An overview of current applications, challenges, and future trends in distributed process-based models in hydrology

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Highlights

- Reasons for use of distributed process-based hydrological models are reviewed.
- Avenues for developments of process-based hydrological models are presented.
- Hydrology will depend on appropriate use of process-based models.

Abstract

Process-based hydrological models have a long history dating back to the 1960s. Criticized by some as over-parameterized, overly complex, and difficult to use, a more nuanced view is that these tools are necessary in many situations and, in a certain class of problems, they are the most appropriate type of hydrological model. This is especially the case in situations where knowledge of flow paths or distributed state variables and/or preservation of physical constraints is important. Examples of this include: spatiotemporal variability of soil moisture, groundwater flow and runoff generation, sediment and contaminant transport, or when feedbacks among various Earth's system processes or understanding the impacts of climate non-stationarity are of primary concern. These are situations where process-based models excel and other models are unverifiable. This article presents this pragmatic view in the context of existing literature to justify the approach where applicable and necessary. We review how improvements in data availability, computational resources and algorithms have made detailed hydrological simulations a reality. Avenues for the future of process-based hydrological models are presented suggesting their use as virtual laboratories, for design purposes, and with a powerful treatment of uncertainty.

1. Introduction

The development of process-based watershed models based on the concepts of observability and scalability of physical hydrological processes has roots that go back almost fifty years with the works of Crawford and Linsley (1966) and Freeze and Harlan (1969). Despite the success of the approach in subsequent decades (e.g., Stephenson and Freeze 1974, Abbott et al. 1986), initial optimism has increasingly been challenged by the scientific community (e.g., Beven 1989). The idea that a mathematical model can provide accurate results across different climates, watersheds, and hydrological extreme conditions based on physical laws and parameters determined *a priori* has been considered a "Hydrologic El Dorado" or an unachievable goal (Woolhiser 1996, Grayson et al. 1992). Furthermore, the challenges imposed by hydrological process non-linearity, temporal and spatial scale dependence, system observability and heterogeneity, and parameter equifinality, among other issues, have led to questioning the usefulness of the approach (e.g., Beven 1989, 2001, Beven and Cloke 2012) and to proposals of alternatives (e.g., Beven 2002, Sivapalan 2003, McDonnell et al. 2007, Wagener et al. 2007, Troch et al. 2008, Clark et al. 2011).

Concurrently, hydrology has gained a broad, international recognition as a geoscience moving from an appendix of textbooks on hydraulics and geology (Klemes 1986, 1988, Bras and Eagleson 1987) to a cornerstone discipline in the geosciences (Bras 2009). Process-based watershed modeling has played an important role in this development, in particular for interdisciplinary efforts such as ecohydrology, geomorphology, cryospheric science, and land-atmosphere interactions (e.g., Bras et al. 2003, Ebel and Loague 2006, Loague et al. 2006, Rigon et al. 2006, Maxwell et al. 2007, Ivanov et. al. 2008a, Yetemen et al. 2015). Process-based modeling approaches are also believed to help provide predictions under a non-stationary climate (Huntington and Niswonger 2012, Sulis et al. 2012, Piras et al. 2014) and for land-use or land cover changes (van Roosmalen et al., 2009, Ogden et al. 2011, Ogden and Stallard

2013, Ebel and Mirus 2014, Pierini et al. 2014, Niswonger et al. 2014). They are also becoming increasingly critical in short-term forecasting of geomorphological hazards or inundation dynamics and in situations where complex feedbacks, such as land-atmosphere coupling, are essential for accurate predictions. The renewed interest has been further boosted by the availability of computational resources and parallel computing approaches (e.g., Kollet et al. 2010, Vivoni et al. 2011, Gasper et al. 2014, Ogden et al., 2015a), as well as some degree of consensus in process representation (e.g., Maxwell et al. 2014).

In this article we review the value of distributed, process-based hydrological models to address a number of questions and highlight key challenges for future developments. We discuss the importance of this fundamental approach in hydrology in the context of existing literature, avoiding descriptions of models and mathematical formulations, which have been recently reviewed (Paniconi and Putti, 2015). In the coming decades, hydrological research and water resources management will depend more heavily on our collective capacity to use models based on physical principles since these are essential instruments to formulate and test scientific hypotheses, investigate spatiotemporal patterns, improve our understanding of hydrological responses to a wide range of potential forcings and changes, and ultimately apply this improved understanding to better manage our finite water resources.

2. Why process-based hydrological modeling?

First, we provide a rigorous definition, to the extent possible, of the main subject of this contribution to lay the foundation for the subsequent discussion. Extending the line of thought suggested by Brutsaert (2005), our definition links two notions: observability and scale. Specifically, a process-based (or equivalently physically-based) hydrological model is a mathematical formulation that explicitly represents and/or incorporates through assimilation approaches, the hydrologic state variables and fluxes that are theoretically observable and can

be used in the closure of assumed forms of the laws of conservation of mass, energy, and momentum at temporal scales characterizing the underlying physical processes. When applied spatially, from hillslope to continental scales, such a model can incorporate the space-time variability of the primary forcings, such as precipitation and radiation, and variations of land-surface properties (e.g., topography, soils, vegetation) at the sub-hillslope scale, while resolving the subsurface domain in horizontal and vertical directions in a way to describe heterogeneity at a scale equal to or larger than a representative elementary volume, for porous media (see Bachmat and Bear, 1987, for a definition of representative elementary volume).

We further generalize the definition of a process-based model to a set of process descriptions that are defined depending on the objectives at hand, be it rainfall-runoff partitioning, vadose zone water fluxes, land-atmosphere exchanges, above and below-ground non-isothermal dynamics, sediment or contaminant source identification, or a complete description of hydrological dynamics. A growing number of these descriptions target one or more processes including coupled subsurface and surface domains, land and atmospheric processes, dynamic vegetation, biogeochemistry, and solute transport, and are applied at the watershed and larger scales (e.g., Kuchment et al. 2000, VanderKwaak and Loague 2001, Downer and Ogden 2004, Panday and Huyakorn 2004, Tague and Band 2004, Bertoldi et al. 2006, Kollet and Maxwell 2006, 2008a, Pomeroy et al. 2007, Qu and Duffy 2007, Li et al. 2008, Ivanov et al. 2008a, Markstrom et al. 2008, Rinehart et al. 2008, Sudicky et al 2008, Ebel et al. 2008, 2009, Kumar et al. 2009, Drewry et al. 2010, Camporese et al. 2010, 2015, Shen and Phanikumar 2010, Mirus et al. 2011a, Maxwell et al. 2011, Weill et al. 2011, Vinogradov et al. 2011, Kolditz et al. 2012, Fatichi et al. 2012a,b, Kim et al. 2012a, 2013, Shen et al. 2014, Endrizzi et al. 2014, Niu et al. 2014a, Shrestha et al. 2014, Xiang et al. 2014, Hwang et al. 2015, representing a non-exhaustive list). Although some of those process-based hydrological models include numerous distinct processes, the degree of complexity and quantity of

processes represented varies between models and influences the suitability of a given model for specific applications.

