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Uncertainties as a Guide for Global Water Model Advancement

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Abstract

Global water models increasingly allow us to explore the terrestrial water cycle in earth-sized digital laboratories to support science and guide policy. However, these models are still subject to considerable uncertainties that mainly originate from three sources: (1) imbalances in data quality and availability across geographical regions and between hydrologic variables, (2) poorly quantified human influence on the water cycle, and (3) difficulties in tailoring process representations to regionally diverse hydrologic systems. New, more accurate, and larger datasets, as well as better accumulated and even improved knowledge, will help to reduce these uncertainties and eventually lead to model advancement. In this review, we explore sources of uncertainty critical to global water models and define actions to reduce them where possible, therefore providing a guide for global model advancement. Following this

path will increase the robustness of model outputs, which is urgently needed to tackle key scientific and societal challenges.

1 Introduction

In 1972, the Blue Marble picture showed us, for the first time, a color image of Earth from space, laying bare its vulnerability and interconnectedness through the water cycle (Eagleson, 1991). It suggested that we require an understanding of the past, present, and future of Earth's freshwater resources to safeguard the blue planet for future generations. Global water models (GWMs) are a central tool to foster this understanding by simulating the global terrestrial water cycle with the help of computer programs. From the first coarse-resolution models with simple process representation in the 1990s, these models have evolved tremendously due to remote sensing (Chahine, 1992; Wulder *et al.*, 2022) and an increased process understanding from regional hydrologic research (Shuttleworth, 1994) (for a history of GWM evolution see Fig. S1). They can now be run at high temporal (hourly-daily) and spatial (up to 1 km) resolutions and include an increasing range of hydrologic processes and anthropogenic influences (Sellers *et al.*, 1997; Pokhrel *et al.*, 2016; Arheimer *et al.*, 2020; Müller Schmied *et al.*, 2021; Hoch *et al.*, 2023). Until recently, these models have been solely based on (sometimes very simplified) representations of hydrological processes, but machine learning and hybrid approaches are starting to emerge (Feng *et al.*, 2023). Here, we use three classes of models representative of GWMs: global hydrological, land surface, and dynamic vegetation models, which have evolved in parallel (Bierkens, 2015). While all three classes were initially built for different purposes, they all model the global terrestrial water cycle and are used to answer questions related to global hydrology (Haddeland *et al.*, 2011; Gudmundsson & Wagener *et al.*, 2012; Schewe *et al.*, 2019; Pokhrel *et al.*, 2021). We chose to jointly discuss them as GWMs as all model classes benefit from a more accurate representation of the terrestrial water cycle, and they all suffer from uncertainties specific to modeling these processes on a global scale.

Because water connects all spheres of the Earth, GWMs have a wide range of applications and offer opportunities for future use in many fields (Fig. 1). In contrast to models of specific places or regions (e.g., catchments or river basins), the capacity of GWMs to generate continuous and consistent global hydrological time series for variables such as streamflow, soil moisture, evapotranspiration, or snow water equivalent makes them a valuable resource. Their global coverage allows usage in regions with limited or no observations, they help to understand spatiotemporal patterns of hydrological extremes (Ward *et al.*, 2014; Emerton *et al.*, 2017; Arheimer *et al.*, 2020) in support of global early warning systems and risk maps (Emerton *et al.*, 2016; He *et al.*, 2020), and they help to assess future risks such as water scarcity, and explore possible adaptation measures (Veldkamp *et al.*, 2016; van Vliet *et al.*, 2021). Other research fields have used GWMs to assess issues related to the Water-Energy-Food nexus (Lodge *et al.*, 2023) or the impacts of climate change on freshwater ecosystems (Döll & Zhang, 2010; Bartosova *et al.*, 2021). Furthermore, GWMs have improved the representation of the Earth system in climate and weather models, because one of the primary outputs of water models, streamflow, naturally integrates various terrestrial hydrological processes and can thus be used to evaluate mass balances of other models (Zsoter *et al.*, 2019; Boussetta *et al.*, 2021).

While GWMs provide global coverage of multiple water cycle components, current uncertainties and their poor quantification may limit their value (e.g., for global change impact analysis) as the reliability of model estimates remains unclear (Wagener *et al.*, 2022). For example, the sixth IPCC assessment report concluded that our knowledge of climate change impacts on groundwater is still poor partly because groundwater remains inadequately presented in many models (IPCC, 2023). Even if implemented, uncertainty of groundwater levels remains high (Reinecke *et al.*, 2024). Complex process interrelationships such as atmospheric CO_2 fertilization and its long-term impact on global water availability are poorly known (Milly & Dunne, 2016), while current representations of anthropogenic impacts such as irrigation, groundwater abstractions (Arheimer *et al.*, 2020; Puy *et al.*, 2021; McDermid *et al.*, 2023), and river regulation (Arheimer *et al.*, 2017) are still in their infancy. This has direct consequences for other impact assessments, such as assessing the economic impacts of floods (Willner *et al.*, 2018) or vulnerability to food insecurity (Betts *et al.*, 2018).

Here, we argue that by identifying and quantifying uncertainties, we can efficiently guide the efforts of the global hydrological community to build better GWMs and, as a result, provide better information to policymakers. By better we mean models that are more consistent with observations and with our system understanding (perception). While we cannot expect global models to represent local observations as well as a locally calibrated model, we have a need for models of the entire terrestrial surface, which can realistically represent our process understanding across diverse hydrologic landscapes and enable a credible (though always uncertain) look into the future across different what-if scenarios.

Much has been said about the topic of uncertainty in the context of local and regional models (Wagener & Montanari, 2011; Beven, 2016; Nearing *et al.*, 2016), but what are the problems and solutions specific to global water models? We focus on so-called epistemic uncertainty, defined by Walker *et al.* (2003) as "uncertainty due to the imperfection of our knowledge, which may be reduced by more research and empirical efforts." If we can identify those uncertainties that can be reduced, they can guide advancements of GWMs and our scientific hydrological understanding in general. Based on a critical review of the current literature, we identify three key sources of uncertainty specific to modeling the terrestrial water cycle on a global scale. We then outline how these uncertainties affect our understanding of past, present, and future water cycles, and suggest ways to reduce them and thus advance GWMs.

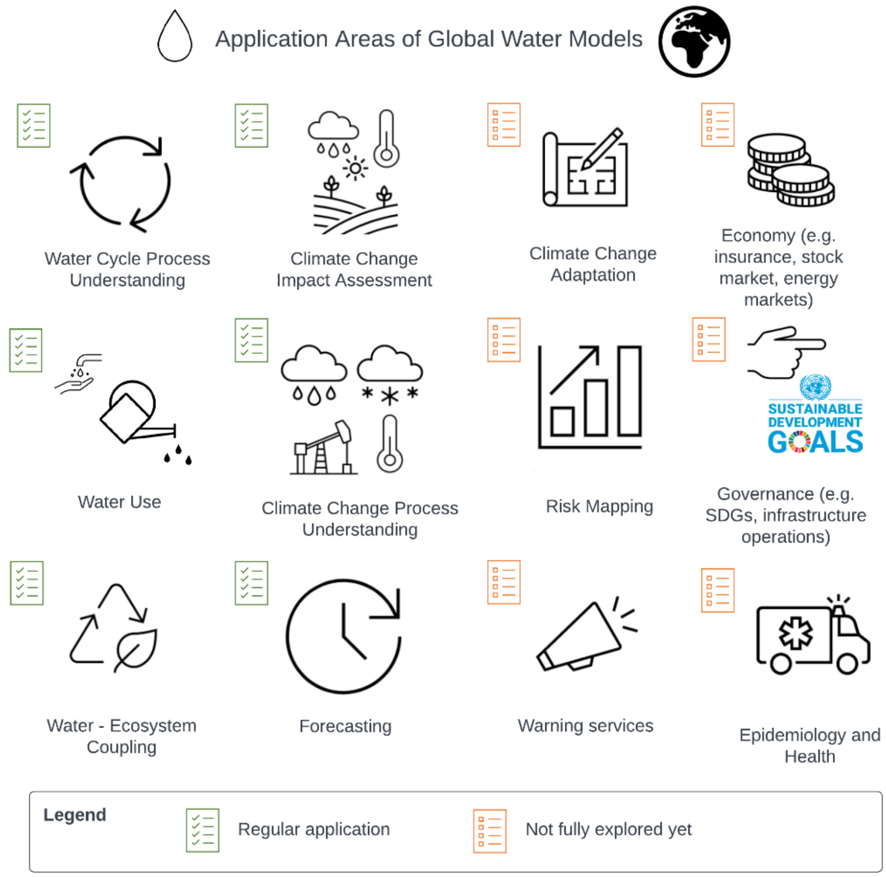

Figure 1: Global water models are relevant for a wide range of applications, but their potential has not been extensively explored in all possible areas. References to examples (for their regular application) and further explanations of potential future applications (not fully explored category in the figure) can be found in Table S1.

2 Uncertainties in building, forcing, and evaluating global water models

In this section, we discuss the main sources of epistemic uncertainty in GWMs and explore from where they originate during the building, forcing, and evaluation stages of the modeling process. All models are subject to uncertainties, as they are, by definition, an approximation and, thus, an imperfect representation of reality. Knowing when, where, and why models are uncertain is a starting point for refinement and improved scientific understanding (Eyring *et al.*, 2019; Gleeson *et al.*, 2021). Importantly, uncertainties can affect the robustness of and confidence in impact assessments, policies, and decisions derived from model results (Haddeland *et al.*, 2011; Puy *et al.*, 2022). Insufficient and inaccurate quantification and communication of existing uncertainties may lead to overconfident decisions and potentially to loss of trust in models (Beven, 2018).

