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Recent advances in integrated hydrologic models: Integration of new domains

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ABSTRACT

Over the past several decades, hydrologic models have advanced from independent models of the surface and subsurface to integrated models that can capture the terrestrial hydrologic cycle within one framework. In recent years, these coupled frameworks have seen the inclusion of biogeochemical processes, ecohydrology, sedimentation and erosion, cold region hydrology, anthropogenic activities, and atmospheric processes. This expansion is the result of increased computational, data, and modeling capabilities and capacities, as well as improved understanding of the processes that drive these integrated systems. Here, we review these recent advances to integrate new processes and systems into existing terrestrial hydrologic models and highlight the significant challenges and opportunities that remain. We identify that with so many models currently available and in development, selecting the most appropriate model is difficult, and we suggest a path for new or novice modelers to find the most appropriate code based on their needs. In addition, data required to parameterize and calibrate these models can often constrain their applicability and usefulness. However, advances in environmental sensors and measurement technology, in addition to data assimilation of non-traditional data (e.g. remote sensing, qualitative data) are providing new ways of addressing this issue. As we expand hydrologic models to integrate more processes and systems, our computational demands also increase. Recent and emerging advances in computational platforms, including cloud and quantum computing, in addition to the use of machine learning to capture some processes, will continue to support the use of increasingly larger and more complex, process-based models. Finally, we highlight that it is critical to develop state-of-the-science models that are accessible to all model users, not just those applied for research and development. We encourage continued development of diverse modeling platforms, considering the user needs, data availability, and computational resources.

1. Introduction

Water is an integral part of all systems and processes in our natural and anthropogenic environments. Water sustains life and supports our quality of life, and maintaining both requires the ability to quantify, simulate, and predict water resources and the impact of water management strategies into the future. Early efforts to simulate and predict the distribution and quality of water resources were compartmentalized into components of the hydrologic cycle (e.g., surface water, groundwater, snow, and evapotranspiration), and/or processes (e.g., geochemical reactions, precipitation-dissolution, overland flow, vegetation water use and response to water availability). With increased understanding of terrestrial hydrologic processes and computational capacity, recent efforts have integrated many of these components and processes in a single computational modeling framework to improve representation of the hydrologic cycle. One such advance is the integration of surface and subsurface hydrologic flow and transport processes which improved representation of the terrestrial water cycle. These physically-based integrated models can take many different forms, but generally couple a representation of Richards' equation for variably-saturated subsurface flow with a version of the St. Venant's equation for surface flow (Aquanty Inc., 2018; Brunner & Simmons,

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2012; Kollet et al., 2017; Kollet & Maxwell, 2008; Maxwell et al., 2014). These equations are then coupled, or integrated, using one of several different techniques. In general, the term 'fully-integrated' is used to differentiate those models that allow for simultaneous solution of the surface and subsurface equations, whereas the terms 'integrated' or 'coupled' is used to indicate models that iterate between solutions of the surface and subsurface (Furman, 2008). The connection between the surface and subsurface can also take many forms, including a first-order exchange flux term that is similar to the Darcy flux, and the common or equilibrium-based approach where the surface and subsurface nodes that connect the two regimes are identical (Aquanty Inc., 2018; Liggett et al., 2012). Due to the integration of discrete surface and subsurface flow equations, these models also require 'spin up' simulations to provide initial conditions that can be appropriately solved during further calibration or simulation runs (Ajami et al., 2014). Several reviews and model intercomparison studies of these integrated hydrologic models have been completed in recent years (e.g., Fan et al., 2019; Maxwell et al., 2014), and the use of these models has evolved to applications that include informing policy and management decisions, and guiding remediation and preventative efforts (e.g., Brookfield & Gnau, 2016; Brookfield & Layzell, 2019; Thatch et al., 2020). Here, we build upon these reviews and comparisons, reviewing recent expansion from the integrated hydrologic models representing the surface/subsurface hydrologic system to include biogeochemistry, erosion and sediment transport, ecohydrology, anthropogenic activities, cold region hydrology, and atmospheric processes that influence the global hydrologic cycle (Fig. 1). Specifically, we focus this review on the expansion of integrated hydrologic models that include:

1) Biogeochemistry - moving beyond basic solute transport to include representation of reactive processes such as complexation, precipitation and dissolution, redox processes, microbial processes and isotopic fractionation.
2) Sediment and Erosion - inclusion of some or all of the sediment budget within study regions, such as fluvial erosion, streambank stability, and depositional processes.
3) Ecohydrology - representation of vegetation dynamics, including growth and mortality, and disturbances including wildfire, and invasive species that influence water and energy fluxes.
4) Anthropogenic activities - inclusion of human activities that directly impact the hydrologic system such as reservoir and dam operation, groundwater extraction, surface water diversion and irrigation.
5) Cold region hydrology - representation of processes and systems related to snow and ice, including accumulation, vapor loss, melt, and permafrost.
6) Atmospheric processes - expanding representation of the hydrologic cycle beyond the terrestrial system, including interactions between surface and subsurface hydrologic conditions to local and regional weather patterns and climate.

Due to the prolific development of modeling approaches and applications, it is not possible to comprehensively include all specific modeling frameworks and advances in these areas. The goal is to present examples of emerging concepts and techniques in order to provide a broad and robust overview of the expansion of integrated hydrologic models and an assessment of ongoing challenges and future directions for further development. We expand on the ongoing challenge of model selection, which was recently highlighted by Melsen (2022), to discuss selecting a model based on a particular objective and data availability. The scope of this work includes a review of the recent expansion of existing integrated hydrologic models to include domains beyond surface water and groundwater systems, as well as innovations in application of these tools for water resources management. It is equally important to develop methods of identifying what simplifications can be made for any particular application to increase the efficiency and useability as it is to develop complex models capable of simulating more processes and systems. While this work focuses on recent advances made with process-based numerical models, we highlight ongoing and emerging research using machine learning approaches in conjunction with process-based models leading to the development of hybrid models.