2.1 Parsimony is convenient but complexity is often necessary

If simple explanations and parsimonious structures are able to highlight the emergence of general rules governing a system behavior, they are very often preferable to complex, high dimensional models. As suggested by Levin (1999) for ecological models: "*…simple models are a good place to start because their transparent features provide clarity. A simple model is something to build on. In its sleek lines and limited assumptions, it can provide a base for elaboration while capturing the essence of a variety of more detailed possible explanations.*"

Simple models have been very useful and elegant in describing large-scale patterns that have features of self-similarity (scale invariance) that can be explained mathematically using fractal theory as well as exhibit the self-organization of complex adaptive systems, such as landscapes (e.g., Mandelbrot 1967, Rodriguez-Iturbe and Rinaldo 1997, Rinaldo 2009), ecosystems (e.g., Levin 1999) or flood quantiles (e.g., Smith, 1992, Goodrich et al. 1997, Ogden and Dawdy, 2003). For example, Muneepeerakul et al. (2008) was able to describe many features of fish biodiversity in the Mississippi-Missouri river network with a few parameters in a meta-community model. Other examples include the application of fundamental physical principles such as Maximum Entropy Production or Maximum Energy Dissipation to explain Earth system and hydrological processes (Kleidon et al. 2009, Wang and Bras 2009, 2010), as well as travel time approaches for reproducing coupled flow and transport processes (e.g., Benettin et al. 2013). These are examples where simplicity is useful and 'beautiful'.

However, there are many cases in which the representation of complexity is necessary to understand how natural and human systems function and interact. Understanding the general

organization of a system does not provide information on how its principal components interact nor does it elucidate the significance of its internal fluxes. The fact is that topology, or where things are located and how they are connected within a watershed, matters (Ogden et al. 2013). As a result, the complex and heterogeneous internal conditions of a watershed escape description by lumped models, which are often difficult to apply to solve within-catchment problems because they rarely describe internal states and fluxes that are observable. In many cases, multiple processes and numerous complex feedbacks lead to non-linear dynamics, instability, and tipping points (Pimm 1984) that can only be predicted with a sufficient level of complexity with preservation of mass, energy, and momentum budgets. Examples come from studies of climate change effects, surface-subsurface interactions, and biogeochemical dynamics (e.g., Maxwell and Kollet 2008, Manning et al. 2009, Tague 2009, Drewry et al. 2010).

Furthermore, the necessity for process-based models is evident when the interest lies in specific variables at the local scale that can be simulated accurately only with detailed representations, such as sediment and contaminant transport (e.g., Ewen et al. 2000, Sudicky et al. 2008, Robles-Morua et al. 2012, Kim et al. 2013, Pradhan et al. 2014, Johnson et al. 2013, Niu and Phanikumar 2015), predicting land management impacts (Fatichi et al. 2014, Pierini et al. 2014), landslide occurrence (Baum et al. 2008, Simoni et al. 2008, Shao et al. 2015, Anagnostopoulos et al 2015), snowpack evolution (e.g., Luce et al. 1998, Lehning et al. 2006, Endrizzi et al. 2014) or permafrost dynamics (e.g., Dall'Amico et al. 2011). Process-based models are also contributing to an improved understanding of different land-atmosphere coupling regimes that are highly sensitive to the spatial heterogeneity of land surface states as well as to the temporal dynamics of atmospheric conditions (Ek and Holtslag 2004, Maxwell and Kollet 2008, Santanello et al. 2011, Rihani et al. 2015, Bonetti et al. 2015, Davison et al. 2015). The use of well-constructed, process-based models should also produce emerging

patterns at large scales that build up from the small-scale complexity of a watershed without tuning specific parameters, as supported by existing examples (e.g., Kollet and Maxwell 2008b, Vivoni et al. 2010, Kim et al. 2012b).

There is a widespread perception that multi-disciplinary process-based models with a high-dimensional parameter space produce results that can span an unreasonably large range of states (e.g., McDonnell et al. 2007). Therefore, the use of these models is often regarded as introducing several layers of uncertainty, including numerous, generally poorly known, parameter values describing different processes. Despite the large dimension of the parameter space, process-based models are less reliant on calibration or tuning because parameter values can be constrained directly by the physical relations or observable quantities (Figure 1). While this is not true for all parameters, many of them can be estimated with a given uncertainty from observations or expert considerations (e.g., Hubbard and Rubin 2000, Kowalsky et al. 2004, Gleeson et al. 2011, Gupta and Nearing, 2014, Bahremand 2015), therefore constraining *a priori* the range of model responses; some claim excessively (Mendoza et al. 2015). Spatial patterns of the inputs imposed by distributed datasets further constrain the basin-internal dynamics. Additionally, the number of sensitive parameters in spatially-distributed process-based models, per process accounted for, is often similar to simpler models (Pappas et al. 2013). Accounting for spatial heterogeneity can complicate parameter identification but surrogate information, such as soil type, land-use, and geology data, can be used to group similar regions into areas with similar parameter values (e.g., Samaniego et al. 2010).

Additional processes and components recently coupled to hydrological models (e.g., vegetation dynamics, soil biogeochemistry, sediment transport, solute and water-age, atmospheric boundary layer, snow and soil thermal regime) not only increase the parameter space, but also the number of constraints on the system response. These constraints emerge from the model internal structure and dependencies, and the larger number of states and fluxes

that can be compared to observations at commensurate scales, rather than from a formal model calibration. These additional simulated processes can involve observable variables and aid in constraining parameter values. For instance, correct simulations of leaf area index seasonal dynamics and stomatal aperture in an ecohydrological model are likely to result in an adequate simulation of canopy radiation exchanges and transpiration fluxes.

2.2 The need for virtual experimentation laboratories

Physics, meteorology, and geomorphology are all examples of fields where the use of model experiments or the definition of theories precedes the validation and test of the theory through observations. For example, the existence of black holes (Schwarzschild 1916, Kerr 1963) and cosmic microwave background (Gamow 1948) were theorized well before the actual observations were made. Other disciplines, for instance structural engineering, soil science and plant physiology, have relied to a larger extent on physical experiments and observations. Consequently, theories have typically followed experiments, though striking exceptions exist, such as the cohesion-tension theory for plant vascular transport (Tyree 1997, 2003). The field of hydrology has evolved with elements of these two categories. Field experiments in hydrology are difficult and expensive due to the relevant spatial scales, instrumentation requirements for measuring a wide variety of variables, especially in the subsurface, and the spatial heterogeneity of hydrological states and fluxes. Nonetheless, both intense field campaigns and long-term experimental watersheds have been conducted at various levels of comprehensiveness (e.g., Swank and Crossley 1988, Hornbeck et al. 1993, Blackmarr, 1995, Western and Grayson 1998, Jones 2000, Slaughter et al. 2001, Tromp-van Meerveld et al. 2008, Ogden et al. 2013). Concurrently, since long-term precipitation and streamflow observations are available globally and have been a hallmark of hydrologic science, our community has also developed many models with the objective to match these sparse observations (see discussion

in Loague and VanderKwaak 2004). As a result, hydrologic science has devoted a minor effort to virtual experiments that can be used to develop theories or propose hypotheses that can subsequently be tested in the field.