We focus our discussion on uncertainties that relate to developing and implementing GWMs, though additional uncertainties originate from the natural variability of human and environmental systems. Such aleatory uncertainties represent variability, imprecision, and randomness, or factors that can generally be modeled as probabilities in statistical frameworks (Beven *et al.*, 2018). In addition, uncertainties might arise when testing specific intervention strategies to guide policymaking, such as land use change or water use scenarios, which cannot be assessed against observations. What is important for our discussion here is that many of the uncertainties currently impacting GWMs originate from a lack of knowledge, i.e., they are epistemic and can be reduced (in principle) through new or better utilized (e.g., through new algorithms or different models) observations, or through new knowledge (Beven *et al.*, 2018). They exist because we lack system understanding, because we cannot measure certain variables in all places, at all times, at the right scale or at all, and because measurements themselves carry uncertainties (Sivapalan, 2018; Condon *et al.*, 2021). In addition, we are often interested in future system states that are possibly very different from the past and thus may lack historical analogs (e.g., due to climate or land use change).

Since GWMs cover the entire terrestrial area of the globe, the degree of uncertainty and potential approaches to address them differ from local and regional hydrologic models. One key problem global models experience more than local or national models is data consistency. Given that GWMs are meant to represent the whole terrestrial hydrology, a key issue is that data support and the uncertainty present will vary hugely between regions. Thus, it is likely that the approaches taken to reduce uncertainty will have to vary as well.

We find that uncertainties largely originate from three sources (Fig. 2): (1) imbalances in data quality/availability across geographical regions and between hydrologic variables, (2) poorly quantified human alterations of the water cycle, and (3) difficulties in tailoring models to regionally diverse hydrologic systems. Imbalances in existing datasets create considerable problems in our ability to assess how consistent models and real-world dynamics are. For example, (in-situ) data availability in temperate regions such as Europe and North America tends to be high, and we generally have more data in regions with higher population densities (Krabbenhoft *et al.*, 2022) (see Fig. 2a). If observations are available, they frequently suffer from inconsistencies due to differences in data collection between administrative boundaries (Fig. 2b), which are challenging to eradicate and can significantly impact model results. In addition, observations are often available in places where anthropogenic influences are considerable but unquantified (often because the data is not publicly available; Fig. 2c). For example, while global datasets on reservoirs and dams are available (Mulligan *et al.*, 2020), their operation schemes are largely unknown (Hanasaki *et al.*, 2006).

Furthermore, it is difficult to tailor GWMs to reflect diverse regional hydrological systems (Fig. 2d) because that regional process knowledge is either not (easily) available or biased (i.e., our perceptual understanding is limited) (Stein *et al.*, 2024) or because we lack the flexibility to implement that knowledge in the current generation of models. In addition, observations rarely represent the scale of model units (Weber *et al.*, 2023). In-situ observations of individual variables (e.g., soil moisture) are often only representative of areas much smaller than the scale of the modeling unit (e.g., a raster cell; this is also true for regional models, but the scale difference is likely more severe for GWMs). In contrast, observations measured at larger spatial scales (i.e., satellite measurements) often integrate over multiple state variables and/or larger areas than the modeling unit. Streamflow observations are a special case as they integrate various processes inside a catchment. However, (especially) for large catchments, the influence of diverse spatially distributed and heterogeneous runoff generation processes cannot be identified easily (if at all) from the signal that arrives at the catchment outlet(van Werkhoven *et al.*, 2008).

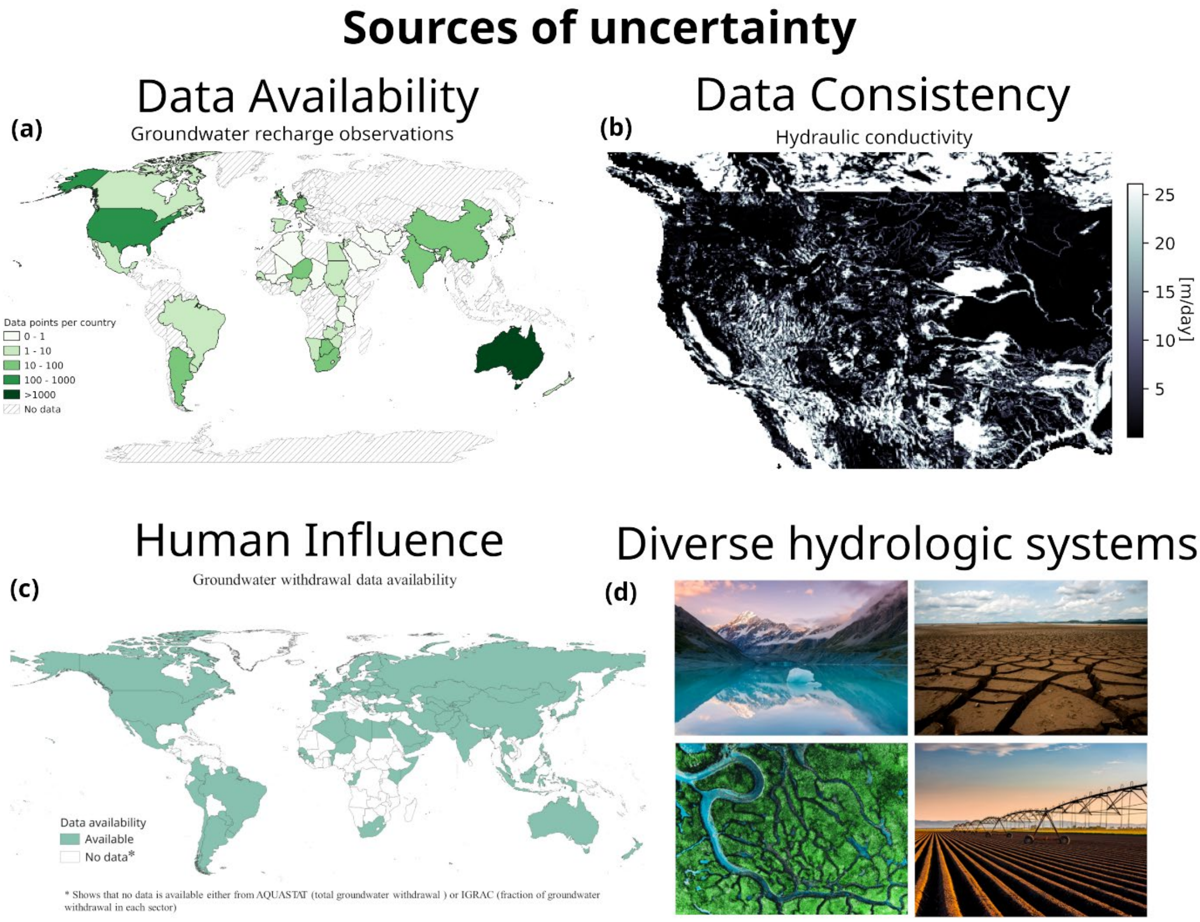

Figure 2: Sources of uncertainty for global water models. Uncertainties mainly originate from three sources: **a**, imbalances in data availability, exemplified by showing the number of available data points in a global dataset of groundwater recharge(Moeck *et al.*, 2020), and **b**, consistency across geographical regions illustrated by a zoom-in showing that hydraulic conductivity in a widely used global dataset (Gleeson *et al.*, 2014) changes abruptly at the border between Canada and the USA, **c**, poorly quantified human influence on the water cycle demonstrated with available data on groundwater withdrawal on a country level in the AQUASTAT and IGRAC database, and **d**, difficulties in tailoring process representations to regionally diverse hydrologic systems.

Building global water models

Any process-based water model, independent of its application scale, is generally built through a modeling process that establishes a perceptual (or conceptual) model of the system under study and ends with a computational model that can be executed (Beven, 2018). For regional models, much discussion has been placed on how these stages are implemented (Beven, 2012). Current GWMs are generally built along the following steps: (1) Given the size of the domain, one or very few representative perceptual models are used (e.g., separating landscapes into mountains and sedimentary basins (Hartmann *et al.*, 2017)). (2) The perceptual model(s) are then translated into model structures applied at the modeling unit (typically a raster cell or a catchment), and routing functions are added to connect the individual modeling units. (3) Each model unit is then tailored to regional conditions (e.g., hydro-climatic) via the model parameters, mostly through a priori estimates directly derived from globally available soil, geology, vegetation, and other datasets. (4) Models may consider different aspects of human interventions, such as water abstractions or reservoirs. (5) The model is then driven by forcing inputs such as precipitation, temperature, and radiation, either using observational records, reanalysis products, or projections from Global Climate Models (GCMs). Sometimes, GWMs are directly coupled to a GCM together with other additional physical, chemical, and biological processes, then referred to as an Earth System Model (ESM) (Clark & Fan *et al.*, 2015). (6) GWMs can be evaluated based on their main outputs, such as streamflow, soil moisture, or evapotranspiration, though whether and how this is done might vary by model and study focus. Calibration of global models to streamflow or other observations is not standard yet (Kupzig *et al.*, 2023) but can be achieved in principle (Döll *et al.*, 2003; Arheimer *et al.*, 2020). While all these modeling steps offer options and choices that introduce uncertainty, they also result in diverse models. However, the current model diversity does not reflect the diversity of hydrologic processes found across the global land surface. It is rather a consequence of different modelling groups selecting a specific underlying model structure to build their GWM with. This diversity can be captured by model ensembles, which offer more robust predictions and help reveal knowledge gaps regarding the appropriate representation of the terrestrial water cycle (e.g., Reinecke *et al.* (2021), Gnann *et al.* (2023)). Even though the ensemble is an ensemble of opportunity and does not necessarily reflect model structural uncertainty in a coherent manner.

