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Global Groundwater Modeling and Monitoring: Opportunities and Challenges

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Key Points:

- A global groundwater framework is needed to address critical gaps in our understanding and predictive capacity of the hydrologic cycle
- We envision a framework that will combine observations and models to provide spatially and temporally continuous groundwater information
- The proposed framework could improve predictability in existing models and provide valuable new information for water management

Supporting Information:

Supporting Information may be found in the online version of this article.

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Abstract

Groundwater is by far the largest unfrozen freshwater resource on the planet. It plays a critical role as the bottom of the hydrologic cycle, redistributing water in the subsurface and supporting plants and surface water bodies. However, groundwater has historically been excluded or greatly simplified in global models. In recent years, there has been an international push to develop global scale groundwater modeling and analysis. This progress has provided some critical first steps. Still, much additional work will be needed to achieve a consistent global groundwater framework that interacts seamlessly with observational datasets and other earth system and global circulation models. Here we outline a vision for a global groundwater platform for groundwater monitoring and prediction and identify the key technological and data challenges that are currently limiting progress. Any global platform of this type must be interdisciplinary and cannot be achieved by the groundwater modeling community in isolation. Therefore, we also provide a high-level overview of the groundwater system, approaches to groundwater modeling and the current state of global groundwater representations, such that readers of all backgrounds can engage in this challenge.

Plain Language Summary

Groundwater is an important part of the water cycle but we are still working on the best ways to include it in global models. This study provides an overview of the state of the science for groundwater modeling and outlines a road map for what is needed to improve global groundwater models.

1. Introduction

Groundwater plays a critical role in the global hydrologic cycle, yet it is the only component of the Earth hydrologic system for which we lack a physically rigorous global modeling framework. While it is true that no global groundwater circulation exists comparable to global atmospheric circulations; groundwater is by far the largest liquid freshwater storage in the hydrologic cycle, and groundwater flow redistributes water over large spatial scales (up to continental scales) and long time periods (commonly days to hundreds of years). Groundwater must be accounted for within our modeling frameworks to fully understand the dynamics of global hydrology. Transient global groundwater modeling is needed to obtain spatially and temporally continuous and consistent information on this critical resource for human well-being given changing global conditions.

This is not a new argument, in fact the need for better global groundwater representations has already been well acknowledged in the hydrologic literature (Bierkens et al., 2015; Clark et al., 2015; Gleeson et al., 2021; Lall et al., 2020; Sood & Smakhtin, 2015). In recent years there has been a push to incorporate groundwater representations into existing global land surface and earth systems models as well as significant progress in continental to global scale groundwater modeling analyses and evaluation (e.g., de Graaf et al., 2017, 2015; Gleeson et al., 2021; Kollet et al., 2018; Maxwell et al., 2015).

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However, as the number and variety of approaches for large scale groundwater representation rapidly grow, we see a critical need for community engagement and interdisciplinary collaboration on best practices. Currently we see a gap between the tools and frameworks being developed by hydrogeologists, often at local to regional scales, and global scale applications. This paper is intended to help bridge the gaps across the diverse modeling community. We have three primary goals (a) to outline a path forward for a unified Global Groundwater Platform (GGP), where "platform" includes not only modeling technologies and tools, but also the data and monitoring efforts needed to build and validate the models, (b) to illustrate how the hydrogeologic community can and should contribute to this platform and (c) to provide some guidance on the complexity and key technical considerations for large scale groundwater simulation relevant to the land surface and atmospheric modeling communities who are working on adding groundwater to their systems.

The manuscript is structured as follows. First, we provide an overview of the role of groundwater in the Earth system and the major outstanding scientific questions that motivate the need for this platform (Section 2). Next, we present a vision for what a community driven Global Groundwater Platform could look like (Section 3). We then identify critical gaps and needs to achieve this vision (Section 4) and highlight the current state of modeling and datasets that we can build from (Section 5). Finally, we close with a suggested path forward and critical next steps that we should address as a community (Section 6). We also acknowledge that the global modeling community comes from diverse backgrounds and may have varying degrees of familiarity with the groundwater system. Therefore, we provide three appendices with background information relevant for global modeling on: groundwater processes (Appendix A in Supporting Information S1), hydrogeology (Appendix B in Supporting Information S1) and groundwater modeling (Appendix C in Supporting Information S1). These appendices also provide foundational information supporting our descriptions of the essential elements or phenomena that need to be included in global groundwater models and metrics that can be used to determine if the global groundwater models are sufficiently reliable.