Yet process-based models can effectively serve as virtual laboratories to quantitatively address questions related to spatial patterns and temporal dynamics of coupled processes. With virtual experiments we refer to numerical simulations carried out to test a scientific hypothesis, which will be difficult or impossible to investigate otherwise. These are different from studies aimed at comparing models among themselves or validating model results. Early efforts were focused on identifying knowledge gaps, such as how soil unsaturated hydraulic properties and snow melt control runoff (Stephenson and Freeze 1974). More recently, virtual experiments have become widely used for hypothesis testing on hillslope-scale processes such as macropore flow (Weiler and McDonnell 2004), surface-subsurface interactions (Park et al. 2011), lateral connectivity (Mahmood and Vivoni 2011), nonlinear storage-discharge dynamics (Camporese et al., 2014b), and throughfall (Frasson and Krajewski 2013). Similarly, the advent of coupled-process models has allowed more sophisticated hypothesis development and testing of runoff generation across the surface/subsurface interface (Niedzialek and Ogden, 2004, Ebel et al. 2007a,b, Loague et al. 2010), channel-land interactions (Shen et al. 2016), and non-uniqueness of soil moisture distribution (Ivanov et al. 2010, Fatichi et al. 2015a) and soil erosion and sediment transport (Kim and Ivanov 2014). This approach further facilitates extrapolation from individual catchments to generalizations across different environmental conditions (Mirus and Loague 2013). For example, ecohydrological process models have allowed virtual experiments related to vegetation dynamics across a range of scales (Ivanov et al. 2008b, Shen et al. 2013, Della Chiesa et al. 2014, Fatichi et al. 2014, 2015, Pierini et al. 2014, Mendez-Barroso et al. 2014). Perhaps the most useful type of virtual experiments for advancing hydrological understanding will be applications that closely match real systems. In fact, process-based

models allow an extension of investigations to temporal and spatial domains and resolutions that are beyond the capabilities of traditional field studies (e.g., Mirus et al. 2011b, Fatichi et al. 2014, Mascaro et al. 2015).

Some studies have already shown the utility of models for the design of experimental hillslopes or catchments with sophisticated monitoring networks, such as Biosphere 2 (Hopp et al. 2009, Ivanov et al. 2010, Niu et al. 2014b). Along these same lines, the development of virtual and physical laboratories such as the Chicken Creek experiment (Holländer et al. 2009) can provide data for unbiased testing of model parameterizations. The continued expansion of coordinated monitoring networks, such as the Critical Zone Observatories (CZOs) (Anderson et al. 2008) and TERENO (Zacharias et al. 2011, Grathwohl et al. 2013), will ultimately rely on numerical modeling to provide generalization to other regions and insights on questions about the value of observations and the limits of our current process understanding.

Finally, high-resolution modeling at large scales (e.g., Wood et al. 2011, Bierkens et al. 2015, Maxwell et al. 2015) can facilitate virtual experiments to address questions that would not be feasible with the current generation of satellite and ground-based measurements alone. This integration will possibly produce a shift from data-driven studies that inform numerical modeling to the use of model-driven hypothesis testing to inform data acquisition.

2.3 Integration is more natural than differentiation

Using the conventional "top-down" and "bottom-up" terminology to describe different approaches (e.g., Sivapalan et al. 2003), process-based modeling approach falls naturally into the latter category. That is, a distributed process-based model relies on multiple components that are combined together to contribute to the overall dynamics at a higher organizational level, such as a watershed. The complexity thus results from interactions of user-selected fundamental process formulations operating at fine spatial and temporal scales. In contrast,

"top-down" models rely on constitutive relations or parameterizations to describe finer-scale behavior from the coarse model scale. Often, this is done with a limited attempt to resolve observable mechanisms, distributed patterns, and feedbacks operating at small-scale levels. Of course, one possible fallacy of the "bottom-up" approach is the inclusion of elements or hierarchical levels in the model that contribute little towards the overall system behavior or overly emphasize dependencies because of lack of process understanding; for instance, interactions between processes that lead to excessive dampening or intensification of the system response relative to actual behavior.

One attractive feature of process-based models is that formulations of individual process descriptions often rely to some extent on first principles for rigor. In theory, at the appropriate scale, these process-level components are verifiable approximations of reality with no, or limited, recourse to empiricism. As such, formulations are independent of immediate data availability, but highly amenable to testing with new observations in a validation procedure. Data sets for testing process-based models may be of heterogeneous types at individual locations or distributed in nature, for example as continuous time series (e.g., soil moisture, energy fluxes, stream flow), instantaneous records (e.g., satellite derived evapotranspiration, biomass, snow water equivalent, tracer concentrations, suspended sediment concentration), or qualitative observations (e.g., presence or absence of snow or inundation), among others. With the increase in the number and quality of remote sensing platforms, the ability to use such observations of internal states and fluxes will rise in importance (e.g., Niu et al. 2014c, Xiang et al. 2014, Mascaro et al 2015, Figure 2).

Finally, the interactions of individual elementary responses represented in process-based models lead to emergent patterns in space and time that are unlikely to be identified using coarse-resolution approaches. For example, discoveries of new mechanisms and feedbacks depending on spatial interactions have already been documented using process-

based models (e.g., Maxwell and Kollet 2008, Ivanov et al. 2008b, Vivoni et al. 2010, Rihani et al. 2010, Le et al. 2011, Mahmood and Vivoni 2011, Hwang et al. 2012, Kim and Ivanov 2014, Bearup et al. 2014, Rahman et al. 2014).

2.4 Non-stationarity: we live in a transient age

Human impacts at the watershed scale have increased since industrialization. Environmental changes, such as those associated with the construction of hydraulic infrastructure, changes in land-use or transient climate alter the amount and distribution of water resources (e.g., Gleeson et al., 2012). An emerging realization is that climate change has likely pushed the hydrologic cycle out of what is considered statistical stationarity (Held and Soden 2006, Milly et al. 2008, 2015, Melillo et al. 2014). A non-stationary future calls for tools that are reliable and sufficiently general, can permit robust assessments and planning, and also operate at the scales of "human action", that is, at space and time resolutions that are immediately relevant for the purposes of design, planning, and management.

In a spatial context, a process-based model can reflect variations at sub-hillslope and stream reach scales, as well as integrate variations of landscape characteristics that control hydrological connectivity in surface and subsurface flow paths. This is close to the localized, "human action" scales (e.g., Piras et al. 2014, Fatichi et al. 2015b, Kim and Ivanov 2015). Process-based models are natural candidates for assessments of non-stationary systems because mass, energy, and momentum fluxes are conserved, and model skills are informed by state variables and fluxes that can theoretically be measured directly. Process-based models also offer a convenient means for addressing the related uncertainty by combining stochastic and deterministic modes of operation (Kuchment and Gelfan 1991). Furthermore, the parameter or forcing variations imposed to the model to address non-stationary conditions can be established either objectively, using a well-defined scenario, or subjectively through the

application of sensitivity (stress) analyses (e.g., Mascaro et al. 2010, Steinschneider et al. 2014, Kim and Ivanov 2015).

2.5 The underpinning of environmental sciences: interdisciplinarity

The problems addressed by hydrological models are interdisciplinary in nature by virtue of the cross-thematic properties of water as a solvent, erosive agent, disease vector, exchange medium for energy, recreational element, human, animal and plant consumable, and, ultimately, an economic quantity. For this reason, interdisciplinarity is at the heart of hydrologic science (Eagleson 1991). Hydrological processes are inherently multi-scale in that the dominant controls on fluxes and residence times within various disciplines are expressed differently across a wide range of spatial and temporal scales. Given the nature of many interdisciplinary problems, process-based models that solve explicitly observable states and fluxes at high spatial and temporal resolution and possess appropriate multi-scale representation capabilities are the most likely candidates for interdisciplinary research.