2. Recent Expansion of Integrated Hydrologic Models

As previously discussed, significant advances in integrated hydrologic models that simulate the terrestrial water system have been made in recent years, including expansion beyond water and solute movement across the surface and subsurface. Here, we identify and review this expansion of integrated hydrologic models into other domains (Fig. 1).

2.1. *Chemistry/Biochemistry/Geochemistry*

A myriad of biogeochemical processes control the production, fate, and transport of solutes and carbon from watersheds. Tracking how land cover, climate, and disturbance impacts solute production and mobility has important implications for water security and critical zone function. The critical zone stretches from the top of the canopy down to the depths

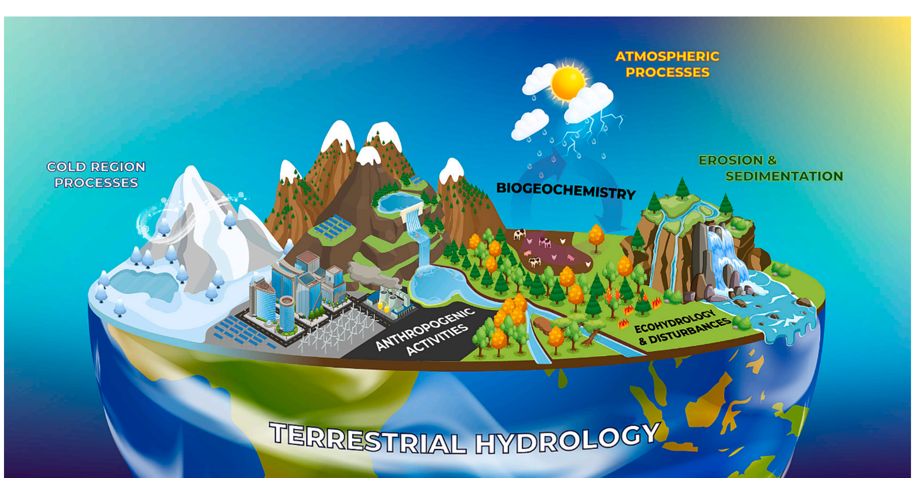

Fig. 1. The scope of this review is to expand beyond existing literature on models representing terrestrial hydrology to include biogeochemistry, erosion and sediment transport, ecohydrology, anthropogenic activities, cold region hydrology, and atmospheric processes that influence the global hydrologic cycle.

of circulating groundwater (Anderson et al., 2007; Brantley et al., 2007; Condon et al., 2020; Council, 2000), and is intricately intertwined with the terrestrial hydrologic cycle (Singha & Navarre-Sitchler, 2022; Sullivan et al., In Revision). Reactive transport models (RTMs) are numerical representations of biogeochemical reaction processes such as respiration or carbonate weathering that allow us to understand how external drivers (e.g., meteoric precipitation) interact with the internal structure of the critical zone (Duffy et al., 2014; Li, 2019; Li et al., 2017a; Li et al., 2017b; Li et al., 2021; Sullivan et al., 2020). Given the numerous processes that may be represented, the dimensionality required to capture these interactions (e.g., 1D-3D), and the timescales of interest, a diversity of RTMs have emerged over the recent decades with varying degrees of integration with hydrologic models.

At the most basic level is the one way coupling between either complex physically-based, spatially-explicit hydrologic models (e.g., Flux-PIHM; Bao et al., 2017) or simpler lumped-parameter models (HBV; Bergström, 1995; Bergström & Lindström, 2015) to geochemical box models (e.g., WITCH–Weathering at the Catchment Scale; Goddéris et al., 2006). Here, the hydrologic model passes soil moisture and water fluxes to the RTM to simulate biogeochemical reactions and thus, processes such as mineral dissolution/precipitation and solute generation and transport (e.g., Sullivan et al., 2019). One advantage of this approach is it simplifies the computational demand for tuning the RTM and allows the end user to focus on the degree of reaction complexity that they will choose to include. If the goal of the numerical simulations is to understand how changes in the solid phase, let say the dissolution of minerals, impact the generation of porosity and augments the permeability, then fully integrated models are needed. CrunchTope (or CrunchFlow; Steefel, 2009) is a widely used RT code that solves for saturated flow (i.e., Darcy flux) while allowing reactions to influence the solid phase. CrunchTope is capable of representing a detailed distribution of soil and rock properties in the subsurface, and has been used to simulate the long-term evolution of the subsurface under “averaged” hydroclimatic conditions (Wen et al., 2021; Xiao et al., 2021). Moving out of solely saturated conditions, there are codes such as Min3P and PFlowtran that can solve for variably saturated conditions in the 3-D tetrahedral mesh (Lichtner et al., 2015; Mayer et al., 2002; Su et al., 2021) and even include processes such as dynamic root architecture. Thus, our ability to represent critical zone processes and numerically explore how it responds to the shifts in the hydrologic cycle is strengthening.

