2015], whereas plants in drought-prone semiarid locations likely have more conservative water use strategies and transport systems that foster moisture retention, reducing embolism risks [*McDowell et al*., 2011]. The mechanistic, physiological conceptualization provides a theoretical basis and a path for testing an optimality hypothesis, but from a modeling perspective, detailed modeling poses a burdensome framework with its own baggage of uncertainty. Resolving the mechanistic complexity into the simpler, emergent statement of optimality has benefits very similar to those of resolving spatial complexity as discussed in section 3.2.

The following tasks regarding development and application of optimality theory in support of hydrologic model development would likely advance the field:

a. Investigate how alternative optimality constructs [see e.g., *Schymanski et al*., 2009a] can be implemented and tested in hydrological models in a comparative way judging to what extent they explain various observations at the scale of interest.
b. Develop and clarify the underlying ecological and thermodynamic theories that explain why optima might be expected to occur, what are the relevant constraints and the related uncertainties.
c. Explore generality and limits for applicability of optimality principles across climates, geologies, levels of human modification, and scales.

Some parts of the watershed system are primarily externally imposed features, such as bedrock geology, topography, or climate, at least at practical time scales. Other parts are more dynamically entangled; particularly, vegetation [*Schymanski et al*., 2015] and soils [*Zehe et al*., 2014], and their consequences for evapotranspiration partitioning can affect a large fraction of the water balance. If the behaviors of these dynamically entangled system components emerge as tendency toward extrema in particular system states or fluxes, tremendous constraints can be placed on expected outcomes. Given the importance of water in ecological process, this vein of work holds promise to be fruitful for development and testing of both ecological and hydrologic theory, potentially increasing robustness of climate change predictions for vegetation communities as well as the coupled hydrologic outcomes.

3.4. Summary: Capitalizing on Existing Theory

The intent of our discussion here is twofold: (1) to focus attention on some key areas where hydrologic theory already exists and (2) to define a set of issues that need to be addressed in order to better represent this existing theory in models. For landscape structure, we recognize the opportunities to improve model representations of how landscape structure affects the space-time variability in hydrologic states and fluxes; and also that there are substantial challenges associated with data limitations and model identification in order to incorporate landscape structure in models with different complexity and with different intended purposes. For scale-emergent behavior, we recognize large advances in our capabilities to explain and predict fluxes of water and energy at larger scales; but note that we still lack information on the general applicability and relative merit of these different explanations and model parameterizations. For optimality, we recognize its potential for greatly focusing the range of likely behaviors of a given catchment; and also that we do not yet understand the limits of optimality-based reasoning or the extent to which it may be useful in different physical settings. These issues bring us to the next two challenges: how can theories be incorporated in models, and how can the theories be evaluated?

4. Model Construction: Implementing Theories in Models

To define a path forward for model construction, we return to our original premise: modern hydrologic models do not reflect the current understanding of hydrologic processes, i.e., theory. At the simpler end of the spectrum, hydrologic models are too often based on empirical postulates (e.g., parsimonious storage-discharge relationships that describe the aggregate response of a catchment to external forcing), without explanations of why those relationships occur. At the complex end of the spectrum, hydrologic models are based on physically motivated partial-differential equations that rely on empirical small-scale closure relations (e.g., the soil water constitutive functions that describe the storage and transmission of water through soils). These small-scale closure relations however do not represent the impact of small-scale heterogeneities on large-scale fluxes (e.g., many physically motivated models neglect the importance of hillslope-scale connectivity and preferential flow in shaping catchment-scale fluxes). Such weak theoretical underpinnings lead several commentators to criticize the current generation of models for "getting the right answers for the wrong reasons" [*Kirchner*, 2006] or for being "process weak" [*McDonnell et al*., 2007].

Improving the theoretical underpinnings of hydrologic models requires a modeling system to systematically evaluate different numerical implementations of current hydrologic theories. As a next step, we propose that the following tasks need to be carried out:

a. Find ways to best encode different theories in our models, to allow for hypothesis generation, testing, grading, selection, and structured model improvement.
b. Investigate how (and where) we can best incorporate algorithmic simplifications of varying complexity, to represent limited knowledge of hydrologic processes and catchment characteristics.