For example, the number of studies that combine process-based hydrological models designed for unsaturated and saturated subsurface flow with models that solve land-surface energy exchanges and/or ecological dynamics are increasing (e.g., Rigon et al. 2006, Maxwell and Kollet 2008, Ivanov et al. 2008a, Siqueira et al. 2009, Maxwell et al. 2011, Banks et al. 2011, Vivoni 2012b, Moffett et al. 2012, Fatichi et al 2012b, Condon et al. 2013, Shen et al. 2013, Ng et al. 2014, Niu et al. 2014a, Endrizzi et al. 2014). However, the integration of process-based hydrologic models within a single modeling framework of the Earth's system that encompasses multiple disciplines is still largely unrealized (e.g., Paola et al. 2006, Flato 2011) and descriptions of hydrology in current Earth systems models do not yet reflect a suitable level of hydrologic process understanding and modeling solutions (Clark et al. 2015).

For hydrologists trained in geology, engineering or geography, making the substantial leap to interdisciplinary research with geomorphologists, atmospheric scientists, ecologists or biogeochemists might not be too difficult. However, human-oriented disciplines such as socio-economics, policy, and law are also essential for taking hydrological modeling expertise and products into stakeholder engagement activities and the valuation of hydrological services to society (Srinivasan et al. 2012, Guswa et al. 2014, Niswonger et al. 2014). Current trends in science and engineering point to greater integration of disciplines and hydrological modeling is considered to be a building block that determines which transdisciplinary, multi-sectorial and multi-objective scenario-based simulations, and output interpretation can be performed. This perception is due in large part to the emphasis that the hydrological modelers have placed on process-based understanding and in building predictive systems that capture the impact of changes in measureable quantities on hydrological parameters and subsequent effects on the fluxes of water and its constituents.

Boundaries of hydrologic science will continue to expand and hydrologists will be integral components of new and emerging fields, which can benefit from the quantitative and computational skills emphasized in process-based hydrological modeling. Much is also to be learned from allied disciplines, where the lack of process-based computational tools has fine-tuned the ability of investigators to pose testable hypotheses through limited field experimentation or the ability to interpret cause-effect relationships on theoretical arguments rather than simulation-based results. Given the likely increase in reliance upon process-based hydrological modeling in multi-disciplinary studies, the responsibility lies with our hydrological community to develop tools that are broadly and conveniently applicable, while continuing to use these tools for hypothesis-driven research. Furthermore, providing non-specialists use of process-based algorithms will help to minimize what Klemes (1986) criticized as "dilettantism in hydrology".

3. Practical issues

Despite the arguments in favor of process-based hydrological models reviewed here, some still resist the use of these models. This is largely due to practical matters. Conceptual models are much easier to use at coarser scales and require a lower threshold of process knowledge and expert training, making them more widely appealing. This occurs at the expense of a considerable time investment in model calibration and possibly a reduced model performance, when used outside of the calibrated range of conditions (Uhlenbrook et al. 1999, Seibert 2003). As a result, a wider dissemination of process-based approaches will require improved model visualization tools, a streamlined approach for model setup, execution and output analysis, and improved communication of the model capabilities and limitations to potential adopters. This is required to avoid the problem of "garbage in, garbage out", where unprepared users operate complex models in an inappropriate fashion obtaining untrustworthy results. Intuitively, direct simulation of coupled processes is more straightforward to understand than a conceptual representation of system response. In reality, the implementation of coupled processes typically requires complex numerical methods with associated risks regarding numerical instability and convergence, whereas conceptual representations are less prone to these problems. Furthermore, consistent applications of process-based models require that the user understands the underlying processes and their interactions as well as the mathematical and computational representation. This requires a deeper understanding of hydrology and numerical techniques, which can be seen as an opportunity to improve the training of students and practitioners in hydrologic sciences.

Hydrological models with the most complete descriptions of processes require data rich settings (e.g., Camporese et al. 2014a,b, Mascaro et al. 2015). However, models that require large amounts of data are unlikely to find widespread use because of data limitations and user limitations to process data. Wider use of these models must hinge on a more systematic

approach for mining existing data repositories from governmental and/or commercial sectors. In the United States, for instance, spatial data needed to drive process-based models are now freely available from a variety of sources, such as the U. S. Geological Survey (USGS) seamless data viewer (http://nationalmap.gov/viewer.html) and the National Resources Conservation Service (NRCS) web soil survey (http://websoilsurvey.sc.egov.usda.gov/App/HomePage.htm). Precipitation data from multiple platforms are available from the National Center for Environmental Information (NCEI, formerly known as National Climatic Data Center, http://www.ncdc.noaa.gov/). It is possible to obtain additional meteorological forcings from the North America Land Data Assimilation System (NLDAS) (http://www.emc.ncep.noaa.gov/mmb/nldas/). Datasets to characterize river hydraulic morphology (e.g., Allen and Pavelsky, 2015) and global hydrogeological maps (Gleeson et al. 2014) are also becoming available. Process-based models that can be driven by readily available geospatial data sources from standard web-based interfaces are likely to be applied more widely by diverse users (e.g., Kumar et al. 2010, Gochis et al. 2014, Bhatt et al. 2014, Formetta et al. 2014).

Since process-based hydrological models mostly rely on non-linear partial differential equations with the aim of solving large domains at fine temporal and spatial resolutions, the model computational burden is a serious issue. Simulation times increase as more processes are included, as process descriptions become more general, and as spatial and temporal resolutions are increased. Even in the case where a single simulation does not require a long time, there are practical issues related to stochastic approaches that might require hundreds or thousands of simulations (e.g., Skahill et al. 2009, Camporese et al. 2009a, Pasetto et al. 2012, Moreno et al. 2013). Since different physical processes (e.g., transpiration, infiltration, snow metamorphism, groundwater flows) have different dominant time scales ranging from a few minutes to many years, approaches using sub-time stepping can be regarded as a way of

improving the computational performance (e.g., Park et al. 2008, 2009). However, the trade-offs between process representation and physical realism remain unevaluated, and different process-based models have various degrees of complexity.

A classic example is represented by numerical solutions of the Richards equation, which are used by process-based models to solve water fluxes in variably saturated porous media. The use of the Richards equation to solve soil-water flow dynamics in process-based models has been criticized for over-emphasizing capillarity and neglecting the role of preferential flow (Nimmo, 2012, Beven and Germann 2013), for being in some ways 'overly simplistic' (Gray and Hassanizadeh, 1991, Niessner and Hassanizadeh 2008), and for being computationally expensive and sometimes unstable and unreliable (e.g., Tocci et al. 1997). The last point posed limitations to large-scale fine resolution applications of process-based models. However, process-based formulations that deal with preferential flows have been introduced (e.g., Gerke and van Genuchten, 1993, Šimůnek et al. 2003) and numerical methods for solving 2D and 3D Richards equation in an accurate and reliable way have been developed (e.g., Paniconi and Putti, 1994, Neuweiler and Cirpka 2005, Mendicino et al. 2006, An et al. 2010, Lott et al. 2012), as well as methods to derive effective soil hydraulic parameters as a function of hillslope topography (e.g., Jana and Mohanty 2012). Recently, an alternative general one-dimensional solution of the vadose zone flow problem has been also presented (Talbot and Ogden 2008, Ogden et al. 2015b,c, Lai et al. 2015) and can considerably reduce computational times in comparison to classic solutions of the Richards equation.