One limitation in RTMs, is their integration into spatially-explicit watershed-scale hydrologic models. While some models do exist, the lack of spatially explicit information on soil, mineralogy, and biotic processes limits the degree to which these models can be applied. One such watershed-scale model is BioRT-Flux-PIHM, which can simulate interactions between land surface, watershed hydrology, and reactive transport at a variety of temporal scales (Bao et al., 2017). These watershed-scale models integrate watershed characteristics such as topography, vegetation, and temporal hydroclimatic variations and have some representation of subsurface structure to allow for predictions of precipitation/dissolution reactions in addition to carbon dynamics (Li, 2019; Xu et al., 2022; Zhi et al., 2019, 2022). But unlike the capabilities in CrunchTope that can update the solid phase distribution, and thus porosity and permeability, these spatially explicit models must first be paused and new parameters assigned to understand how changes in the subsurface could alter hydrologic and therefore, biogeochemical fluxes. To this end, some integrated hydrologic models have begun to include reactive transport (Moulton et al., 2015; Usman Munir & Frei, 2021; Z. Xu et al., 2022). While these developments have limited reaction pathways and/or the limited hydrologic conditions (e.g., saturated vs variably saturated), they are one manner by which RTMs are growing to be more fully integrated in large watershed and even regional scale models.

Recent advances in RTMs allow for the heterogeneous and dynamic nature of the critical zone to be better represented in numerical experiments. For example, geologic heterogeneity can lead to complex and variable fluid flow dynamics and thus, solute transport, creating challenges in our ability to predict geochemical processes (e.g., Navarre-Sitchler & Jung, 2017; Wen & Li, 2017). Efforts are underway to understand the discrepancies between laboratory and field based dissolution rates that arise from differences in physical heterogeneity, by providing correction factors to linear transition state theory (Hyman et al., 2022), elucidating the propagation of reaction fronts through fracture networks (Andrews & Navarre-Sitchler, 2021), and developing rate laws that account for the overall degree of spatial heterogeneity in the domain (Wen & Li, 2017, 2018). Advances in our understanding of isotope chemistry are now emerging as reaction capabilities within RTMs, particularly CrunchTope. Here the isotopic composition of both fluid and solid phase shed light on the dominant controls of reactions (e.g., spatial variability in microbial growth, order of rate laws, and dominance of kinetic vs equilibrium fractionation; Druhan et al., 2012; Druhan et al., 2013; Druhan et al., 2014). Modeled isotopic signatures are improving our understanding of the interaction between critical zone structure and function, for example: 1) multiple fractionation pathways and flexible transit time distributions are necessary to capture intra-site variability in silica stream water concentrations (Fernandez et al., 2022), 2) a fairly rapid supply of fresh bedrock is required to reproduce the parabolic shape between dissolved lithium and weathering intensity observed in global data (Winnick et al., 2022), and 3) unraveling the critical zone's past (e.g., changes in climate and vegetation) recorded in speleothems is possible through the modeling of stable- and radio-carbon isotope data (Druhan et al., 2021). By including root exudation processes into CrunchTope (REWTCrunch; Roque-Malo et al., 2022), it is now also possible to vertically resolve root-soil-microbe-water interaction and their influence on solute fluxes at a daily time scale.

Overall the development of RTMs allows us to explore both the impacts of the Anthropocene on critical zone function (Kumar et al., 2018; Sullivan et al., 2022) and to elucidate how long term changes in Earth's atmosphere has controlled weathering rates (Goddéris et al., 2010; Maher et al., 2009; Moore et al., 2012). We can now explore how changes in land cover influence stream water chemistry (Wen et al., 2021), how variations and hydrologic connectivity influence the export of dissolved organic carbon to streams (Wen et al., 2020), and the impact of changing climate on solute export across environments of varying subsurface heterogeneity (Wen et al., 2022).

2.2. Sediment and erosion

Accurate representation of streamflow generation processes and near surface hydrologic dynamics impact the overall sediment budget of a catchment and are important for understanding sediment transport processes (Heppner et al., 2006; Huang & Niemann, 2008). Many empirical and physically-based models have been developed to simulate erosion and sediment transport processes with various levels of complexity and data requirement (Merritt et al., 2003). While application of empirical models such as the Universal Soil Loss Equation is preferred due to a smaller number of parameters, these models assume that watershed properties are stationary (Zi et al., 2019). Physically-based models implement various formulations to represent detachment, transport and deposition processes, and use different model structures for representing hydrologic processes. With the exception of few models such as GEOtopSed (Zi et al., 2016), tRIBS-OFM (Kim et al., 2012) and InHM (Heppner et al., 2006), many erosion and sediment transport models simplify representation of subsurface hydrologic processes due to differences in temporal and spatial scales of the phenomena and computational demand of solving surface water-groundwater equations simultaneously (Francipane et al., 2012).

Existing coupled surface water-groundwater-sediment transport models either simplify surface water-groundwater coupling by using the first order exchange coefficient approach (e.g., Integrated Hydrology

Model; InHM, Heppner et al., 2006), reducing subsurface heterogeneity by using soil classes and geological layers parallel to bedrock (e.g., GEOtopSed; Zi et al., 2016), or simplifying vadose zone and groundwater processes by using a gravity-dominated formulation and the Boussinesq's equation under the Dupuit–Forchheimer assumptions, respectively (e.g., tRIBS-OFM; Kim et al., 2012 and tRIBS-Erosion; Francipane et al., 2012). Physically-based integrated hydrologic models such as ParFlow.CLM (Kollet & Maxwell, 2008; Maxwell & Miller, 2005) that simulate the terrestrial hydrologic cycle as a continuous system by solving the 3D Richards' equation over the entire subsurface and has a fully integrated overland flow simulator and a land surface model (CLM 3.0, Dai et al., 2003) to solve water and energy budgets at the land surface are valuable tools for integrating erosion and sediment transport processes. The integrated hydrologic model, HydroGeoSphere (HGS; Aquanty Inc., 2018; Brunner & Simmons, 2012; Hwang et al., 2014), which also simulates the terrestrial hydrologic cycle as a continuous system has been coupled to surface water operations model, OASIS (HydroLogics, 2009), and was developed to solve for fluvial erosion using the excess shear-stress approach (Brookfield & Layzell, 2019) and is linked to a streambank stability module (Wei, 2022). Despite these advances, inclusion or integration of sedimentation and/or erosion processes into integrated hydrologic models remains limited and computationally challenging as changes in land surface elevation due to erosion or deposition processes can lead to numerical instability for continuous simulations.