2. The Role of Groundwater in the Earth System

Groundwater's connection to land surface processes and surface water bodies is multi-scale, creating patterns that connect small headwater catchments' recharge zones with continental aquifers and basins. These connections maintain flows along river corridors and to wetlands during droughts, ultimately resulting in continental streamflow and shelf discharge into the oceans. These interactions across spatial scales close the hydrologic cycle from the continent to the oceans in a dynamic equilibrium (Wörman et al., 2007). Groundwater abstraction is also a critical component of the human water budget. Groundwater makes up 35% of all freshwater withdrawals globally (Döll et al., 2012). This groundwater abstraction and subsequent usage, results in large-scale redistribution of freshwater resources that is critical to the dynamics of both human and natural systems as well as the ultimate sustainability of our combined systems (Gleeson et al., 2020).

Still, current estimates of groundwater storage and fluxes are highly uncertain due to data scarcity and model uncertainty, and have been continuously revised over the past decades (Abbott et al., 2019). For example, estimates of the global volume of fresh groundwater storage vary broadly from 1 to 60 million km^3 (Gleeson et al., 2016; Richey et al., 2015). The effects of climate change on groundwater processes, including potential changes in groundwater recharge and discharge over large spatial and temporal scales, are also uncertain; this fundamentally undermines attempts to determine effective strategies for integrated water resources management that can satisfy demands of human ecosystems.

Although groundwater is often treated as a simple storage term in global analyses, it is not an isolated reservoir. As illustrated in Figure 1, dynamic interactions between groundwater, surface water and land surface processes provide an additional control on earth system dynamics and are critical to accurate simulations and ultimately more accurate predictions. For example, Miguez-Macho and Fan (2012) studied the potential contribution of groundwater to evapotranspiration in the Amazon Basin. They demonstrated that the local interactions that drive subsurface flow may result in non-local effects via groundwater recharge, cross-watershed flow, and continental drainage and discharge by continental scale stream networks. Additionally, the hydraulic connections between shallow and deep fresh groundwater systems, and the fact that most of the worlds groundwater pumping comes from deep confined or semi-confined aquifer systems, means that global groundwater models need to represent

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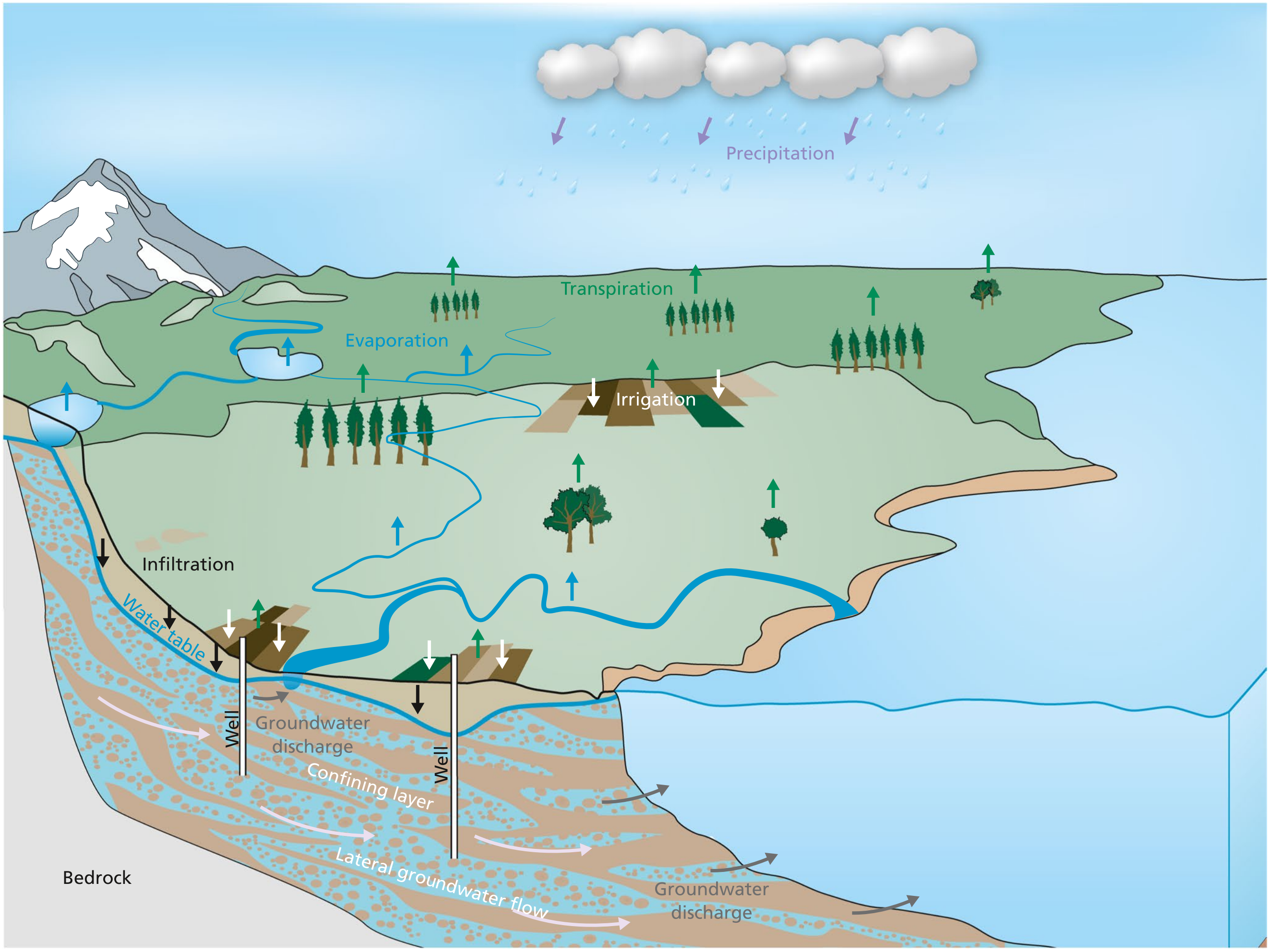