More generally, code parallelization is an essential requirement to reduce computational times for large problems (Kollet et al. 2010, Vivoni et al. 2011, Eller et al. 2013, Ran et al. 2013, Hwang et al. 2014, Ogden et al. 2015a). The Message Passing Interface (MPI) and Open MP set of tools, which provide open-source libraries for developing parallel computing capabilities within model codes, can reduce simulation times significantly on multi-processor desktop

machines. One alternative for massively parallel computations is the use of General Purpose - Graphical Processing Units (GP-GPUs) based on the GPUs originally developed to improve graphics rendering of computer animations, with initial applications underway in hydrological and hydraulic modeling (e.g., Kalyanapu et al. 2011, Hughes and White 2013, Anagnostopoulos et al. 2015, Le et al., 2015, Lacasta et al, 2015, Falter et al., 2015).

4. Avenues for future advances

4.1 Toward fully integrated natural and virtual laboratories

A key challenge facing hydrological modeling is the integrated use of natural and virtual laboratories to advance theory and process understanding, and develop and test new approaches. Too often, the model development occurs in isolation from field experimental activities or within specific geographic regions where the model is desired. While model generality is an admirable goal, it should not justify disconnecting modeling activities from field knowledge. Natural laboratories or physical models of natural systems (laboratory-scaled versions of plots or hillslopes) are likely to become an indispensable part of a hydrological modelers' toolkit. At experimental sites, instrumentation networks and field sampling allow coordinated, simultaneous measures of the states and fluxes of the hydrologic, atmospheric, geomorphic, ecologic or biogeochemical processes of interest. Along with knowledge of system characteristics, natural laboratories provide essential datasets to test the ability of models to capture the system behavior under different forcing or initial conditions, thus challenging the accuracy and fidelity of individual processes and the emergent behavior at specific locations and averaged over a spatial domain.

Fortunately, prior calls to reduce the disconnection between experimentation and modeling and to reconcile soft and hard hydrological data (e.g., Seibert and McDonnell 2002) have led to substantive progress. A growing number of hydrological modelers are participating

in multi-disciplinary experimental sites, such as the Critical Zone Observatories, Landscape Evolution Observatory and Long-Term Ecological Research sites (e.g., Hobbie et al. 2003, Anderson et al. 2008, Huxman et al. 2009), where modeling and observation activities are coordinated. A number of small-scale (100s of m^2) artificial catchments and experimental sites, where boundary conditions can be carefully controlled (Kendall et al. 2001, Nicolau 2002, Gerwin et al. 2009), are also available for this purpose. However, few of these sites, with some exceptions (Hopp et al. 2009, Vivoni 2012a), have used hydrological modeling for formulation or testing of hypotheses, presenting an opportunity to expand the utility of process-based modeling tools.

In addition to natural observatories, a new generation of distributed hydro-geophysical measurements (e.g., light detection and ranging, ground penetrating radar, distributed fiber optic temperature sensors, electrical resistivity tomography, phenological cameras, large aperture scintillometers) and remote sensing products from satellite and aerial platforms, including unmanned aerial vehicles, are also being used to improve the characterization of hydrological systems and to provide spatiotemporal patterns of hydrological states and fluxes (e.g., Robinson et al. 2008, Steele-Dunne et al. 2010, Panciera et al. 2014, Vivoni et al. 2014, Singha et al. 2014). Measurements aimed at improved process-level understanding naturally aid in the simulation of those processes. Long-term investments for collection of datasets specifically designed for testing process-based hydrological models would pay substantial dividends to model development and to the closer integration of natural and virtual laboratories.

In many cases, the breadth and depth of the data generated from natural observatories and remote sensing is astounding, raising significant questions on how to properly use them in hydrological modeling development and testing. The current widespread field-scale data collection in natural laboratories and proliferation of data-sharing requirements by funding agencies and journals should be helpful to hydrological modelers in multiple ways – helping

in the design of sensor networks, aiding in the appropriate level of spatiotemporal aggregation of data for use in models, and providing model-based insights into the key variables to measure for advancing theory and process-level understanding. Process-based distributed modeling can in fact benefit from improved model-data fusion (e.g., Vrugt et al. 2005, Hyndman et al. 2007, Camporese et al. 2009a,b, Hinnell et al. 2010, Kerkez et al. 2012, Mascaro and Vivoni 2012, Pasetto et al. 2012, Vrugt et al. 2013, Mirus 2015). Furthermore, improved assimilation of data with different origins (i.e., *in situ*, remote sensing, Lagrangian sampling, point-, 2D and 3-D scales) will speed model testing and process-level validation.

4.2 From watershed scales to stakeholder scales

Hydrological models have traditionally focused on watershed-scale quantities such as streamflow or integrated water budgets. However, localized scales - a stream reach, a floodplain, an agricultural field, or a stormwater sewer - provide societal relevance and interest in the impacts of land-use or climate changes that are typically much stronger when predictions concern local, "backyard", problems such as urban flooding, water quality and aquatic habitats, or morphological variations in a channel or landscape. Addressing problems at these scales very often require interdisciplinary models based on physical processes. What is more, these scales are in some ways ideal for process-based approaches. For instance, the computation of metrics, such as shear stress and turbulent kinetic energy, are pivotal for investigating streamflow effects on the aquatic environments for fishes (Crowder and Diplas 2002, 2006). In practice, this can only be achieved by coupling process-based hydrological, hydrodynamics and sediment transport models (e.g., Heppner et al. 2007, Kim et al. 2012a,b, 2013, Kim and Ivanov 2015).

Furthermore, the hydrological modelers should continue to demonstrate that state-of-the-art hydrological predictions are useful to society. Demonstration of this worth is a laudable

objective. This might seem obvious to hydrologists as our education, practical training, and research experiences have largely been motivated by the desire to improve the public good through, for example, enhanced warning systems, more resilient and robust infrastructure or better water resources management plans. However, in the process of building, testing and deploying modeling systems, there is a real risk of creating a disconnection from stakeholders who, ultimately, will benefit from or be impacted by the hydrological predictions. This can be attributed to the difficulty in communicating complex ideas or modeling structures, but also to the lack of training and expertise currently in our field in the realm of stakeholder engagement activities (e.g., Hatzilacou et al. 2007, White et al. 2010). It is noteworthy that the keystone of hydrological modeling in engineering and regulatory practice remains today the curve number approach, despite all its empiricism and established shortcomings (e.g., Garen and Moore 2005).