2.3. Ecohydrology

Transpiration accounts for roughly 70 % of precipitated water, although this proportion varies dramatically with space and time (Jasechko et al., 2013). Given the importance of transpiration, most hydrologic models consider the direct impact of vegetation on evapotranspiration. In simple, conceptual hydrologic models, vegetation may be implicitly represented as a parameter but in some integrated hydrologic models vegetation is explicitly represented via a combination of parameters and submodels (Fatichi et al., 2016a) that can include transpiration partitioning (Maxwell & Condon, 2016). These submodels generally account for vegetation's direct control on transpiration and indirect influences on evaporation, soil moisture, and snow accumulation and melt via canopy interception and shading but vary substantially in terms of the inclusion of other coupled ecological processes (see reviews in Brewer et al., 2018; Fatichi et al., 2016a).

Climate change is expected to alter not only vegetation function (water use) but to accelerate changes to vegetation composition and structure (size, density, rooting depths, heights, etc.) (Hauser et al., 2021; McDowell et al., 2022) as well as disturbances (e.g., fire, disease; Seidl et al., 2017). Disturbance driven changes in species are also expected to intensify with climate change (e.g., Serra-Diaz et al., 2018). These changes to vegetation structure and function will have substantial hydrologic impacts (e.g., Mankin et al., 2019) and thus there is a growing need to represent vegetation growth/mortality, community change and response to disturbances including fire in many integrated hydrologic model applications.

Models of ecohydrology vary along several dimensions (Fatichi et al., 2016a). The realism of the relationship between vegetation structure and radiative forcing varies from simple submodels, such as Beer's Law with a leaf area index, to complex submodels where tree-spacing and gaps, height, overstory/understory and/or sunlit and shade leaves are accounted for in estimates of the radiative forcing of plant transpiration (Bonan et al., 2021). Plant hydraulics or how plants mediate the flux of water from soil to atmosphere similarly vary from simple models of stomatal conductance to models that track vertical and horizontal root distributions, stem conductance and more complex stomatal physiology (e.g., Javaux et al., 2008, 2013; Lin et al., 2019; Trugman et al., 2019). Ecohydrology models also vary in how they account for changes in vegetation structure and composition through time, including changes that are coupled with hydrologic conditions e.g., declines in leaf area with drought (e.g., Garcia et al., 2016). Ecohydrology models that couple hydrologic models with carbon and nutrient cycling to grow vegetation have been available for decades and used within the land surface submodels in General Circulation Models (GCMs) or Earth System Models. These coupled carbon-hydrology models represent incremental changes to parameters that are relevant to hydrology (such as height, root depth and leaf area) with variation in the availability of light, water and nutrients (Arora, 2002). More recently coupled models that represent disturbances such as fire and disease are available (Seidl et al., 2017). These models can account for how climate drivers including drought alter the probability and severity of disturbances such as fire and disease that have dramatic consequences for vegetation (e.g., Hanan et al., 2021) and ultimately hydrology (e.g., Ren et al., 2021). Similarly several recent terrestrial biosphere models account for shifts in species distributions with climate (Fisher et al., 2022), although the representation of hydrologic processes in these models remains limited. Considering not only species differences but also between species interactions can have important hydrologic consequences (Pretzsch et al., 2015) but this level of plant ecosystem complexity is rarely included in hydrologic models.

For hydrologic models that resolve channel flow, ecohydrology includes the impact of riparian vegetation on hydrodynamics (e.g., effects of vegetation on fluid flow) and morphodynamics (including vegetation impacts on change in channel structure itself) (Camporeale et al., 2013; Marjoribanks et al., 2014). The representation of vegetation change in hydrodynamic models is generally less well developed relative to coupled ecohydrology models used in the terrestrial environments. Approaches for accounting for in-stream vegetation impacts range from simple roughness parameters to models that represent changes in riparian vegetation communities as a function of hydrologic conditions (Camporeale et al., 2013). Similarly, modeling within channel biogeochemistry, including hyporheic flow and exchanges, has advanced in recent years but these models of within stream and river ecological processes are rarely included in models that account for both upland and within river flows (Jan et al., 2021).

Finally, the impact of human intervention on vegetation can be significant. Both simple and complex ecohydrology models typically represent human intervention as an external forcing (e.g., prescribed land cover change, irrigation, fuel treatments, etc) (Wagner et al., 2019; Yalew et al., 2018).

2.4. Anthropogenic activities

Humans modify the terrestrial hydrologic cycle in numerous ways, including construction and operation of dams and reservoirs, surface water diversions, groundwater extraction, irrigation, and land use change including urbanization. Within the last millennium, 75 % of Earth's land surface has been modified by human activities (Luyssaert et al., 2014). These modifications can substantially alter infiltration capacity via impermeable surfaces and changes in evapotranspiration by altering the type, density and distribution of vegetation. Some processes related to these modifications have been included in hydrologic models for decades, including groundwater pumping and land use change, yet challenges remain. For groundwater pumping, the inclusion of numerous discrete groundwater wells and variable pumping rates, common in agricultural regions, remains numerically challenging. The representation of land use change is challenged by the variety of ways it can impact the hydrologic system, including changes to evapotranspiration due to changes in vegetation (see ecohydrology), and local scale routing of water in urban environments due to the construction of impermeable surfaces and water collection and distribution systems (e.g. storm water management).