Addressing these issues is possible through recent model development efforts that pursue the method of multiple working hypotheses [*Chamberlin*, 1890; *Clark et al*., 2011]. Modern model implementations of the method of the multiple working hypotheses now exist, offering a "master template" from which it is possible to incorporate different modeling decisions, process parameterizations, and spatial organization [*Kraft et al*., 2011; *Niu et al*., 2011; *Essery et al*., 2013; *Clark et al*., 2015b,c]. Recent advances in the development of multiple hypothesis modeling frameworks include: (1) the capability to represent all the biophysical and hydrologic processes thought to be relevant, extending beyond traditional land surface models as well as traditional hydrology models, and including options for model simplification (e.g., ignore or implicitly represent specific state variables and fluxes); (2) implementation of modeling approaches in a clear and modular fashion, in order to incorporate multiple competing hypotheses of hydrologic behavior; (3) flexible and hierarchical spatial organization, in order to experiment with different model representations of spatial variability and hydrologic connectivity; and (4) incorporation of different strategies to estimate and adjust model parameters [*Clark et al*., 2015b]. These advances notwithstanding further developments to multiple hypothesis modeling frameworks are required to better incorporate existing hydrologic theory (as proposed in this paper).

A key research priority is to define a community-based approach to incorporate hydrologic theories in models, building on the successful implementation of community models in the atmospheric science and land-atmosphere interactions communities [*Lawrence et al*., 2011; *Hurrell et al*., 2013]. This issue has received some attention in the hydrologic literature; most recently where *Weiler and Beven* [2015] consider the need for a community hydrologic model. Weiler and Beven offer an interesting and wide-ranging discussion on the challenges of agreeing on the modeling concepts, of adequate support and effective governance, and, critically, in the context of this paper, of the need to evaluate alternative formulations of subelement parameterizations at different spatial scales and hydrologic regimes. Weiler and Beven argue that "*the most important aspect of a Community Modeling Initiative is to instigate a discussion* [on what process parameterizations should look like], *test the potential alternatives, understand their domain of applicability, and agree on a formulation, before such a model is released for general use*." *Weiler and Beven* [2015] deliberately avoid defining what a model should look like and how a model can be tested, and they leave as an open question whether such a community model could be programmed in a way that is agile enough to be used as an effective learning tool.

Here we propose a specific path forward for community modeling that is more focused than the path proposed by *Weiler and Beven* [2015]: our primary aim is to evaluate alternative hydrologic theories and associated process parameterizations as well as alternative modeling concepts. We impose no requirement that we attain *agreement* on modeling concepts, and we hence deliberately take a model agnostic position to implement and test multiple theories and associated process parameterizations. Our proposed approach is the unified approach to hydrologic modeling defined by *Clark et al*. [2015b]. This modeling approach cleanly separates the conservation equations from the flux parameterizations, providing the flexibility to incorporate multiple modeling options to calculate the flux across the boundaries of model control volumes. The modeling approach employs hierarchal data structures, providing the flexibility to define multiple representations of spatial variability and hydrologic connectivity, including models with different spatial architecture and complexity. This flexibility enables users to isolate and evaluate individual modeling decisions, enabling the use of models as virtual laboratories [*Weiler and McDonnell*, 2004; *Sivapalan*, 2005; *Blöschl*, 2006; *Wagener et al*., 2010] to help formalize and evaluate alternative hydrologic theories.

An important point here is the need for a community modeling *process* rather than a community hydrologic model. Given the diverse range of questions that the discipline of Hydrology seeks to answer, it is unreasonable (and unwise) to formulate a single community model for all purposes. The critical need is to further develop the "community of practice" of hydrologic modeling to consistently test and compare competing hypotheses and algorithms, i.e., to test and compare competing modeling approaches. This requires strong community engagement in formulating and evaluating multiple competing hypotheses. Such community efforts should be conducted within modeling frameworks that recognize the similarities among extant models, and control for their differences, and hence help form general conclusions of widespread relevance across models with very different objectives. A key metric of success will be seeing our "best" theory incorporated in a wider range of multidisciplinary modeling efforts, such as improving the representation of hydrologic processes in Earth System Models [*Clark et al.*, 2015a], to ensure robust predictions of global environmental change.

5. Model Evaluation: Developing a Rigorous Approach to Evaluate and Select Among Competing Theories

A key issue in hydrologic model development, and also in achieving the solidification of theory, is the rationale used to select among competing alternatives. Our principles for model development are often based on individual philosophical penchants for either physics or parsimony [*Ebel and Loague*, 2006; *McDonnell et al.*, 2007], but neither is fully supported by data nor model analysis [*Smith et al.*, 2013; *Mendoza et al.*, 2015]. Here we argue for a more systematic and robust approach to discriminate among model alternatives.