Figure 1. Illustration of the role of Groundwater in the hydrologic cycle.

deeper groundwater systems that influence not only the water table and land surface processes, but also the availability of groundwater for extraction by wells.

As the slowest flowing component of the terrestrial hydrologic cycle, groundwater often acts to buffer variability in both the water and energy cycles. Also, due to its inertia, it can be a potential source of increased predictability (Sutanto et al., 2020). Extremes such as droughts can be buffered by groundwater-surface water exchanges that provide relatively stable flow to rivers during low flow periods, and allow roots to take up water from the groundwater store (e.g., Marchionni et al., 2020). Similarly, fluctuations in groundwater depth have been shown to play an important role in the potential switching of groundwater-dominated ecosystems from carbon sinks to carbon sources due to groundwater abstractions and natural and anthropogenic climate changes (Genereux et al., 2013; Ma et al., 2014). Studies have already demonstrated the role of soil moisture (Koster et al., 2010, 2011) and more recently of vegetation states (Koster & Walker, 2015) in improved predictive skills of atmospheric processes at sub-seasonal-to-seasonal time scale. Accurate representation of anomalies in shallow groundwater, and their connections to soil moisture and evapotranspiration dynamics could further improve forecast performance at these time scales and longer (i.e., decadal) (Bierkens & van Beek, 2009). This is especially important for assessment of long-term impacts of global change (Erler et al., 2019; Ferguson & Maxwell, 2010; Goderniaux et al., 2009; Markovich et al., 2016; Maxwell & Kollet, 2008; Stoll et al., 2011; Sulis et al., 2012; Tague et al., 2008; Taylor et al., 2013).

Quantifying the temporal dynamics of groundwater systems across spatial and temporal scales is an active research area. Connections from the atmosphere to groundwater are well established; put simply, precipitation drives water infiltration, ambient atmospheric conditions drive evaporative demand and plant water usage, and recharge is the net effect of these exchanges. Many studies have demonstrated periodic oscillations of groundwater levels in response to climate indices at the continental scale (Perez-Valdivia et al., 2012; Rust et al., 2018, 2019). It is well established that watersheds and aquifers can act as low-pass filters dampening and attenuating climatic signals as the propagate through hydrologic systems (Duffy & Gelhar, 1985; Dwivedi et al., 2020; Eltahir & Yeh, 1999; Zhang & Schilling, 2004). There has been some work using the concept of groundwater response times to provide rough analytical estimates of the timescales of groundwater response to systematic changes at the global scale (Cuthbert, Gleeson, et al., 2019). Still, the temporal lags in groundwater response to climate variability caused by the slow processes of percolation through the soil-aquifer system remain uncertain at continental scales.