Integrated hydrologic models that simulate the terrestrial water cycle (e.g. ParFLOW; Kollet & Maxwell, 2006), HGS (Aquanty Inc., 2018), GSFLOW (Markstrom et al., 2008) were originally developed to simulate natural hydrologic systems, with limited abilities to incorporate anthropogenic activities. Almost all watersheds have anthropogenic activities and impacts, therefore including these processes is critical for proper representation of the hydrologic conditions. In addition, these models are increasingly being used for integrated water management planning, which also requires inclusion of the anthropogenic water uses and management infrastructure for proper assessment. In response, integrated hydrologic models have advanced to better include the interactions between humans and the terrestrial water system. However, one of the biggest challenges in integrated hydrologic model application is limited data availability of human water use (e.g., groundwater pumping, canal deliveries).

More recently, a number of packages have been integrated into hydrologic models to capture anthropogenic activities. Building upon existing frameworks that capture groundwater and surface water pumping, modules were developed to capture irrigation application, including variability in evapotranspiration and infiltration (often termed irrigation return flow) due to irrigation strategy (e.g. flood irrigation, center pivot, subsurface drip) and water rights structure (e.g., Kitlasten et al., 2021). These modules include specific agricultural packages for GSFLOW (Niswonger, 2020), and processes integrated directly into the integrated hydrologic modeling codes such as ParFlow and HydroGeoSphere (Aquanty Inc., 2018; Condon & Maxwell, 2013). Hydrologic modeling in urban settings is particularly challenging due to the high resolution and spatial complexity of urban land cover (Salvadore et al., 2015). Flow networks in urban environments are also complex, and hydrologic models applied to urban areas (e.g SWMM; Niazi et al., 2017) include submodels that integrate storm sewer networks, green infrastructure and stormwater control measures (SCMs), and differentiate between connected and disconnected impervious areas (e.g., Bell et al., 2019). High resolution data is increasingly available for urban areas and assimilation of this data is expected to improve hydrologic modeling (Hutchins et al., 2017). The high spatial resolution required to account for these changes to flow networks can be a barrier for regional scale IHMs application (Golden & Hoghooghi, 2018). However fine scale hydrologic model applications can be used to derive parameters based on land use classification (e.g., high density urban, suburban) to support larger scale application (e.g., Shields & Tague, 2015).

Many codes are modified to include methods of integrating reservoirs, canals, pipe networks and other water storage and distribution systems into the hydrologic models. While natural processes and physical conditions can constrain operation of these engineered structures, the distribution of water is dictated by human decisions, regulations, and policies. Integrating these non-physics based operations into an integrated hydrologic modeling framework often requires coupling to other existing models that use rule-based optimization strategies (e.g., Brookfield et al., 2017; Morway et al., 2016) or incorporating often inflexible boundary conditions based on historic operations. A significant drawback of the latter approach is that operations cannot be easily adapted for future scenarios as opposed to the former which has operational structures built into the coupled model.

2.5. Cold-region Processes

Snow-dominated headwaters provide water resources to 1/6th the world's population (Barnett et al., 2005) and support ecologic and social-economic services (Immerzeel et al., 2021). Cold regions are considered especially vulnerable to climate change (Milly & Dunne, 2020; Portner et al., 2019), with low-land dependence on these snow water resources expected to increase in the near future (Viviroli et al., 2020). The amount and timing of snow and glacial melt are critical to hydrologic processes related to transpiration (Knowles et al., 2018; Parida & Buermann, 2014), recharge (Carroll et al., 2019; Godsey et al., 2014; Meixner et al., 2016) and streamflow generation (Hammond et al., 2018; D. Li et al., 2017a; Millan et al., 2022). Likewise snow and ice loss and permafrost degradation have important implications on biogeochemical reactions, trace gas release and riverine export of organic matter, inorganic nutrients and major ions (Broadbent et al., 2021; Frey & McClelland, 2009; Jafarov et al., 2018; Milner et al., 2017; Miner et al., 2021; Pongracz et al., 2021). Snow and ice cover also play an important role in weather and climate through surface albedo, sublimation, sensible heat exchange with the lower atmosphere and insulation of soil by snow (Clark & Serreze, 2000; Lo & Clark, 2002; L. Xu & Dirmeyer, 2011). The interactions of snow and ice across atmospheric, hydrologic, ecologic and biogeochemical subcomponents is further complicated by the scale-dependence of snow processes (Bales et al., 2006; Broxton et al., 2015; Clark et al., 2011; Deems et al., 2006; Mott et al., 2018; Tennant et al., 2017). As a result, representation of snow and ice dynamics in integrated hydrologic models remains a major challenge.