The issue at hand is the process for theoretical development outlined in Figure 1. At the stage where the data confronts the model, there is an option to detour on a side-loop where we calibrate model parameters—perhaps parameters derived from the theory in question, or perhaps parameters in other parts of the model. It is well understood that we can take that side-loop many times to avoid "the slaying of a beautiful hypothesis by an ugly fact" [*Huxley*, 1894]. Put differently, the process of model calibration can render model hypotheses unfalsifiable. This leads us to wonder whether we are actually in a situation where the current state of hydrology is too accepting of competing theories, and where hydrologic applications rely on calibration at the expense of understanding because explanation cannot be established with sufficient confidence.

Addressing the following questions will help to challenge and refine our hydrologic theories:

a. How can we best distinguish among competing theories? How can we best balance quantitative and qualitative insights to challenge and refine theories [*Seibert and McDonnell*, 2002; *Freer et al.*, 2004; *Winsemius et al.*, 2009; *Euser et al.*, 2013; *Seibert and McDonnell*, 2013; *Birkel et al.*, 2014; *Wrede et al.*, 2014], especially given limitations of information on internal model states and fluxes?
b. What are the best model application practices for testing theories as opposed to continuing to increase model complexity when confronted with additional data?
c. What does a falsification framework look like? How can we improve understanding of the worth of data and the sensitivity of model rejection to assumptions and experimental designs? How can we meaningfully discriminate among competing hypotheses in the presence of incomplete and inexact information?
d. What are the applications (and limits) of information theory to select among competing theories [*Gupta and Nearing*, 2014; *Nearing and Gupta*, 2014]?

We suggest performing at least the following tests to evaluate a hydrologic model or a land surface model: (1) evaluate model simulations at internal locations within a given model element (e.g., eddy covariance stations, cosmic ray probes, streamflow gauging stations, and snow depth measurements) not used during parameter estimation [*Freer et al.*, 2004; *Smith et al.*, 2013; *Rakovec et al.*, 2015]; (2) evaluate model simulations at many locations, especially those with climatic regimes different from that used for parameter estimation [*Nijssen et al.*, 2001; *Seibert*, 2003; *Wenger et al.*, 2010; *Coron et al.*, 2012]; (3) evaluate internal model states across multiple spatial scales [*Kumar et al.*, 2012]; (4) test the flux matching condition between simulated fluxes across scales [*Samaniego et al.*, 2010; *Kumar et al.*, 2013]; and (5) assess comparability and reproducibility of model results [*Ceola et al.*, 2015]. The fundamental goal is to evaluate energy fluxes at the native scales at which observations can be made, for example, from control volumes varying from 10^2 m (cosmic ray probe) to 10^5 m (GRACE satellite footprint). The common practice in hydrology of using univariate signatures to infer model parameters provides only weak constraints on model simulations of the terrestrial hydrologic cycle [*Gupta et al*., 2008; *Rakovec et al*., 2015].

The path toward meaningful model evaluation must embrace, or at least acknowledge and account for, underdeterminism [*Kleinhans et al*., 2005; *Beven*, 2006a,b]. One path forward is to conduct controlled experiments, e.g., through targeted collection of the necessary data to test specific model constructs and hypotheses. This path was proposed by *Zehe et al*. [2014] to test their ideas of using functional units to represent the spatial organization of hydrologic processes. While critical, resource constraints invariably mean that such controlled experiments are limited in extent, constraining our capabilities to generalize. A parallel path forward is to evaluate individual model hypotheses in isolation [*Clark et al*., 2011]. This involves first decomposing a high-dimensional model into the individual decisions made during model development (as discussed in section 4), and then making better use of the data that we do have to evaluate different model development decisions (which are ideally formulated as falsifiable concepts; see Figure 1). In this context, underdeterminism can be reduced by defining metrics, or diagnostic signatures, that provide insight into the internal states and fluxes [*Kirchner et al*., 1996; *Gupta et al*., 2008; *Euser et al*., 2013; *Birkel et al*., 2014], using new measurement technologies that provide information at higher spatial and temporal resolution or that cover larger spatial areas [*Tyler et al*., 2009; *Zreda et al*., 2012], and qualitative insights [*Winsemius et al*., 2009; *Wrede et al*., 2014]. Underlying both of these paths is uncertainty in myriad sources. Uncertainty in model inputs, in the details of landscape structure, and in evaluation data are all important factors limiting the extent to which it is possible to discriminate among competing model alternatives; hence, characterizing these uncertainties in a meaningful way is crucial to avoid incorrectly rejecting behavioral model structures [*Beven et al*., 2012; *Clark et al*., 2012]. Ultimately, if the outcome of the evaluation procedure is the inability to test a given hypothesis with our current observation capabilities, this would indicate a need for additional theory development, the need to identify priorities for future observing capabilities, or both.