Presenting detailed hydrological predictions to a scientific audience is a challenging task. Conveying the nuances and difficulties associated with modeling assumptions, spatial and temporal resolutions, parameter estimation, or coupled model components to non-technical audiences is even more difficult. Despite this, we believe that an effort to disseminate the capabilities of process-based modeling to non-technical decision makers is crucial, because of its central role in quantifying the complex interplay between hydrological processes and human decisions (e.g., Srinivasan et al. 2012, Sivapalan et al. 2012, 2014). In this context, the requirements of hydrological models are far greater when a system description includes humans and their interventions. For example, it is not uncommon that the biophysical and geochemical processes represented in hydrological models would need to interact with active agents who make individual or group decisions that affect these coupled processes in nonlinear ways (e.g., time-varying water extractions or diversions, pollution sources, land cover changes) (e.g., Parker et al. 2003, Bomblies et al. 2008). Building realism into the simulation of these

complex interactions necessitates the use of process-based hydrological models that can be coupled to models that represent these decision dynamics at a compatible scale.

4.3 Short-term predictability of hazards and engineering design

One of the most common and perhaps justified criticisms of process-based models is that they produce limited improvement over calibrated operational models for short-term streamflow predictions. This is due to the large uncertainty in the knowledge of boundary and initial conditions, as well as the difficulty of a formal calibration of the large parameter space (e.g., Senarath et al. 2000). However, the ability of calibrated models to mimic short-term hydrological responses also leads to over-confidence in their predictive skills. Calibration procedures that do not account for uncertainty in input and output observations and model structure inevitably lead to biased parameter values (e.g. Restrepo and Bras 1985, Ajami et al. 2007, Renard et al 2010). We argue that process-based models are equally useful tools for short-term predictions of natural hazards and for engineering design; additionally, they are less subject to biased parameters arising from intensive calibration exercises. Short-term predictions using process-based models typically involve minor computational efforts, therefore stochastic simulations that account for uncertainty ranges of parameter values, forcings and initial conditions are feasible.

In fact, process-based models are increasingly used to provide alerts and mitigation measures for short-term hazards, such as floods, avalanches and landslides. For instance, the U.S. National Weather Service (NWS) is now implementing a process-based hydrological model as its centralized national modeling system (Gochis et al. 2015). While NWS will also still run lumped conceptual models, the fact that it is embarking on this new direction is a confirmation of the idea that process-based models could improve complete hydrologic cycle forecasting. The clearest advantage of process-based models is their ability to bring critical

information about state variables, such as flow depth, into the simulation through the use of data assimilation of non-conventional variables and/or properly formulated dynamic boundary conditions (Figure 3). A classic case is coastal flooding due to tides and storm surge (Lin et al. 2012). For certain episodic flooding events, such as Hurricanes Irene and Sandy that affected the northeast U.S. coast, these effects are the dominant flooding process. In these events, encouraging examples come from the U.S. Army Corps of Engineers, which provided, with the process-based hydrological model GSSHA (Downer and Ogden 2004), predictions of flooding extent and depth that were used to plan evacuations (Massey et al. 2013). Another example is potential for real-time prediction of landslide hazards, including the proof of concept system built upon the model GEOtop (Rigon et al. 2006, Endrizzi et al. 2014) or the exploration of rapid operational application of TRIGRS (Raia et al. 2014).

An area where high-resolution process-based models could be used effectively is in the engineering design of structural controls (e.g., flood control, sediment abatement, and pollution control). While the effect of individual controls is mostly localized, the system of different structural controls influences the entire watershed or river reach of interest. Within a conceptual modeling framework, the effect of controls can only be approximated by an *a priori* estimation of the effect of individual structures, thus the entire system effect is the estimated sum of the individual parts without accounting for locations and feedbacks between various controls. On the other hand, a process-based approach can explicitly simulate features at the approximate locations, sizes and with varying functions. For instance, urban flood control measures may include surface retention, subsurface drainage, levees, pumping and water diversions. Unexpected feedbacks between these controls can render them inadequate, useless, or even detrimental. Process-based models capture boundary effects, flow paths, and effects of topology and thus solve for the total system response, facilitating the design and collocation of critical components. For example, the use of the process-based GSSHA model (Downer and

Ogden, 2004) in designing a flood control system in Florida by the U.S. Army Corps of Engineers led to a documented savings of over $40 million over standard practice using separate hydrology and hydraulics models (Downer et al. 2015).

4.4 Introducing the stochastic component

There is no doubt that the current use of process-based models is mostly deterministic, with few examples merging theoretical frameworks (Kuchment and Gelfan 1991, Kuchment et al. 1996) and ensemble approaches to date (e.g., Forman et al. 2008, Mascaro et al. 2010, Kim and Ivanov 2015). This is likely a result of the large computational requirements of process-based distributed simulations rather than an underestimation of the involved uncertainties. While the deterministic nature of current process-based models is a limitation, it also leaves room for improvements using stochastic approaches. An exact and detailed knowledge of all the system properties (e.g., bedrock topography, soil-hydraulic properties, vegetation physiology) will likely remain elusive in the foreseeable future. As a result, uncertainty will unavoidably persist in several parameters as well as in the model structure. It immediately follows that uncertainty must be treated using an appropriate framework (e.g., Montanari and Koutsoyiannis 2012). Many approaches and methodological tools have been presented to deal with uncertainty in hydrological modeling (e.g., Beven 2006, 2008, Montanari 2007, Koutsoyiannis 2010). However, applications of these approaches have been mostly carried out using coarse, conceptual models applied to watersheds (Beven and Freer 2001, Montanari 2005, Vrugt et al. 2005) or groundwater hydrology models (e.g., Hill and Tiedeman 2007). Making these varying approaches suitable for use with process-based models coupling surface and subsurface domains requires an easing of the large computational burden of numerical stochastic techniques (e.g., Pasetto et al. 2013).

More importantly, we need a systematic approach to rank the sources of uncertainty and address primarily those implying larger effects on the results of interest. Regardless of the

computational issues, many theoretical problems still remain to be tackled, such as how to deal with system non-stationarity, the definition of likelihood distributions for inputs and model parameters, and the cross-correlations among the various sources of uncertainty. While computational and theoretical problems can currently represent a daunting challenge, treating uncertainty through a synthesis of process-based models and stochastic approaches may represent a fundamental leap forward in the field of hydrologic science. The recent progresses in surrogate modeling or meta-modeling (Razavi et al. 2012a,b, Castelletti et al. 2012, Wang et al. 2014) or specific downscaling techniques to increase output resolution (Pau et al. 2016) suggest that the use of process-based models in settings that require thousands of model evaluations may be feasible. These advances may alleviate the issues of prohibitive computational cost in optimization or uncertainty quantification contexts.