As a consequence, classic representations of snow processes in hydrologic models have relied on relatively simple temperature-index approaches that correlate snowmelt to air temperature (e.g., Martinec, 1975). These empirical relationships are most often associated with glacial applications, snowmelt in open sites and operational forecasting (Kumar et al., 2014) with recent models incorporating wind speed, vapor pressure and radiation into the approach (Li & Williams, 2008). More accurate representation of cold-region hydrology must describe the distributed water- and energy-balance between the atmosphere and land surface (Clark et al., 2015; Shrestha et al., 2015). Modeling approaches that account for water and energy distributions across space tend to also account for their vertical distribution in the snowpack. Some integrated hydrologic models use only two snowpack layers to account for radiant, convective and conductive exchanges (e.g. GSFLOW) while others are more finely resolved (e.g. Parflow-CLM). These modeling approaches are largely based on the parameterization of individual processes related to albedo, snow compaction, turbulent and radiant energy transfer (Chen et al., 2014; Kumar et al., 2013; Magnusson et al., 2015). Representation of wind redistribution (e.g., Liston & Elder, 2006) remains a significant challenge (Zhou et al., 2021) and is rarely included directly in integrated hydrologic models due to computational expense and lack of process understanding. However, the redistribution of snow is potentially important in capturing the amount and timing of snowmelt with significant ramifications on the water budget. As a consequence, several hydrological studies have corrected precipitation inputs to account for preferential distribution using airborne lidar mapping of snowpack (Carroll et al., 2019; Lahmers et al., 2022), satellite-derived data assimilation strategies (Bennett et al., 2019) or accounting for topographic effects on gravitational and wind transport of snow (Freudiger et al., 2017).

Representation of permafrost processes in earth system models have advanced in recent years but there remains significant uncertainty and variation in how model representations account for freeze/thaw processes and how released melt water moves through the subsurface to rivers (Andresen et al., 2020). More detailed representations of permafrost hydrology are available and these approaches provide more accurate estimates of permafrost change on river flow and chemistry (e.g Cold Regions Hydrological Modelling Platform (CRHM; Pomeroy et al., 2007), Advance Terrestrial Simulator (ATS, Painter et al., 2016). However, strategies are needed to integrate learning from these data intensive permafrost models into integrated hydrologic models (Krogh & Pomeroy, 2021).

2.6. Atmospheric processes

Atmospheric processes control the weather (short-term conditions) and climate (long-term conditions) and are critical drivers of the hydrologic cycle, governing the hydrologic and energy fluxes between the air and land surface. Most hydrologic models include weather-related parameters, such as precipitation and potential evapotranspiration. In early hydrologic models, the weather conditions were included as a boundary condition with prescribed precipitation and potential evapotranspiration. These models advanced to include algorithms and models that calculated actual evapotranspiration based on both weather and hydrologic conditions and subsequently to actual weather and climate models that provided one-way and two-way feedback to the hydrologic model (Davison et al., 2015, 2018; Maxwell et al., 2007; Maxwell & Condon, 2016; Sorooshian et al., 2008; Zhang et al., 2009). The treatment of atmospheric conditions varied between surface water and groundwater models, where the direct link to weather was included earlier in the surface water models (e.g., Benoit et al., 2000; Walko et al., 2000) compared to groundwater models (e.g., York et al., 2002). Groundwater models traditionally prescribed recharge fluxes that are often indirectly attributable to mean weather conditions (e.g., Maxey & Eakin, 1949). This is likely due to the direct connection between the land and atmosphere compared to a more in-direct connection to the subsurface.

In the frameworks that integrate atmospheric and hydrologic models, computational difficulties arise from the complexity of the processes included and the mismatch between the spatio-temporal resolution and scales between the two model types (Davison et al., 2018; Fatichi et al., 2016b; Maxwell et al., 2011). The domain required to simulate weather/climate is significantly larger than that required for terrestrial hydrology, and associated cell sizes also have significant mismatch. This is driven by the relatively fast rates of atmospheric processes, in comparison to slower rates of the surface water domain, and even slower rates of the groundwater domain. Approaches to address these issues include coupling existing models of each system, such as in the Terrestrial Systems Modeling Platform (TerrSysMP; Shrestha et al., 2014). This approach uses an external coupler to couple three independent models (an atmospheric model (Consortium for Small-Scale Modeling; COSMO), a land surface model (the NCAR Community Land Model, version 3.5; CLM3.5), and ParFlow with different spatial and temporal resolutions in an integrated framework. Results show explicit representation of groundwater processes in TerrSysMP reproduce observed heat waves statistics compared to regional climate models (Furusho-Percot et al., 2022).

3. Challenges and Future Directions

While the continued development of integrated hydrologic models, including those that have expanded to include the domains described above, provide new capabilities and opportunities for application, it also continues to face, and develop new, challenges for their use. These challenges include those related to process-based representation, such as the ability to upscale parameters and constitutive equations and represent spatial heterogeneities, however, detailing these challenges for all the processes reviewed here is beyond the scope of this paper, and can be independent review papers in each discipline. Here, we aim to discuss and reiterate some of the challenges related to the expansion of integrated hydrologic models into these other domains and bringing together models and methods from across traditional discipline boundaries and to propose potential solutions.

3.1. Model selection

With the number of available modeling frameworks expanding, the first challenge often faced by model users is selection of modeling frameworks. Despite the expectation that the 'best model for the job' should be selected, recent research indicates that technical considerations often do not determine what model is used, instead more 'social' aspects, including familiarity with the model, and interactions with others who have used the model previously are considered (Melsen, 2022). A challenge remains to balance these 'social' aspects of model selection with a less-biased assessment of what model would best meet the objectives of the project. In the supplemental document to this paper we suggest a model selection pathway that we feel balances these aspects which can provide more novice model users with guidance on model selection (see supplemental information). Several of the aspects and challenges discussed in reference to model selection, such as data availability and computational resources, are further discussed in this section.