As with model construction, evaluation should be a community effort: that is, where the community actively compares and debates the merits of alternative evaluation approaches using a framework that helps minimize the differences among models and model configurations [*Ceola et al*., 2015; *Clark et al*., 2015b]. This enables the community to move forward from developing models for particular basins to models maintained by a community and tested everywhere. The key to progress is to find cases around the world in which community models (sets of hypotheses) do not work well, and also where data exist with sufficient quality and density to evaluate why. These cases will provide the hints on how to move forward—failures are therefore the key to improve our theories. The ultimate goal is to have open source community models that are in principle applicable worldwide, and have open source multivariate and multiscale data available for comprehensive model evaluation (recognizing data paucity and uncertainty). This requires substantial breadth of information across a diverse range of watershed types along with demonstrated depth of observing capabilities in specific locations [*Gupta et al*., 2014]. With that, we anticipate that the community will drastically advance model evaluation frameworks, gather and bring together relevant data, extensively test hypotheses, and accelerate progress for the discipline of hydrology as a whole.

6. Concluding Remarks

Many have argued that there is a need to “discover” new laws and theories in hydrology. These discussions have tended to focus on particular problem areas (e.g., floods) or processes (e.g., hillslope storage). An underlying common theme has emerged where laws and theories are lacking to address these challenges in a common way—that there are no general principles, only separate applications to unique catchments [*Beven*, 2000; *McDonnell et al*., 2007]. In this Commentary, we depart from earlier narratives by arguing that substantial bodies of theory already exist for hydrology, but are rarely recognized as such; moreover, important elements and insights drawn from existing theories are not widely or consistently implemented and tested in hydrologic models, particularly for regular applications outside of watersheds where individual models have been developed and tested. More generally, we argue that the growing gap between models and theory is impeding the progress of hydrologic science.

We propose here that it is possible to improve the theoretical underpinnings of hydrologic models by focusing attention on three related issues. First, we propose that a useful starting point is the synthesis of our understanding of hydrologic processes (hydrologic theory), based on commonly observed behavior in research watersheds (formulated as hydrologic laws). Ultimately this synthesis will result in multiple algorithmic simplifications of the components of hydrologic theory, including algorithms of varying complexity. Second, we propose that these multiple theory-based conceptualizations be systematically incorporated into community models, encoding theory into models as multiple testable hypotheses, to enable systematic scrutiny of competing hypotheses. Third, we propose that comprehensive, multiscale, diagnostic, model evaluation be designed and systematically carried out to apply, challenge, and subsequently refine current hydrologic theory and its instantiations in hydrology models. Our proposed synthesis effort requires research to systematically formulate, organize, encode, and evaluate hydrologic theories, so that our models synthesize the best process understanding and are used as an avenue to evaluate and refine hydrologic theories. A key challenge is to develop methods that use incomplete and inexact information to effectively evaluate competing hypotheses, and to improve the extent to which we can scrutinize and refine hydrologic theories. Such a synthesis will strengthen the link among algorithms, theory, and observations, improving our understanding of the impact of model simplifications, increasing the fidelity of model simulations, and, ultimately, increasing our confidence in model predictions.

Pursuing the questions defined in this paper will be challenging, and requires strong community engagement. The questions we pose require a broad range of interdisciplinary expertise; the quest for generality requires synthesis across a broad range of hydrogeoclimatic regimes, and an enhanced model-based synthesis and evaluation procedure require developing creative and effective methods for model construction and analysis. We therefore welcome collaborations from scientists interested in the synthesis of process explanations and modeling approaches across diverse physical environments, in constructing models to encode the components of hydrologic theory as testable hypotheses, and in advancing model evaluation efforts to provide meaningful and comprehensive evaluation of model alternatives (i.e., model evaluation under uncertainty). Such strong community engagement will enable the community to move forward from developing models for particular basins to theoretically grounded models maintained by the community and tested everywhere, which will accelerate the continuing refinement of hydrologic models and the grounding theory they encode.

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