5. Conclusions

Several compelling motivations for a wider use of process-based hydrological models exist. We describe a series of opportunities and modeling challenges where a high spatial and/or temporal resolution and a refined representation of hydrological processes are required by the complexity of the real world and by the fact that flow path and heterogeneity of land surface properties are important. Distributed estimates of soil moisture, evapotranspiration, sediment and pollutant transport are examples where explicit modeling of flow paths and residence times are warranted because they have a dominant effect on the solution. Interdisciplinary studies of ecohydrology, carbon cycle, riparian processes, flood and landslide hazard predictions, cold season processes, and land-atmosphere interactions benefit from process-based hydrological models because conservation of mass, energy and momentum is often a pre-requisite for these problems. They also fall in the class of question that require explicit representation of spatial patterns and temporal dynamics of fluxes and state variables

(e.g., soil moisture and temperature, snow water equivalent, runoff generation, etc.). Better understanding and simulation of human disturbances of hydrological systems, for instance climate and land use changes, are also strong incentives to implement process-based solutions. We review reasons why the integration of small-scale complexity is likely to succeed in establishing causal relations between processes, parameters, and outcomes in reproducing emergent responses and patterns at larger scales. Using process-based models based only on *a priori* information could be foreseeable in the near future, but this strongly hinges on the capability of using large amount of information currently available in constructing, testing, and setting-up the models, and appropriately accounting for the related uncertainty through stochastic approaches. Practical issues connected with process-based models, such as difficulty in their use, scalability of physical laws, prohibitive computational times and a large number of parameters, have hampered widespread adoption of these tools. Arguably, detailed characterizations of hydraulic properties of the subsurface and flow paths still represent the most significant obstacle for widespread use of process-based hydrological models. This should challenge the hydrologic science community to develop innovative ways to measure these key variables. Recent developments in parallel computing resources, new ground-based or remote sensing tools and data collection methods, and new data sources (e.g., tracers and geophysical techniques), will hopefully help resolve some of these barriers and facilitate a more comprehensive treatment of uncertainty. Better integration between virtual and natural laboratories can additionally help in developing model validation datasets and further refining the representation of specific processes. There are ample opportunities for leveraging the utility of process-based models beyond what has been achieved so far and we encourage hydrologists to seize this opportunity.

Acknowledgments

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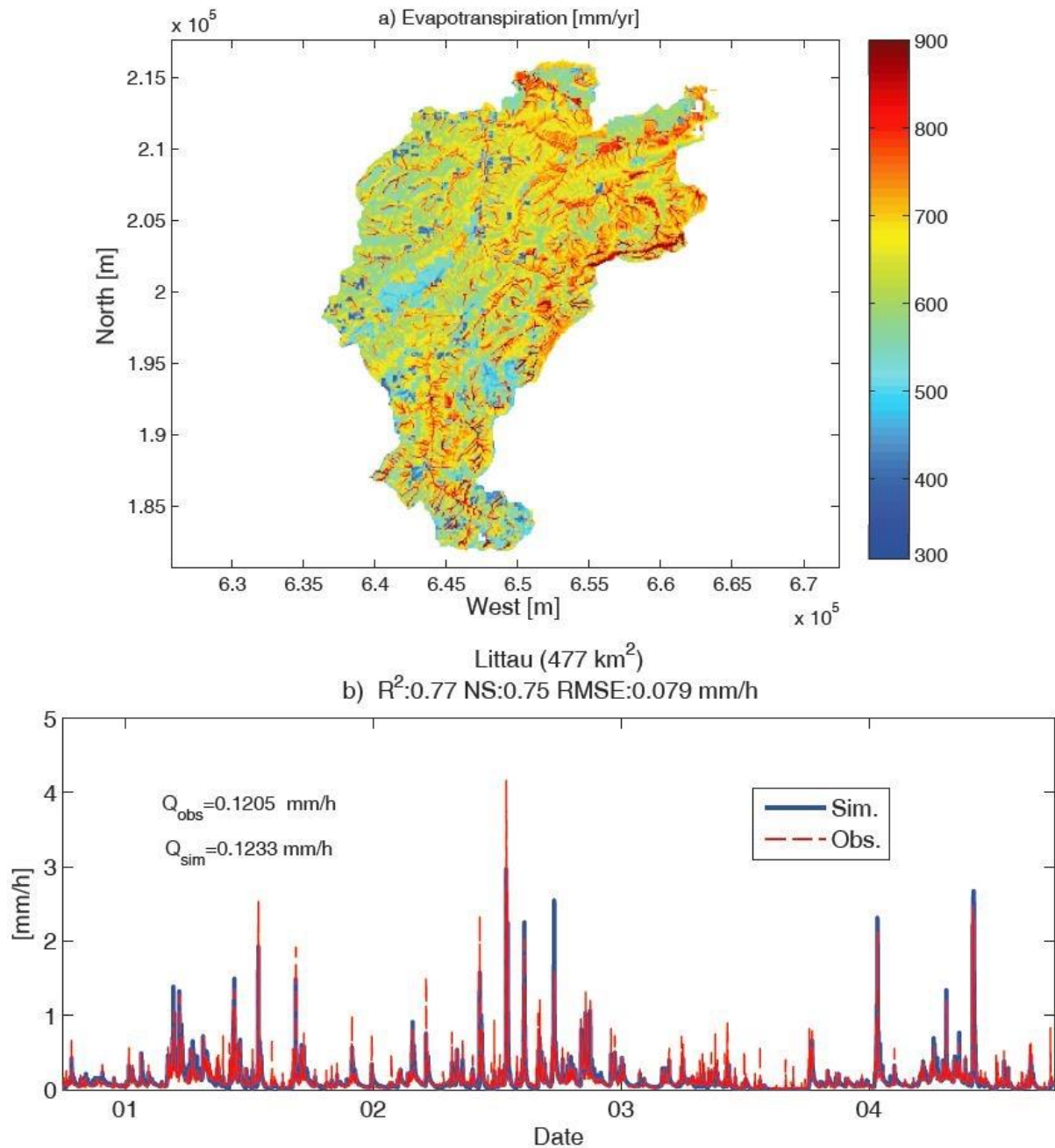
Figure 1. High-resolution (~100 m) un-calibrated hydrological simulations with the process-based ecohydrological model Tethys-Chloris at the hourly time scale for the Kleine-Emme catchment (477 km^2) (Switzerland) for the period 1st October 2000 to 30th September 2004. Spatially distributed forcing was provided by Meteo-Swiss and includes hourly station measurements of air temperature, wind speed, relative humidity, shortwave radiation and a gridded precipitation product RhiresD. Simulation results are presented for distributed evapotranspiration averaged over the four years (a) and streamflow at the catchment outlet (b). The match in water budget amount (Q_{obs} and Q_{sim} are the observed and simulated annual mean