3.2. Data

Sources of uncertainty in integrated hydrologic models include uncertainty in model inputs, structure, parameters, and observations used to constrain model parameter sets (Liu & Gupta, 2007; Moges et al., 2021). While there are variety of techniques to address model uncertainty, including approaches for calibration, sensitivity analysis and uncertainty quantification, widespread adoption of these approaches within the integrated hydrologic models remains challenging due to computational demand of methods such as the Bayesian inference (Herrera et al., 2022; Kavetski et al., 2006; McMillan et al., 2018). Community standards, training in the application of these core techniques and the development of easy to use, well documented tools, are still needed, particularly within the integrated hydrologic model context where a 'one size fits all' approach to model parameterization and calibration is rarely appropriate for all sub-models (McMillan et al., 2018; Moges et al., 2021). Further existing uncertainty analysis techniques do not typically explicitly address structural uncertainty (Blöschl et al., 2019).

The exponential increase in, and accessibility of, earth system science datasets, including remote sensing data, distributed networked sensors and new innovations in geophysics, are both an opportunity and a challenge for integrated hydrologic models. On one hand, integrated hydrologic models benefit from new data for assimilation, parameterization and calibration (e.g., Hutchins et al., 2017); as integrated hydrologic models account for multiple processes, and have the ability to incorporate multiple data sets. The diversity of data sets, within differing spatial–temporal scales, and a wide range of accuracy, presents a challenge, however, for assimilation. Community cyberinfrastructure and training for ensuring appropriate techniques are used for disparate datasets will be needed (Fer et al., 2021). Recent studies showed that variability in the magnitude and resolution of commonly used gridded precipitation and air temperature products for forcing integrated hydrologic models results in large uncertainty in simulated water budget in a mountainous catchment (Schreiner-McGraw & Ajami, 2020, 2022). Therefore, development of data fusion strategies are needed to create accurate climate products particularly in regions with large topographic gradients.

3.3. Computational needs

The computational needs of integrated hydrologic models can vary significantly with model size, resolution, and complexity. The challenges related to computing in hydrologic modeling are not new and research is constantly striving to simultaneously increase the complexity of the models and develop methods to reduce the computational demand (Gan et al., 2018; Ghorbanidehno et al., 2020; Zhang et al., 2009). This challenge remains for integrated hydrologic models, particularly as we continue to develop more complex and more integrated models. To address this challenge an additional hurdle emerges, the ability to modify existing models to use new computational platforms, such as the recent transition to cloud computing and prior to that, the transition to parallel computing. This transition often requires changes to the model and solver structure, which requires some expertise in computer science. Many groups developing the leading-edge advances in integrated hydrologic models include researchers with diverse expertise required to make these transitions, and it is critical to maintain this diversity as new computing capabilities and platforms emerge.

Another method of addressing computational challenges is integration with other methods, such as machine learning methods. We can identify 5 potential synergies in the application of machine learning (ML) and integrated hydrologic models: 1) integrated hydrologic models can help to identify the underlying mechanisms that give rise to patterns revealed by machine learning in observational data sets. 2) Patterns identified by ML can be used to parameterize, calibrate and evaluate integrated hydrologic models (e.g., Kim et al., 2019; Tsai et al., 2021). Using patterns or behaviour for calibration rather than calibrating with observations directly can improve hydrologic model reliability (Schaefli et al., 2011). 3) ML can reveal patterns within integrated hydrologic model outputs. Many integrated hydrologic models can estimate 1000 s of variables at multiple time scales. ML can be used to simplify this output (e.g., Burke et al., 2021). 4) ML can be used to construct emulators of computationally intensive integrated hydrologic models, which can substantially expand sensitivity analysis (e.g., Fer et al., 2018). 5) Physical theory from integrated hydrologic models can be incorporated into ML methods (Jiang et al., 2020; Zhao et al., 2019), sometimes referred to as physics informed ML or Hybrid modeling. There are many emerging approaches for augmenting physically-based models with ML or using theory to guide the ML models (Bergen et al., 2019).

3.4. Applicability, Accessibility, and ease of use

Applicability, accessibility and ease of use are intricately linked. Complex models that require extensive expertise and have intensive data and computational requirements are able to be used in research applications, but are not often accessible beyond those in the research realm. Their results may be accessible, but the interpretation of their results may still require extensive hydrologic knowledge. Recent work has pushed towards more accessible applications of the complex integrated hydrologic models, including frameworks that allow for limited manipulation by users for engagement and decision-making (e.g., Ewing et al., 2022; Jadidoleslam et al., 2020), and teaching tools that simplify the hydrologic system (e.g., Gallagher et al., 2021; Gannon & McGuire, 2022). Examples of these applications are limited and a challenge remains in incorporating advanced tools and 'state of knowledge' into frameworks that are applicable and useful across the spectrum of potential users. We need to work towards accessibility of state-of-the-science to all users, identifying the technical background and knowledge of the intended users and the computational and data resources required. It is important to note that any one modeling framework does not have to meet the needs of all users, nor do variations of every modeling framework need to be made, but clear intention about the purpose of framework development is needed. Broadly, the spectrum of models that need to be available include:

- Research-focused models that are more complex and difficult to use, have high computational and data requirements but will move the fundamental science and understanding forwards. This includes developing models, in addition to methods of incorporating different information and data types (e.g., remotely sensed, qualitative) and using a variety of computational resources (e.g., cloud, parallel processing, and quantum computing).
- Application-based models that are used by the broader hydrologic community to address ongoing societal issues. These are often commercial or open source models that still require expertise, but are not as complex and intensive as research-focused models to develop and run. These models lag behind the research focused models but aim to keep users (e.g., consulting, government, etc.) as up to date on proven approaches as possible.
- Teaching-focused models that are simple to use and modify, and computationally inexpensive with results that are easy to interpret. These models focus on tools that can inform students/shareholders/general public - anyone with an interest but limited expertise. These models that are critical to effective communication and stakeholder involvement in the modeling process have shown to increase identification of interventions and model outcomes (Maskrey et al., 2016). These models are also valuable for training and adoption of advances in hydrologic models (e.g., Gallagher et al., 2021).