Data availability is a key problem for all steps of the model-building process for GWMs. It starts during perceptual model development, where the availability of data limits how detailed our system perception can be. Given that modelers are also limited in their knowledge of global hydrologic diversity, this limitation influences what structural representations we might even consider. While local experts may have a thorough understanding of a certain hydrologic system, collecting and combining that local knowledge into a coherent global database has not yet been achieved. Even though the first steps have been made (McMillan *et al.*, 2023), the transferability of system understanding, especially across scales, remains difficult (Wagener *et al.*, 2010). Ultimately, the lack of trustworthy (not uncertainty-free) perceptual models limits our capability of tailoring global models to the diversity of hydrologic systems that we find on Earth.

A chosen perceptual model is then translated into a model structure and tailored to different hydrologic systems, mainly through global datasets (Table S2). The datasets are used to estimate a priori model parameters, and in many cases, these data may have already influenced the equations that were used to build the model structure in the first place. For example, the Harmonized World Soil Database (HWSD) (Nachtergaele *et al.*, 2010) is utilized as a soil map in eight GWMs in the global water sector of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP) (Frieler *et al.*, 2017), and is playing a crucial role in estimating soil-related parameters. Without alternative datasets, quantifying the uncertainty that this choice introduces remains a challenge. Some processes, such as groundwater recharge, for which there is a lack of direct measurements of the relevant system properties are parameterized by combining geology, soil, topography, and permafrost datasets, as well as expert knowledge (Döll & Fiedler, 2008). However, such a complex combination of different sources of information may lead to the inability to explain model differences (Reinecke *et al.*, 2021).

Our ability to represent the processes we assume to be present is related to finding an adequate model structure, especially for scales far finer than the spatial or temporal resolution of GWMs. Adequate here means that the model can be used for its intended purpose (see also Fig. 1). The representation of sub-grid scale processes and their variability is a challenge to GWMs, with long-lasting debates around the issues of model and parameter adequacy as well as data limitation and uncertainty (Beven & Cloke, 2012; Clark *et al.*, 2017). Reasons for this ongoing dispute are questions regarding the validity of theories when applied beyond their scale of derivation, the representation of interactions and feedback among processes, strategies to describe the effects of sub-grid scale heterogeneity, and the availability of data to parameterize and test model formulations. A prominent and illustrative example is the structural representation of the land surface, particularly the representation of soil processes (Fatichi *et al.*, 2020; Or, 2020; Weber *et al.*, 2023), whose description is generally rooted in theories and limited observations (Vereecken *et al.*, 2016). As mentioned, most models use maps of soil types (e.g., HWSD (Nachtergaele *et al.*, 2010) or SoilGrids (Poggio *et al.*, 2021)) and correlate them with the model parameters of interest via pedotransfer functions (PTFs). However, current parameterizations of soil hydraulic properties based on PTFs rely on geographically limited data, generally derived from small samples taken from agricultural fields, thus not accounting for soil structure effects and spatial heterogeneities (Or, 2020; Gleeson *et al.*, 2021). Such effects may significantly alter infiltration-runoff and other exchange processes at larger scales (Fatichi *et al.*, 2020; Bonetti *et al.*, 2021). Recent research showed that it is possible to incorporate soil structure corrections into pedotransfer functions based on remotely-sensed vegetation metrics and local soil texture (Bonetti *et al.*, 2021). The uncertainties in soil process representation influence multiple other processes within GWMs. Besides infiltration and runoff, different soil and land use representations can also influence model translation from radiation forcing into evapotranspiration, thus significantly altering the water balance representation of the model (Gnann *et al.*, 2023).

Another critical aspect of process representation and parameter estimation are anthropogenic alterations of the terrestrial water cycle through land and water management. Humans have profoundly impacted freshwater systems by changing land use patterns, expanding irrigation, building dams, transporting water across catchment boundaries, and pumping groundwater (Abbott *et al.*, 2019). It is challenging to represent these human water cycle alterations in GWMs, making it very difficult to distinguish natural and anthropogenic components in hydrological signals as a consequence (Salwey *et al.*, 2023). Many GWMs now represent water management processes (e.g., irrigation, reservoir operation, and groundwater pumping), but with great difficulty, especially when trying to capture complex human decision-making processes and field-scale management practices (McDermid *et al.*, 2023). The representation of water management is often challenging because of data paucity, especially at the global scale (e.g., water used for irrigation, source of water withdrawal, reservoir operation rules (Pokhrel *et al.*, 2016; Wada *et al.*, 2017)). Future projections considering human activities are even more problematic because scenarios of future water use and management practices are almost nonexistent due to limited data of the past and lack of approaches to model the future. On the positive side, there is a growing body of literature on attributing observed changes to natural versus human drivers (Felfelani *et al.*, 2017), even though a comprehensive quantification is often challenging. For example, the desiccation of the Aral Sea is likely primarily caused by anthropogenic disturbances, but a reliable quantification is lacking (Pokhrel *et al.*, 2017).

Increasing awareness of the problem of model structural uncertainty has led to a range of modular modeling frameworks that maximize flexibility to allow users, in principle, to tailor models to the specific perceptual model of a particular system (Clark *et al.*, 2008; Fenicia *et al.*, 2011; McMillan *et al.*, 2011; Dembélé *et al.*, 2020). It has also led to increasing efforts to highlight and demonstrate the need to explicitly formulate perceptual models to distinguish uncertainty in system perception from uncertainty in model implementation (Wagener *et al.*, 2021; McMillan *et al.*, 2023). GWMs have not yet fully explored the possibility of modularity. This is due to the high diversity of the subsystems (Fig. 2d) and missing approaches to disaggregate them sensibly and efficiently on the global scale (models already separate between, e.g., humid and arid (Müller Schmied *et al.*, 2021), or mountains and plains (Hoch *et al.*, 2023), but that does not account for the full hydrologic diversity). Also, current GWM software architectures are rarely flexible enough to allow for flexible parameterization of different subsystems with diverse process equations. Second, we lack strategies and initiatives to collect, verify, organize, store, and share the vast knowledge of diverse hydrologic systems in a structured way that allows a robust, transparent, and computationally efficient integration in GWMs. Finally, the diversity of global hydrologic systems also underlines the need for methods to analyze and evaluate the diverse outputs of GWMs. Likely, the lack of structural tailoring and, thus, limited flexibility of current global models entails significant structural uncertainty. Some studies suggested that calibration should also consider the hydrologic diversity and would benefit from tailoring the model structure to different regions (Beck & van Dijk *et al.*, 2017; Santos *et al.*, 2022; Kupzig *et al.*, 2023).

Despite all these challenges, there are multiple possibilities for improving GWM building. Regional information can be collected through community data portals (Crochemore *et al.*, 2020; Zipper *et al.*, 2023), increasingly high-resolution satellite products are available, and some studies have shown that structural improvements can be derived from more informed and diverse perceptual models, e.g., the inclusion of preferential recharge in karst regions, an important yet often omitted process (Hartmann *et al.*, 2017).

Forcing global models

Once a model is established and a priori parameter values have been defined based on available data, GWMs are driven by time-varying inputs of meteorological variables such as precipitation, temperature, and radiation. These inputs may be based on historical observations, most likely reanalysis products that combine observations with simulations (Beck & Vergopolan *et al.*, 2017), or climate projections of future conditions, possibly with additional downscaling and bias correction steps (Maraun *et al.*, 2017) (see also section 3). A less common forcing for GWMs (so far) are reconstructions of the deeper past with paleo-hydro-climatic conditions (Gladstone *et al.*, 2007) to understand how the hydrologic cycle has evolved over long time scales.

Reanalysis products depend strongly on existing observations, which means that any uncertainties (due to uncertainties in the measurements themselves and in interpolation and modeling techniques to derive spatial data fields, e.g., for precipitation (Viviroli *et al.*, 2011)) will propagate into the final forcing product. For example, precipitation stations cover only a small area of the world (likely less than 1% of the Earth's surface is represented (Kidd *et al.*, 2017)) and generally, fewer (and poorer) observations are available in mountainous or economically poorer regions, leading to unbalanced datasets (Viviroli *et al.*, 2011). This availability issue also affects simulations of the future, e.g., for climate impact studies, because uncertainty in historical observations still matters as we require them as reference data (Tarek *et al.*, 2021).