streamflow, respectively) and temporal dynamics (coefficient of determination R^2, Nash-Sutcliffe efficiency, NS, and Root Mean Square Error, RMSE) between simulations and observations is very satisfactory, despite strong spatial heterogeneity in simulated evapotranspiration (not testable with current observations) and lack of calibration at the catchment scale.
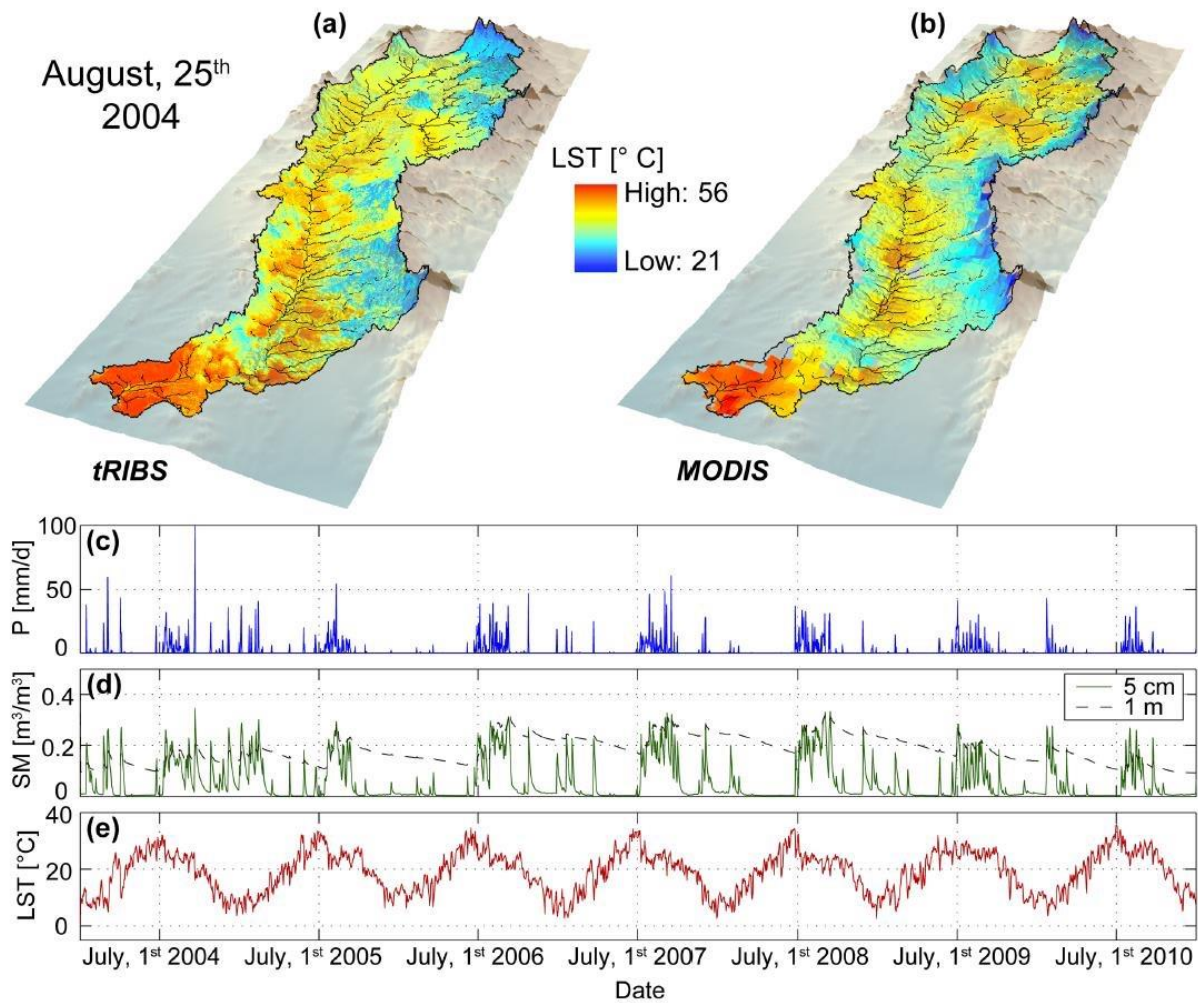

Figure 2. High-resolution (~70 m) hydrologic simulations with the tRIBS model in the Rio San Miguel basin (3796 km^2), Mexico, from January, 1st 2004 to December 31st, 2010. Spatially-distributed hydrometeorological forcings were provided by hourly products from the North America Land Data Assimilation System (NLDAS), bias-corrected with ground observations. Hydrologic simulations were validated by comparing (i) time series of simulated and observed soil moisture (SM) and land surface temperature (LST) at nine distributed locations, and (ii) simulated SM and LST maps against remote sensing products from the 2D-Synthetic Aperture Radiometer (2D-STAR) and Moderate Resolution Imaging Spectroradiometer (MODIS), respectively. The LST maps simulated by tRIBS and observed by MODIS on August, 25th 2004 are presented in panels (a) and (b), respectively. A root mean square error of 4.0 °C and a correlation coefficient of 0.67 were obtained after resampling the

simulated LST at the coarser MODIS resolution (1 km). The basin-averaged time series of (i) daily total P, (ii) daily average surface (top 5 cm) and root zone (top 1 m) SM, and (iii) daily average LST are reported in panels (c)-(e). Adapted from Mascaro et al. (2015).
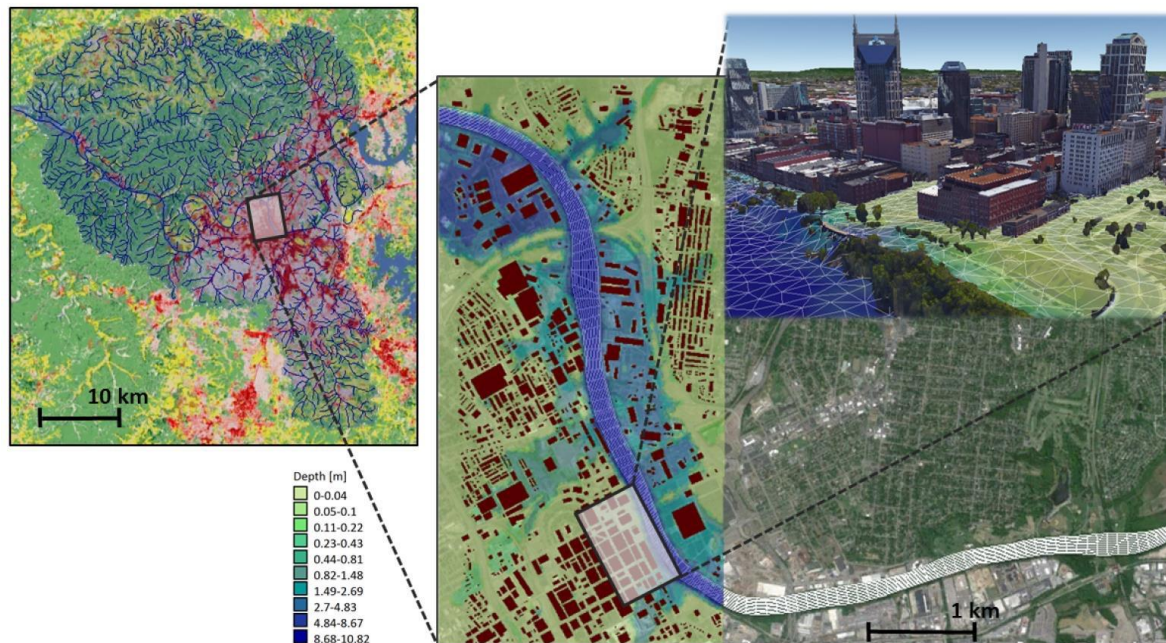

Figure 3: A watershed scale – urban flood simulation with a coupled hydrologic and hydrodynamic model, tRIBS-VEGGIE-FEaST for a 'thousand-year' flood event in early May 2010, Nashville (TN). A ~1,000 km^2 watershed (the left panel) contains naturally vegetated and agricultural areas, an urban center (over 500,000 buildings), contiguous channel and floodplain areas, and several upstream reservoirs. Seamless flood modeling for such a diverse domain requires a suite of interacting process-based models, ranging from spatially explicit rainfall-runoff partition to reservoir controls, and to hydraulic modeling that accounts for flood wave propagation and impediment by buildings. Multi-scale resolutions are necessary, ranging from few hundred meters for the watershed area, few decameters in the channel and floodplain, and few meters in the city downtown. The land-use and inundation maps (flow depths) are presented in the right panels, in which the downtown of Nashville with inundated water levels is highlighted. Satellite imagery and 3D buildings are based on satellite imagery processed by Google Earth.