Furthermore, the influence of groundwater on land surface and atmospheric processes and two-way feedbacks remain poorly understood. The effect of soil moisture on precipitation has already been elucidated through the delineation of hot-spot regions (Koster et al., 2004; among many others). Two-way feedbacks between groundwater depth, soil moisture and evapotranspiration are also well established up to the continental scale (e.g., Christoffersen et al., 2014; Fan & Miguez-Macho, 2010; Pokhrel et al., 2013; Staal et al., 2018). Recently, Furusho-Percot et al. (2019) presented the first groundwater-to-atmosphere climatology in an evaluation simulation over Europe. Still, the causal mechanisms, and inherent timescales explaining whether and under which conditions groundwater helps to drive or merely responds to atmospheric variability is missing, and a theoretical framework has yet to be established (Anyah et al., 2008; Li et al., 2019; McGregor, 2017). Likewise, establishing the two-way feedbacks between global groundwater states and natural modes of variability (e.g., ENSO and MJO), which are dominant sources of predictability at the subseasonal-to-seasonal time scale, appears less straightforward and hinges on adequate observational datasets, which are currently unavailable.

There has been significant progress in continental to global scale groundwater modeling and analyses in recent years. However, much work remains to be done and the following basic questions remain unanswered:

1. How will future groundwater availability for humans and ecosystems change in response to climate change and anthropogenic influences?
2. How do the slow processes of groundwater recharge and lateral groundwater flow influence spatial patterns and temporal lags in groundwater response to change?
3. How much water is recharged to shallow and deep groundwater storage and what is its spatial distribution globally?
4. How much does groundwater contribute to evapotranspiration and streamflow under natural and human-influenced conditions?
5. What is the impact of groundwater on global atmospheric circulation and can we better quantify the chain of processes that control this interaction?
6. Are there teleconnections in groundwater timeseries in addition to natural modes of atmospheric variability related to for example, ENSO, NAO, PDO and AMO?
7. What role does groundwater storage play in the overall hydrologic responses to global change in both natural and managed systems?

3. Vision for a Global Groundwater Platform for Monitoring and Prediction

To address these questions, a Global Groundwater Platform (GGP) is needed to simulate groundwater processes in a scientifically rigorous and reproducible way, and to integrate groundwater observations in a consistent framework. This requires global tools that can simulate interactions from the water table, across the vadose zone and land surface, through the atmospheric boundary layer, all the way to large-scale atmospheric processes responsible for regional-scale precipitation regimes. These interactions need to be unraveled in light of transient climate scenarios, accounting for the role of emerging human-induced groundwater depletion, and considering the frequency, duration, propagation, and intensity of extreme events such as floods, heatwaves and droughts. Additionally, any platform must include the characterization and quantification of model structural and observational uncertainties. This constitutes a grand technical and scientific challenge. Also, it is clear, considering the current rate of global change and great uncertainty we are facing over the time scale of a generation (∼25 years), that this challenge needs to be tackled now.

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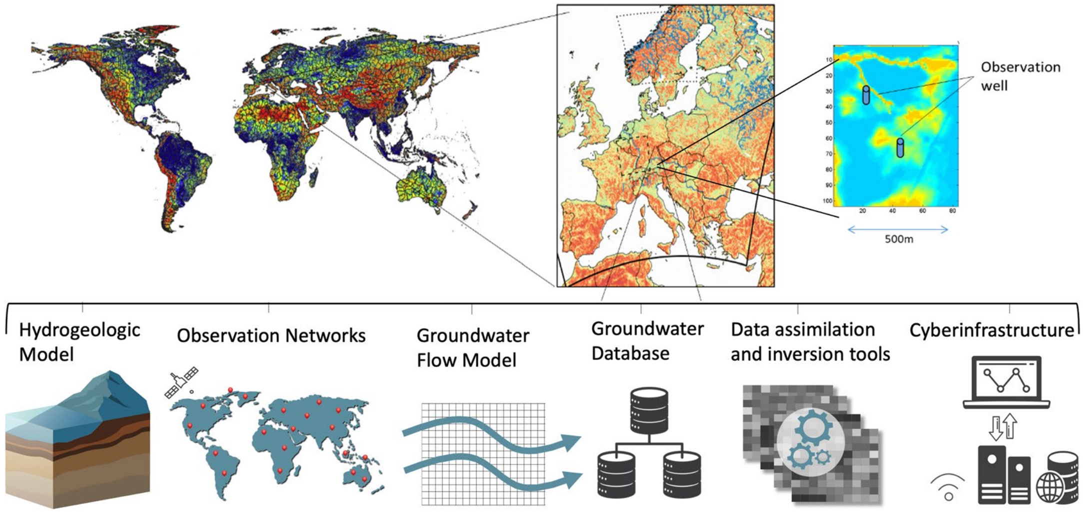