Uncertainty in GWMs forcing for projections of future climates is caused by three primary factors: GCM/ESM or structural uncertainty (e.g., different models giving different outcomes for the same data or initializations), scenario-related uncertainty (e.g., differences in outcomes due to varying scenarios/input specified, e.g., atmospheric composition), and uncertainty caused by internal variability (i.e., arising from natural processes such as multi-decadal oscillations) (Deser *et al.*, 2020; Lehner *et al.*, 2020). The specific contribution of these three components to the total uncertainty generally depends on the time horizon considered (the more distant the time window is from the present states, the higher the uncertainty), the variable of interest (e.g., uncertainty in precipitation is generally higher than for temperature), the GCM/ESM used, and the geographic region (Schwarzwald & Lenssen, 2022). While structural and scenario uncertainties are important, uncertainties from internal variability can account for over 50% of the total uncertainty in climate projections (Xie *et al.*, 2015; Kumar & Ganguly, 2018; Deser *et al.*, 2020; Schwarzwald & Lenssen, 2022). This implies that the uncertainty in climate forcing should be a key consideration in future projections by GWMs, for example, by utilizing model ensembles. Among different climate forcing variables, precipitation is a key field, distant projection of which can be highly uncertain and can directly influence streamflow and other outcomes in hydrological models (Deser *et al.*, 2020). The uncertainty from GCM/ESM structure and scenarios is usually considered in hydrologic studies by using projections from multiple GCMs/ESMs and radiative forcing scenarios, respectively (Bartosova *et al.*, 2021).

Evaluation of global models

Evaluation is a key step to assess a model's ability to perform a specific task, or to adjust its parameters as part of an iterative calibration process (sometimes referred to as tuning). Ideally, model evaluation should be diagnostic (Gupta *et al.*, 2008) and help to identify model deficiencies in, e.g., capturing water fluxes and storage dynamics. Evaluating process realism is an important step towards enhancing the credibility of GWMs' multiple uses (Fig. 1), for example, for climate change impact assessments (Krysanova *et al.*, 2020). GWMs are mostly evaluated by comparing simulated and observed streamflow time series (Arheimer *et al.*, 2020), given that streamflow is relatively widely available and provides information for model performance across a larger region - the upstream catchment. Other fluxes and states such as evapotranspiration, snow, terrestrial water storage and soil moisture are less commonly used (Pimentel & Arheimer *et al.*, 2023), but are gaining more traction with new evaluation protocols (Collier *et al.*, 2018). Globally, datasets of streamflow are biased towards large rivers (Downing, 2012) with extensive anthropogenic influences (Wagener & Montanari, 2011; Krabbenhoft *et al.*, 2022), while other variables like groundwater recharge are often only available as long term averages and certain climatic regions (dry regions) (Moeck *et al.*, 2020). Some variables are not measured at all (e.g., lateral groundwater fluxes, macropore flow) and others are measured at scales which are very different from the current model scales (e.g., evapotranspiration (Wartenburger *et al.*, 2018), soil moisture (Crow *et al.*, 2012), or groundwater table depth (Reinecke *et al.*, 2020) and groundwater recharge (Moeck *et al.*, 2020)). Due to insufficient length and homogeneity of observational records, long-term variations and trends in components of the water cycle can only be quantified with large uncertainty (Dorigo *et al.*, 2021).

The uncertainties of observation data themselves is rarely accounted for (even if they can be substantial (Westerberg & McMillan, 2015)) during GWM evaluation (or calibration) (Moges *et al.*, 2021), and little is known about how this in turn affects the predictive uncertainty of GWMs. Direct comparisons with observations are difficult in data-sparse regions, in regions with substantial anthropogenic impacts (Döll *et al.*, 2014), and generally not possible for the future. Thus, alternative evaluation strategies have been proposed. To provide information for evaluation also in regions without measurements, we may use regionalized streamflow characteristics (Troy *et al.*, 2008) or functional relationships that capture the co-variability of forcing and response variables in space (e.g., Koster and P. Mahanama (2012), Gnann *et al.* (2023)). As a complimentary method to point-by-point comparisons with historical data, evaluation focusing on input-output relationships can help to reveal additional insights into model functioning (e.g., Luo *et al.* (2012), Gnann *et al.* (2023)). This is particularly relevant for climate change impact studies, where response-based analysis methods can provide insight into whether a model is fit for purpose, for instance, by showing whether a model's sensitivity to changing forcing is as expected (Wagener *et al.*, 2022).

If the evaluation shows discrepancies between observations and model results calibration is a potential strategy to reduce them. Few global models so far have been calibrated against observed variables to improve a priori parameter estimates (Kupzig *et al.*, 2023). In light of the equifinality of parameter sets and the risk that the model is adjusted only for the variable that is used for calibration, but not for other flux or state variables, multi-criterial calibration of GWMs with different observables and signatures has been recommended (Döll *et al.*, 2016; Pimentel & Crochemore *et al.*, 2023). Model calibration beyond streamflow with multiple remote-sensing-based observations such as evapotranspiration, snow cover, snow water equivalent, soil moisture, water level, surface temperature, among others, has been realized for several river basin studies (Meyer Oliveira *et al.*, 2021). However, neither single- nor multi-objective calibration has become general practice for GWMs (Telteu *et al.*, 2021). Apart from a lack of observational data for many regions, the observations themselves may carry large uncertainties (Pimentel & Crochemore *et al.*, 2023) and calibration procedures can be computationally expensive. With km-scale models and nested catchments, calibration can be very time and resource consuming. Ultimately calibration on historical observations does not ensure that GWMs are also providing robust projections of future changes (Wagener *et al.*, 2022), e.g., a particular parameter might not be adequate to represent streamflow processes if conditions have changed substantially due to climate and land use change (Milly *et al.*, 2008).

Evaluating or calibrating GWMs requires observations of (at least some) simulated variables. Given that in-situ observations do not seamlessly cover all land areas, there is prospect of using satellite-based products with global coverage. Terrestrial water storage (TWS) is a variable estimated using satellite gravimetry (GRACE, GRACE-FollowOn) (Landerer *et al.*, 2020; Rodell & Reager, 2023) and has become an important observation for assessing GWM performance as TWS is an integrative hydrological state variable (Lee *et al.*, 2023). First efforts have been made to assimilate GRACE data in GWMs (Tian *et al.*, 2019). However, TWS products for model evaluation also hold substantial uncertainties due to the coarse spatial and temporal resolution (Scanlon *et al.*, 2018; Rodell & Reager, 2023) and complex attribution to specific water storage components (Döll *et al.*, 2014). Other satellite missions like Landsat (e.g., extents of surface water bodies, surface temperature, land use change), altimetry missions for water level of inland water bodies and SMAP (Soil Moisture Active Passive) have also proven to be essential sources to evaluate and build GWMs (McCabe *et al.*, 2017), although they may also include considerable uncertainties (Pimentel & Crochemore *et al.*, 2023). Among recent satellite missions, the Surface Water and Ocean Topography (SWOT) mission is expected to be an important step for assessing surface water dynamics and storage variations of inland water bodies (instead of water level only) with unprecedented spatial resolutions and global coverage, providing insights into small and otherwise ungauged water bodies at scales of about 100 meters (Papa & Frappart, 2021).

To facilitate a more structured comparison between models, model intercomparison projects have gained importance by providing modeling protocols that define standardized forcing data, scenarios, and other modeling choices. These have been carried out very successfully in the climate community with the Climate Model Intercomparison Project (CMIP) (Eyring *et al.*, 2019). The Earth System Modeling community has implemented the ILAMB (International Land Model Benchmarking) benchmark, which offers a structured comparison of models to observations in a standardized software package (Collier *et al.*, 2018). The ISIMIP project, specifically the global water sector (Frieler *et al.*, 2017), has also developed standardized protocols for joint simulations to evaluate models, which have already yielded multiple insights on model deficiencies and uncertainties (e.g., Zaherpour *et al.* (2018), Reinecke *et al.* (2021)). Model intercomparison projects offer a powerful framework to diagnose differences between GWMs and their potential reasons, as well as GWM uncertainties.

To summarize, building GWMs remains challenging regarding the identification of an adequate model structure, building complex simulations software, estimating parameters, simulating human activity, driving models with uncertain inputs, and evaluating them with limited observations. All these issues require further study to understand and quantify existing uncertainties and their origins, and to understand their implication for GWM applications. On the positive side, new and growing datasets, alternative methods for model evaluation, and increasing computational resources have the potential to push forward the development of GWMs.

3 Uncertainties in simulating the past, future, and near future water cycle

In this section, we discuss how GWM uncertainties influence simulations of past, future, and near-future water cycles. We focus on six essential hydrological variables: streamflow, evapotranspiration, groundwater recharge, soil moisture, terrestrial water storage, and anthropogenic water use (Table S3).

Simulating the (recent) past

Reconstructions of the terrestrial water cycle over the last 100 years include different sources of uncertainty, such as model conceptualization and parameterization, meteorological forcing, and anthropogenic influences that will impact simulated hydrological variables (see Section 2). This period largely covers our observational records (and thus enables the use of reanalysis products) and includes the main upswing of global economic growth after the Second World War. Multiple model comparison studies and global water balance studies that include GWM outputs reveal substantial uncertainties, even for global average fluxes.

For streamflow, studies estimate ranges from less than 40,000 km^3/y to over 60,000 km^3/y globally [< 300 mm/y to > 450 mm/y] (Haddeland *et al.*, 2011; Schellekens *et al.*, 2017; Abbott *et al.*, 2019; Rockström *et al.*, 2023) (see Fig. 3a for differences in a GWM ensemble). Correspondingly, estimates of evapotranspiration range from approximately 60,000 to over 80,000 km^3/y [450 to 600 mm/y] (Haddeland *et al.*, 2011; Schellekens *et al.*, 2017; Abbott *et al.*, 2019) (see also Fig. 3b and 5d). The (relative) disagreement is similarly large for fluxes such as groundwater recharge, ranging from approximately 12,000 to 25,000 km^3/y [90 to 190 mm/y] (Abbott *et al.*, 2019; Rockström *et al.*, 2023) (see also Fig. 3c), with a recent data-based study suggesting that models generally underestimate diffuse groundwater recharge (water that percolates down to groundwater rather evenly across the landscape, in contrast to focused recharge that enters groundwater at certain "focused" points, such as rivers and lakes) compared to observations [observation-based estimate: 218 mm/y] (Berghuijs *et al.*, 2022).