We have not listed specific models in the categories defined above because often the same modeling framework can be applied in multiple categories, depending on how they are implemented. For example, while ParFlow is a research-focused model (e.g., Kollet and Maxwell, 2008; Condon and Maxwell, 2013), it has also been used in teaching-focused applications including the Sandbox model (Gallagher et al., 2021). In addition, different variations of the same base model (e.g., MODFLOW; Harbaugh, 2005), which is used extensively in application- and teaching-focused purposes, are also used for predominantly research (e.g., GSFLOW; Niswonger, 2020). While some modeling frameworks are mostly used in one focus area, such as RT-Flux-PIHM (Bao et al., 2017; Zhi et al., 2022) and HydroGeoSphere (Aquanty, 2018), they are beginning to see use in other applications as these advances become more established.

4. Conclusions

Numerical models in hydrology have advanced significantly in recent decades, from simplistic models of one process and component of the hydrologic cycle, to advanced models integrating across several processes and components. There are a wide variety of models and model combinations under development that provide the diversity of frameworks needed to cover the wide range of environments and applications to which they are applied. Consistent with this, continued model development should seek to not converge upon one modeling approach or framework, but remain diverse to meet the needs across the spectrum of users, sites, and objectives. The challenges currently faced in model development, some of which were discussed here, also present opportunities to continue diverse model development through the pursuit of different paths to overcome the challenges. We encourage taking this diverse approach to model advancement across three main components of development: model, data, and platform (Fig. 3).

To advance our understanding of the processes and systems included in each model it is important to investigate them using many different modeling approaches. This includes the processes included in the modeling framework (Model development in Fig. 3), and the approach of the model itself, whether that is deterministic, statistical, etc. Much like the integration of different processes within one model framework, we also believe that the recent advances integrating different approaches (e.g.,Tsai et al., 2021) are an ideal path forwards towards not only improving our understanding of the inherently complex systems we seek to represent, but also improving the efficiency of the models themselves.

As we increase the processes and approaches used in integrated hydrologic models, the data required to parameterize and calibrate them also changes. In addition, recent advances in sensor technology provide an opportunity to use non-traditional data and data types in our model design and development. This requires continued advancements in our data assimilation methods to integrate these new data types into modeling frameworks. Research has demonstrated that the careful integration of different data, in-situ and remotely sensed products, into our modeling development provides significant improvements in model skill (Stisen et al., 2011; Tang et al., 2019), and we believe that there is significant potential to improve them further.

Computational resources and platforms used for integrated hydrologic models continue to advance and evolve. The accessibility of these resources, from cloud to high performance and quantum computing, provides opportunities across the spectrum of model users. For example, for educational and training purposes, web-based models can be used to allow users to modify model scenarios and experiment with the model and results, yet are readily accessible and can be easy to use. Conversely, while high-performance computing systems are not readily available and accessible to most users, the large-scale, complex models developed

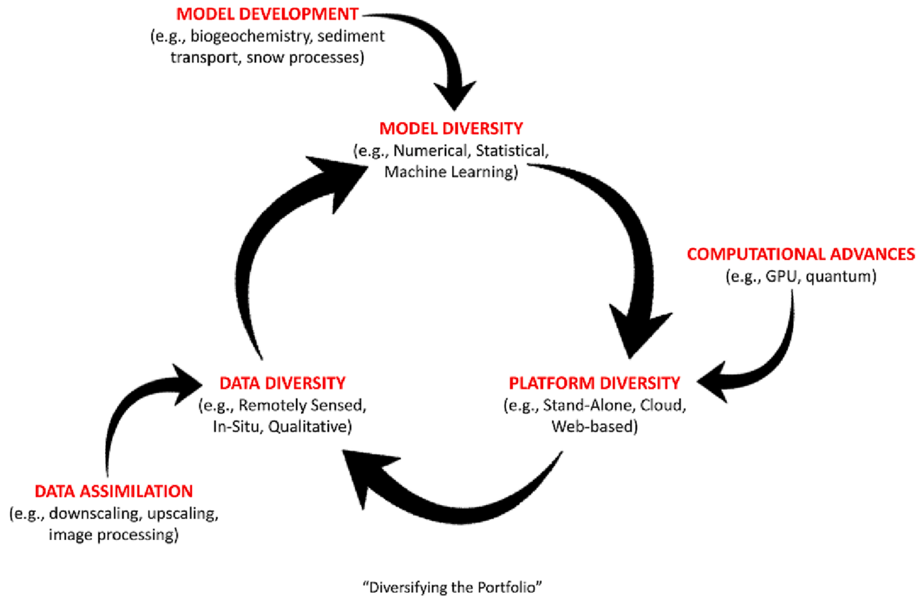

Fig. 3. An integrated approach to model development, with a focus on encouraging the diversification of models.

for research purposes are often best developed using these platforms for efficiency. Developing a diversity of modeling frameworks that operate across the spectrum of computational resources will help advance hydrologic sciences for all users.

We feel inclusion and diversity is the future of integrated hydrologic modeling – not only in developing new modeling frameworks, but also in the developers and users of these models. There is room for a multitude of modeling frameworks, including those not currently in use in hydrologic science, and by diversifying the model, data and computational platforms we are allowing for the greatest opportunities for advancement in hydrologic modeling.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

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