For terrestrial water storage, we can only assess relative differences between models and observations, often done by examining anomalies and trends. For example, Scanlon *et al.* (2018) noted substantial uncertainties among different models, reporting that terrestrial water storage anomaly trends (summed over all investigated basins) are "positive for GRACE (∼71–82 km^3/y) but negative for models (−450 to −12 km^3/y)". Storages, such as groundwater, accumulate errors (in contrast to fluxes) and may exhibit long-term memory. This is often not captured by the current generation of models that usually contain very simplified representations of groundwater systems, for example, bucket models that may not be able to represent long-term storage depletion (Fowler *et al.*, 2020).

Anthropogenic water use is particularly uncertain, especially for irrigation, which accounts for ~70% of global water withdrawals, with estimates collated by a recent study ranging from 1571 to 3,800 km^3/y (McDermid *et al.*, 2023) (i.e., differences by a factor of 2; Fig. 3d). Uncertainties of water use are, however, not necessarily a direct consequence of GWM uncertainty but a reporting issue since minor changes to definitions can change reporting of water consumption of, for example the US energy system, substantially (Grubert *et al.*, 2020). Another example is the area equipped for irrigation data, which is used in multiple global water models and datasets (Siebert *et al.*, 2015). If a municipality or private entity reports an area as being equipped with irrigation equipment, it includes planned-but-not-implemented, and existing-but-not-used equipment as well. While challenges especially remain in correctly allocating withdrawals to their sources (e.g., surface water or groundwater), determining the withdrawals in the first place is highly uncertain as, for example, uncertain information on where irrigation equipment exists is fed into an uncertain irrigation model to determine irrigation estimates (McDermid *et al.*, 2023).

While global long-term averages already reveal large differences, these uncertainties are even larger in specific regions and during specific time periods. Streamflow is typically more uncertain, in relative terms, in dry regions (Zaherpour *et al.*, 2018; Heinicke *et al.*, 2024), and in lake-rich and snowy places (Giuntoli *et al.*, 2015; Beck & van Dijk *et al.*, 2017; Gädeke *et al.*, 2020). Possible reasons are that in these regions, precipitation is a weaker or less direct control on streamflow, because other processes (e.g., related to filling and spilling the storage) and their representation in GWMs are more important. For example, seasonal dynamics are often poorly captured and timing bias of the annual flow maximum is regularly more than one month, in part because of poor representation of snow, lake dynamics, and other storage processes (Gudmundsson & Wagener *et al.*, 2012; Zaherpour *et al.*, 2018). Also, studies tend to find larger uncertainties for extremes such as high and low flows (Gudmundsson & Tallaksen *et al.*, 2012; Schewe *et al.*, 2019), which are particularly important for flood and drought impact analyses. For instance, assessing modeled streamflow during the European heatwave in 2003, Schewe *et al.* (2019) found that many models underestimate low flows compared to observations, likely because these models poorly represent groundwater flow to streams that become particularly important during dry conditions. Devitt *et al.* (2021) tested four global models regarding their ability to simulate historical floods in the USA and found that two models underestimated floods by more than 25% in roughly two-thirds of all catchments, while the other two overestimated flows by the same amount in a similar fraction of catchments.

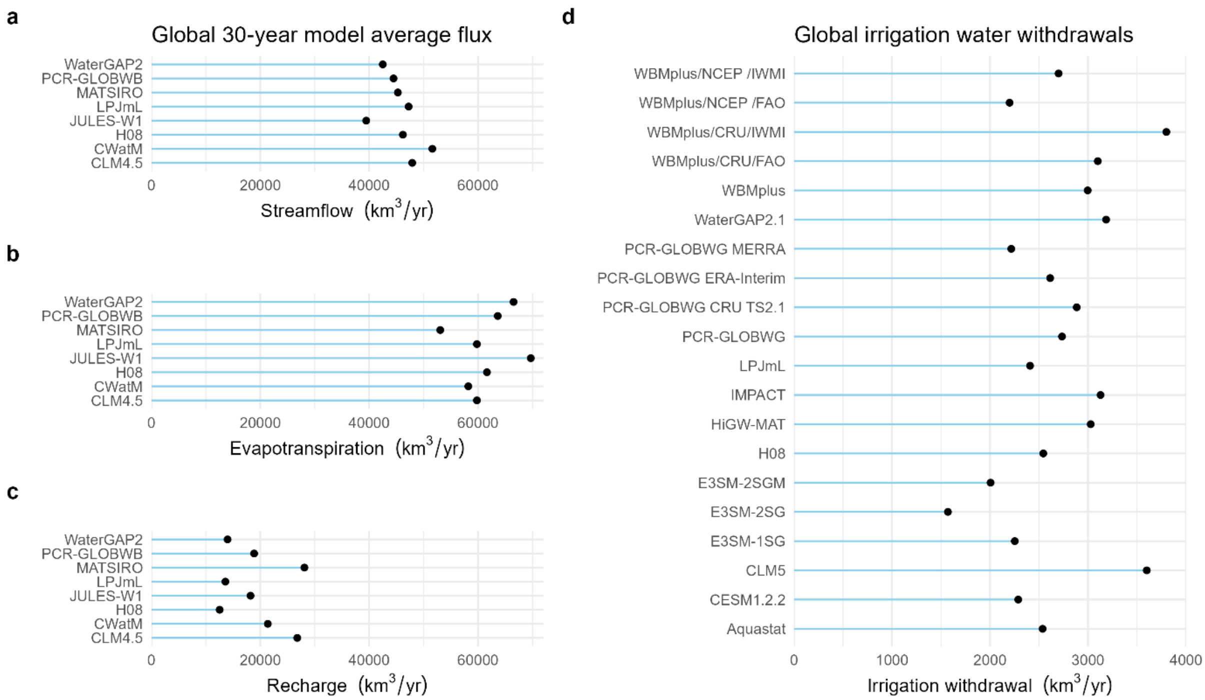

Figure 3: Disagreements between key variables of global water models. **a-c**, Differences between multiple global water models for streamflow, evapotranspiration, and groundwater recharge (replotted from Table S5 in Gnann *et al.* (2023) with a factor of 132 for conversion to km³, which is an estimate of average model cell size). **d**, Irrigation: Estimated global irrigation water withdrawals show large disagreement between models, with global water models tending to show larger values than reported

by the United Nations Food and Agriculture Organization in Aquastat (replotted from McDermid *et al.* (2023)).

Simulating the near future – seasonal forecasts

Generation of near-future (seasonal to sub-seasonal) climate and hydrological forecasts is crucial for integrated water resources management as well as for generating early warnings for hazards, such as floods and droughts, which can have long transition periods. While seasonal climate predictions (see Fig.S2 for mapping meteorological to hydrological forecasts based on timescales) are common practice, their utilization for global hydrological forecasts remains uncertain and is largely under development and not yet operational, except for flood forecasting (https://www.globalfloods.eu). The quality/accuracy of global seasonal hydrological forecasts is driven by three major factors: (a) initial hydrological conditions, which consider various observed variables (both hydrological and meteorological), (b) GWM uncertainties (WMO, 2023), and (c) seasonal climate forecasts accuracy, which depends on historical climate data and climate forecasts (temperature and precipitation being of utmost significance to hydrological models; Fig.S3). However, contribution of a) - c) to the uncertainty of the seasonal hydrological forecast vary with hydro-climatic zones (Shukla *et al.*, 2013), size of the catchment (Paiva *et al.*, 2012), chosen reference year(s) (Shukla *et al.*, 2013; Sinha & Sankarasubramanian, 2013), and prediction method (Wood *et al.*, 2016). An important component to counteract these uncertainties is data assimilation (see also 4.1.) which is pivotal for state updates when simulating the near future (Zhang *et al.*, 2021).

Simulating the far future - climate change and water use projections

The further we move away from the instrumental record of observations, into the past or future, the more we expect uncertainties to grow due to the influence of scenarios and other choices (e.g., quantification of human influences, land-cover changes) (Collins *et al.*, 2012). Uncertainties related to the reconstruction of the recent (50-100 years) water cycle by GWMs are thus naturally smaller than the uncertainties related to future projections. This is because meteorological forcings are constrained by data assimilation (reanalysis data instead of climate model projections), actual land use data are obtained from remote sensing (at least in recent decades), and socio-economic forcings (GDP, population, water demand) are constrained by regular country reporting. In addition, GWMs may become more uncertain in future regimes for which they were not developed or calibrated, for example, because of changes in biophysical processes related to CO_2 fertilization.

A question often posed is if input uncertainty or model structure uncertainty dominates the uncertainty in the model output. Is the uncertainty in climate forcing originating from GCMs or are the differences related to the GWMs? While this has been evaluated in multiple studies (Prudhomme *et al.*, 2014; Schewe *et al.*, 2014; Giuntoli *et al.*, 2015; Wartenburger *et al.*, 2018; Reinecke *et al.*, 2021), the answer depends on which models, variables, time periods, and geographic regions are included in the analysis. Wartenburger et al. (2018) showed that evapotranspiration differences between different model choices largely explain overall variability but that the spatio-temporal differences can mainly be explained by forcing uncertainty. Schewe *et al.* (2014) (depicted in Fig. 4) compared sources of uncertainty for streamflow and found high spatial variability in what sources dominated. In some warm arid regions, GWMs dominate uncertainty more than GCMs while at least in some humid and in some cold regions forcing is the major contributor to output uncertainty. This is comparable to results by Giuntoli *et al.* (2015), who evaluated sources of uncertainty separately for low and high streamflow. In their analysis, GCMs generally dominate uncertainty for both flow regimes with exceptions in snow dominated and arid regions. They conclude that GWMs dominate uncertainty where flow processes are more relevant than precipitation input. Somewhat similarly, if we investigate subsurface water fluxes like groundwater recharge, GWM uncertainty becomes more important because these hydrological processes are less directly controlled by climatic input. For instance, Reinecke *et al.* (2021) (depicted in Fig. 4) found that in most regions the variability in process representation for groundwater recharge modeling has a larger impact on output differences than GCMs. While these studies suggest that the ratio of GWM to GCM uncertainty depends on climate characteristics and hydrological processes, a comprehensive review of sources of uncertainty across different variables is currently lacking. It would be worthwhile studying systematically for which variables, which time periods, and which regions each of these uncertainties dominate globally to show where future model improvement would have the most leverage.

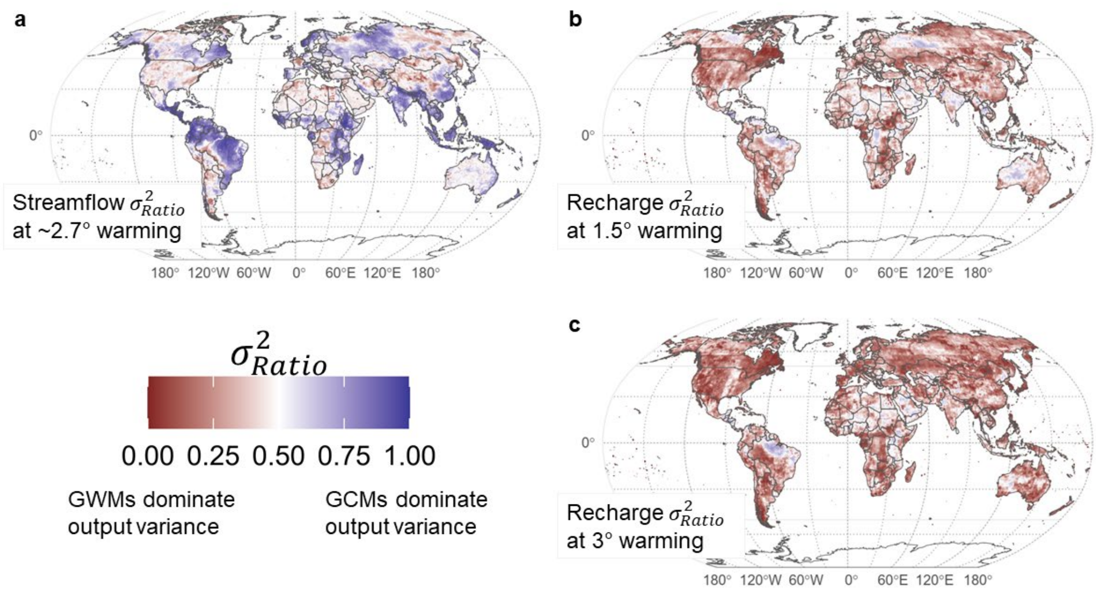

Figure 4: Do Global Water Models or their forcing (Global Climate Models) dominate output uncertainty? Figures a-c show maps of GWM output variance of different GCM forcing divided by total output variance for different variables and warming scenarios (in comparison to pre-industrial temperatures). **a**, Variance ratio for streamflow replotted from Schewe et al. (2014)(Schewe *et al.*, 2014). **b-c**, Variance ratio for groundwater recharge replotted from Reinecke et al. (2021).

Uncertainty originating from the GWMs in the context of climate projections is at least partially related to the representations of various biophysical processes, such as those related to vegetation and soils (Wartenburger *et al.*, 2018), which influence how future atmospheric moisture and energy translate into hydrologic impacts variables (Samaniego *et al.*, 2017). How, for example, the function of the vegetation-soil sub-system will evolve under different climate change trajectories is uncertain, thus adding uncertainty to estimates of evapotranspiration or percolation. One would expect that the overall uncertainty increases with longer projection horizons, yet current literature is inconclusive whether GCMs or GWMs dominate projection uncertainty. For example, Pokhrel *et al.* (2021) found that for terrestrial water storage, GCM uncertainty is significantly larger than GWM uncertainty for any given Representative Concentration Pathway (RCP) scenario, with variations between regions (e.g., Fig. 5a). However, GWM uncertainty increases with time within a scenario, potentially surpassing GCM uncertainty for the distant future (e.g., a century into the future) (Pokhrel *et al.*, 2021). While one might expect GCM uncertainty to become increasingly dominant in the future, this does not always seem to be the case. One reason might be that variables like TWS accumulate errors from different compartments, which is linked to a not fully closed water balance, and thus become increasingly uncertain. Another reason might be that some water models reach thresholds at which certain processes or their numerical representations change unpredictably. Some models, for example, may encode a specific fixed process behavior or factor for dryer and wetter regions, respectively; e.g., Müller Schmied *et al.* (2021). If a region shifts from wet to dry in the future, this may lead to inconsistent model behaviors, thus amplifying GWM uncertainty. The uncertainty arising from socio-economic and water use scenarios is challenging to quantify owing to the lack of data and thus limited model accuracy (see also section 2). The limited number of studies that have quantified this uncertainty indicate that future projections of water availability and use, especially for irrigation, are greatly influenced by the scenarios considered (Wada *et al.*, 2013; Rosenzweig *et al.*, 2014).

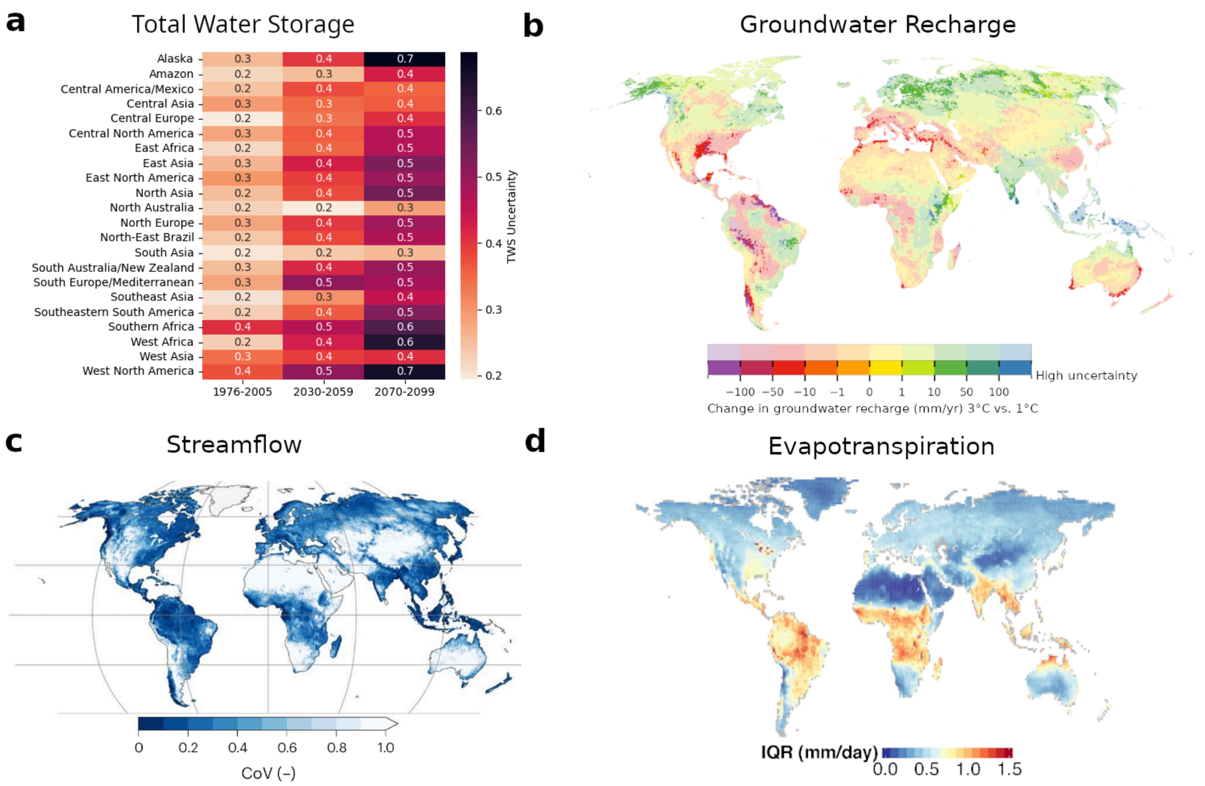

Figure 5: Uncertainty in projected total water storage (**a**) and groundwater recharge (**b**), replotted from Pokhrel *et al.* (2021) and Reinecke *et al.* (2021) respectively. Uncertainty in streamflow (**c**) and uncertainty in evapotranspiration (**d**) reproduced from Gnann *et al.* (2023) and Wartenburger *et al.* (2018) respectively. In (b) only regions where model agreement is significantly large are plotted in solid colors, all other regions are shown in an opaque color. In (c) the coefficient of variation (CoV) is calculated for an ensemble of eight GWMs over a 30-year period. In (d) the interquartile range (IQR) is shown for an ensemble of 11 GWMs. The ensembles of all four studies may not use the same models.

One aspect of projection uncertainty is that different processes may be active or in-active; or play a dominant or minor role during changing conditions. For example, CO_2 levels can increase leaf-level water use efficiency of plants, potentially offsetting reductions in water availability due to higher temperatures through reduced evapotranspiration (Rosenzweig *et al.*, 2014; Berg *et al.*, 2016; Lemordant *et al.*, 2018; Hatfield & Dold, 2019). However, recent work also suggests that the change in water use efficiency is already exhausted due to an increased vapor pressure deficit (Li *et al.*, 2023). Water use efficiency has been suggested to strongly influence total terrestrial runoff and evapotranspiration (Gedney *et al.*, 2006; Piao *et al.*, 2007), and is not represented in some GWMs despite predictions of CO_2 fertilization effects being credited as a source of uncertainties. This can lead to contradicting findings regarding the extent to which a climate induced decline in water availability and improved plant water use efficiency counterbalance each other (Mankin *et al.*, 2019; Adams *et al.*, 2020; Singh *et al.*, 2020). Uncertainty from CO_2 fertilization effects have also been linked to the uncertainty in future projections of crop productivity, irrigation water use, and groundwater recharge (Fig. 5b) (Elliott *et al.*, 2014; Rosenzweig *et al.*, 2014; Reinecke *et al.*, 2021). A second example are cold regions, many of which will experience considerable change as rising temperatures will affect frozen water storage in snow, glaciers, and permafrost. Given that some models are already associated with considerable uncertainty in cold and lake-rich places (Giuntoli *et al.*, 2015; Beck & van Dijk *et al.*, 2017; Gädeke *et al.*, 2020), it is unclear how robust future projections are and what role threshold behavior will play. For example, reduction in snow cover and/or greening due to vegetation growth can lead to albedo feedback, reducing streamflow due to increased net radiation (Milly & Dunne, 2020). Better representation of glaciers increasing runoff in glacierized basins is already included in some models (Cáceres *et al.*, 2020; Wiersma *et al.*, 2022). Other aspects related to human decisions, such as land use change (Sterling *et al.*, 2013) and water regulation (Arheimer *et al.*, 2017), may even mask climatic change but are difficult to investigate due to a lack of historical data as discussed earlier.

4 Uncertainties as a guide for the advancement of global water models

The use of global water models is unavoidably associated with uncertainties that arise during model-building and execution. These uncertainties influence simulations of past, near-future, and future water cycles. Key sources of uncertainties in GWMs are deficits and imbalances in data quality and availability across geographical regions and between hydrologic variables, poorly quantified human influences on the water cycle, and difficulties in tailoring process representations to regionally diverse hydrologic systems. Due to these GWM uncertainties, we have a limited understanding of when and where our models provide reliable and consistent results. Specifically, it is unclear to what extent the models realistically reflect regional hydrological behavior, and a distinction between natural variability and human impacts remains challenging. The scientific community can use uncertainties to guide future GWM development by gathering new, more accurate, and larger datasets, improving process knowledge, and ultimately building more reliable and consistent models.

4.1 Towards more consistent and reliable information

We have discussed in depth that limited information is a core issue causing GWM uncertainty. So where is new information likely to come from? Upcoming satellite missions will provide information on variations in inland water bodies at unprecedented spatial resolutions, providing new insights into the hydrology of ungauged regions (Papa & Frappart, 2021). Some initiatives, like ESA-CCI (https://climate.esa.int), offer possibilities for better parameterization of, for example, land cover, which would lead to a better representation of surface heterogeneity, and many other essential climate variables to be used for model forcing, parameterization, calibration, or evaluation (even if they may also carry substantial uncertainties (Pimentel & Crochemore *et al.*, 2023)). Recent efforts have also shown that remote sensing data can be used to monitor human alterations of the water cycle such as dam construction (Zhang & Gu, 2023) and can be used to extend in-situ observations of streamflow (Elmi *et al.*, 2024).

Beyond satellites, there are ongoing efforts to collect high-resolution data such as HydroBASINS (Lehner & Grill, 2013), which are not yet fully utilized. For example, increasing spatial resolution of digital elevation data offers new possibilities for high-resolution river routing (Yamazaki *et al.*, 2019). However, to profit from such advancements requires new methods to utilize this high-resolution data in the current comparably coarse-scale models. Advances in data availability also require advancements in how we merge data and models. Data assimilation methods established in other communities can be utilized to adjust GWMs and have already been adopted (Gerdener *et al.*, 2023). Importantly, satellites, and in fact any observations, carry uncertainty that should be propagated through GWM estimates. While propagating this uncertainty into model results is computationally expensive, the main problem again is that information about uncertainty is rarely available for existing datasets.

The spatial resolution of GWMs is increasing, with the hope of improving model accuracies because parameter heterogeneities and spatial variability can be better resolved (Wood *et al.*, 2011; Beven & Cloke, 2012; Bierkens, 2015). However, existing problems in process representation and data availability will not be eliminated through increased resolutions (Beven & Cloke, 2012). Hoch *et al.* (2023) showed that improvements may be found for streamflow but not necessarily for other hydrological variables, owing to a lack of accurate high-resolution forcing data, inaccurate scale transitions of model parameters, and challenges in realistically representing scale-dependent processes (Beven & Cloke, 2012). However, increasing resolutions might enable more regional information to be used in GWMs, for example, by assimilating regional system conceptualizations.

Data is used in all stages of the model-building and execution process. Hence, new and improved data will be critical for advancing GWMs, including data on local/regional hydrologic knowledge, newly measured or collated datasets, and more information on data uncertainties. The scientific community started investing resources in collecting local knowledge to improve model structures and tailor them to specific regions. For example, community portals (Crochemore *et al.*, 2020; 2023) allow uploading existing local models (including data, code, and documentation) or perceptual models (McMillan *et al.*, 2023) that encode the hydrological knowledge and human influences of particular regions. We can extract and synthesize information from such databases to tailor global models to specific areas.

New research may also extract knowledge from the enormous number of existing publications, which could be automatically built into new global datasets of regional knowledge (Stein *et al.*, 2022). Existing data may also be found in non-scientific resources and can be combined into valuable products of human influences on the water cycle, e.g., freshwater demand for energy production (Gerbens-Leenes *et al.*, 2024). Existing data can be combined into joint datasets such as the Global Gravity-based Groundwater Product (G3P) (Güntner *et al.*, 2023), which combines different observational products into one global product of groundwater storage variations (other examples of combined datasets exists such as (Moeck *et al.*, 2020)). Further, datasets often lack uncertainty quantification, which would be valuable to rigorously test how uncertainties affect GWM output uncertainties (when used to force or calibrate models) and allow for a more improved model evaluation (Kiang *et al.*, 2018; Beven *et al.*, 2020; Pimentel & Crochemore *et al.*, 2023). Model evaluation should also include not just streamflow but other components of the water cycle as well, such as evaporation (Pimentel & Arheimer *et al.*, 2023), groundwater recharge (Wan *et al.*, 2024), soil moisture (Crow *et al.*, 2012), and snow (Arheimer *et al.*, 2017). However, this again requires datasets that are less biased towards specific regions, quantified uncertainties of the measurements themselves, and methods to compare point measurements to coarse-scale models estimates.

4.2 Toward more consistent and reliable models

Collecting existing regional knowledge provides the opportunity to tailor GWMs to particular regions. However, current modeling frameworks (Clark *et al.*, 2008; McMillan *et al.*, 2011; Clark & Nijssen *et al.*, 2015) that allow for a more modular approach to hydrologic modeling require information about the model structure that best fits particular hydrologic settings, something we rarely have. Modular catchment-scale modeling mainly works through model structure comparison using performance metrics, which does not allow for upscaling to largely ungauged global settings and suffers from model structure equifinality (Knoben *et al.*, 2020). New approaches that express global hydrologic diversity in a model without the computational and diagnostic drawbacks of existing frameworks (i.e., sampling a multitude of model structures) are necessary. One path might be better utilization of perceptual models to guide a priori model component selection based on our hydrologic understanding (Kiraz *et al.*, 2023). During the model-building process, different assumptions may lead to different models. Making the perceptual (or conceptual) model explicit (e.g., through a graphical representation) can help to understand assumptions about the underlying system and resulting uncertainties (Wagener *et al.*, 2021). Making the computer code of these models openly available is equally important as it enables the community to work towards open science goals and make internal assumptions such as hard-coded empirical factors (Hutton *et al.*, 2016) more transparent.

Another pathway to GWM improvement lies in evaluation strategies that use the global process variability represented already in these models as an advantage. Compared to single catchment models, GWMs simulate a large diversity of regions simultaneously. This enables us to search for similar patterns of hydrologic behavior, for instance, functional relationships between forcing and response variables, which can be used for model diagnosis and improvement (Gnann *et al.*, 2023). Also, the wider application of diagnostic signatures (Gnann *et al.*, 2021; McMillan, 2021) provides a pathway to improve GWM evaluation. Methods for uncertainty attribution can guide the necessary reduction in data and model uncertainty (by focusing on main sources of uncertainty) and help evaluate the models' sensitivity to future changes (Wagener *et al.*, 2022). Connected to those ideas is the development of calibration in general and new calibration schemes adapted for GWMs as mentioned in Section 2. Currently, most of the existing methods have been developed in a catchment or regional modeling context and lack the flexibility to account for the hydrologic diversity of GWMs (Kupzig *et al.*, 2023).

The GWM community increasingly couples their models with those developed by other communities (climate models, flood models, crop models, water quality models, groundwater models, socio-economic models, and many more) to obtain a more integrated Earth system view. The hope is that these models will be able to represent feedback loops that could otherwise not be simulated, such as land-atmosphere feedback (Koster *et al.*, 2004; Zipper *et al.*, 2019) or groundwater-surface water interactions and the supply of groundwater to the atmosphere through capillary rise (Reinecke *et al.*, 2019). These coupled systems can then be used to, for example, investigate the nitrogen cycle (Vilmin *et al.*, 2020), the carbon cycle (Zhang *et al.*, 2020) or in the future possibly to better represent human interaction, e.g., by coupling socio-economic models with GWMs.

However, it is still unclear how model coupling affects model uncertainty. Coupling requires additional assumptions and thus likely increases uncertainty, yet examples of coupling land surface processes with atmospheric processes have shown that coupling might help to constrain model dynamics and possibly reduce uncertainty (Lewis & Dadson, 2021). While some efforts already achieved online coupling (allowing feedbacks to flow into both model domains (Furusho-Percot *et al.*, 2019)), others are limited by the computational burden of one model or the resulting coupling feedbacks (e.g., flood modeling (Hoch & Trigg, 2019)). In addition, the challenge of multi-parameter calibration (e.g., for energy and water fluxes) escalates for these coupled systems (Sellar *et al.*, 2019).

Finally, an aspect which is often overlooked is the modeling software itself. Several GWMs have been developed for almost 30 years (e.g., WaterGAP since 1996 and VIC since 1994 (Liang *et al.*, 1994)) by many students and researchers with diverse programming experience (Reinecke *et al.*, 2022). While some have been published as open-source, most models remain closed-source projects primarily used by one research group (Melsen, 2022). Openly available models rarely contain comprehensible documentation of the code itself, i.e., internal documentation, and of how to use and modify it, i.e., external documentation, and require experts to be executed. The unavailability and complexity of the models and their code mean that they usually do not comply with FAIR principles (Findability, Accessibility, Interoperability, Reusability) (Barker *et al.*, 2022; Nyenah *et al.*, 2024), affecting the reproducibility of research relying on GWMs. It is currently unclear to what extent the code complexity and lack of application of established software engineering best practices affect model uncertainty (Nyenah *et al.*, 2024). Poorly documented code may lead to unintentional wrong use, missing rigorous automated tests may lead to mistakes, and hidden physical constants and assumptions contribute to uncertainty (Mendoza *et al.*, 2015; Cuntz *et al.*, 2016; Hutton *et al.*, 2016). Still, efforts have been made to make underlying assumptions and equations more transparent (Telteu *et al.*, 2021). A likely source for this missing compliance with FAIR principle is that current funding and hiring practices undervalue model development efforts (Reinecke *et al.*, 2022; Nyenah *et al.*, 2024). GWMs should strive to make their code openly available, including comprehensive internal and external documentation. Open code will lead to fewer hidden and implicit assumptions, reducing model uncertainty and will lead to faster progress. Modular software, for example, offers the possibility to transfer implementations (e.g., human water use, routing) between models. In addition, a more flexible code would allow for a more flexible implementation of different model structures, which in turn would be an essential step towards achieving regional tailoring. Reproducible experiments will provide a pathway to more in-depth knowledge of model differences, and more modular and modern software code will lead to experiments that can pinpoint uncertainties in process understanding more accurately.

4.3 Machine learning as a complementary modeling approach

Machine learning (ML) methods are rapidly entering global hydrology and will likely help gather better information, fill knowledge gaps regarding hydrologic processes, human dynamics, etc., and build better models (Tsai *et al.*, 2021). Purely data-driven ML has already demonstrated high performance in predicting hydrologic variables across the water cycle (Shen *et al.*, 2021), including streamflow (Feng *et al.*, 2020), soil moisture(Fang *et al.*, 2017; O & Orth, 2021), snow water equivalent (Meyal *et al.*, 2020), and groundwater levels (Wunsch *et al.*, 2022). One benefit of ML is that it absorbs information directly from data. This produces models that are inherently consistent with data, but which also inherit the imbalances and uncertainties of these data. In addition, purely data-driven models may be hard to interpret or helpful in making a specific scientific inquiry as they do not directly encode physical concepts. As an important mission of GWMs is to create long-term projections under future climate, it remains unclear (and difficult to evaluate) if pure ML models are suitable for such long-term tasks. At the same time, ML models have already shown to provide more accurate real-time flood forecasts than state-of-the-art global modeling systems, indicating their potential (Nearing *et al.*, 2024).

Other approaches have shown the capability of ML approaches to emulate complex physical models, which could foster future uncertainty quantification in continental to global scales water models (Bennett *et al.*, 2024). ML models can also be used to estimate human water uses and thus reduce uncertainty in GWMs (Shrestha *et al.*, 2024). Hybrid models of classical GWMs and ML (Kraft *et al.*, 2022; Slater *et al.*, 2023), such as differentiable models (Shen *et al.*, 2023), are developed to reap the benefits of both worlds while circumventing their respective limitations. Differentiable models mix process-based equations with neural networks and offer the ability to learn unknown physical relationships. By finding new relationships that govern large scale processes of the water cycle they could help to reduce GWM uncertainty. While ML models potentially carry less of the uncertainty as they can skip steps in the classical modeling chain (Nearing *et al.*, 2021), they will ultimately also suffer from limited global hydrological information and thus will equally benefit from new, more accurate, and larger datasets (Beven, 2020; Nearing *et al.*, 2024). In the future, machine learning and process-based models are likely to be particularly powerful when used as complementary approaches that can both efficiently learn from data and be enriched with hydrological and other process knowledge (Reichstein *et al.*, 2019).

5 The future of global water models

The water cycle is a central element in the Earth system, transporting and storing water and energy, nutrients, sediments, and pollutants. Thus, the water cycle influences our climate, societal development, and the evolution of ecosystems. Global water models have evolved into widely used tools that help us understand and predict the terrestrial water cycle under past, current, and potential future conditions. Key water fluxes such as streamflow, evapotranspiration, groundwater recharge, and water storage in its various forms can now be simulated consistently across the whole global land surface. Outputs of these models support critical global discussions and scientific analyses around the central resource of all life on Earth and are a dominant source of disaster risk assessments for society.

However, considerable uncertainties remain despite significant advances in GWMs in recent years. Reasons for these uncertainties are that data quality and availability are hugely imbalanced worldwide, imprints of human alterations on the water cycle are poorly quantified, and the diversity of hydrologic systems makes it challenging to represent process diversity adequately. Yet, these uncertainties are mostly epistemic in nature and can be reduced if knowledge gaps are closed. We think that reducing these gaps will happen through new observations, the synthesis of existing regional hydrologic knowledge, diagnostic model evaluation strategies tailored to the specific characteristics of GWMs, and through improved and new modeling approaches, including machine learning and hybrid strategies.

In the future, new data sources, including those from new satellites and new and open collections of existing observations, will provide considerably more information that can be assimilated into GWMs to improve model structures, parameters, and, ultimately, predictions. How quickly this might happen will depend on how new approaches, including those from Machine Learning, enable us to interrogate large and diverse datasets to estimate model parameters and structures (with more or less stringent physical constraints). Increasing the space-time resolution of existing models further means that model parameters and state variables become closer in scale to the variables we can observe. Whether this will lead to improved model performances, as seen in meteorology (Bauer *et al.*, 2015), is questionable (Beven & Cloke, 2012) and examples show that increasing hydrologic model resolution does not necessarily lead to better results (Hoch *et al.*, 2023). Also, blind spots in our observations of properties and dynamics of hydrologic systems remain despite advancements in observations. Lastly, significant opportunities for advancement remain in the context of GWM evaluation. Few strategies have so far been developed that benefit from the nature of GWMs, e.g., by looking across large gradients in the model domain or by establishing contrasting expectations of model form (structure and parameters) and behavior.

Keeping track of and utilizing advancements in machine learning, observational capabilities, computer science, and other relevant fields will be increasingly difficult for individuals and groups. Integrating diverse knowledge and skill sets will be critical to developing and maintaining a highly dynamic research field. In addition, various other fields also attempt to establish global modeling capabilities across the Earth sciences, e.g., vegetation modeling, to understand carbon fluxes. Cross-communication and exchange will likely be highly beneficial for all areas where similar problems of building, testing, and utilizing global models exist. Therefore, the reasoning put forward in this review goes beyond the topic of GWMs but provides a wider blueprint for how understanding epistemic uncertainties can be a light to guide knowledge discovery and accumulation for global model improvement.

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RR led the writing of the draft and conceptualization together with LS, SG and TW. MB, SM, YP, SK, CS, SB, BA, JA, JS, CP, SN, NM, and AG contributed to writing of specific sections of the draft, provided figures and data, and commented on the overall document.

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