Figure 2. Schematic of the Global Groundwater Platform (GGP). The top portion of the figure is an illustration of what multiscale groundwater simulations might look like starting from the global and working to the local scale. The primary required components of the platform are shown in the bottom portion of the figure.

The ultimate goal of a GGP is to identify and predict continental to global scale patterns and trends in groundwater storage and divergences due to natural variability and global change (including climate change and anthropogenic groundwater interventions). We envision a platform that will combine observations and models to provide spatially and temporally continuous and consistent groundwater system information. This platform should consist of a monitoring component, focused on historical analysis and the present state of the system, as well as a prediction component for generating short and long-term projections and scenario analysis. Both the monitoring and prediction systems can be applied for water management and decision making as well as scientific analysis to answer the questions listed above and improve process understanding. The envisioned platform would encompass major technologies that do exist within other communities but have yet to be taken up fully in the hydrogeologic community in a consistent framework at continental to global scale.

As illustrated in Figure 2, the envisioned platform consists of several components: (a) global hydrogeologic model; (b) in situ observation networks and remote sensing; (c) groundwater flow model (or models); (d) high performance data storage and data base management system; (e) data assimilation and inversion technologies; (f) cyberinfrastructure including telecommunication systems and web services for user interaction to perform pre- and postprocessing, visualization and analyses. All components (source code and data) must be open, accessible, sharable, modifiable. In the following we provide a brief non-exhaustive overview of the different components, with an ensuing description of the two primary modes of operation for the platform: monitoring and prediction.

- The ***hydrogeologic model*** comprises the parameterization of the global hydrogeology in terms of aquifer structures and types as well as hydraulic parameters such as porosity, permeability, to be used in the (numerical) groundwater flow model. The hydrogeologic model will be based on well-defined metadata standards that are consistent with existing approaches and the flow model. More importantly it will also allow ingestion of regional and local data from existing well-established groundwater flow models that are available for many groundwater systems.
- The ***observation networks*** will pull together observations from in situ sensor networks directly measuring groundwater levels, including the water table, and remote sensing, such as the GRACE-FO satellite mission as well as surface water and land surface observations.
- The ***groundwater flow model*** is the numerical platform to simulate hydrologic fluxes in the subsurface. This platform may accommodate simulation of the entire terrestrial hydrologic cycle using integrated or coupled modeling approaches. However, here we focus on the groundwater simulation portions of the model. The flow model will include initial conditions and boundary conditions representing external groundwater fluxes with all the complexity that is possible today. The physical representation and parameterization of the subsurface will be based on the *hydrogeologic model* and might include multiple realizations to account for parameter uncertainties.

- The ***data assimilation and inversion tools*** include formalized ensemble methods to merge the numerical flow model with observations resulting in a correction of the hydrogeologic states and fluxes as well as improved parameter estimates. In this component, the ensemble methods also account for model and observation uncertainty.
- Downstream, of the confluence of all observational and simulation data is the high-performance ***Groundwater Database*** for data storage and data base management *system* for data storage and retrieval that is required for handling the data in research and applications globally at the long term.
- In addition to data storage dedicated ***cyberinfrastructure*** will be needed to support platform operations. The numerical implementation of the GGP platform will be based on state of the art massively parallel technologies implemented in distributed supercomputer environments to achieve the required spatial resolution and computing times. The observation data will be transmitted via dedicated telecommunication systems that may be maintained in a distributed fashion at the global scale. Users will have access to the platform via open gates consisting of web services allowing the user to perform analyses, visualization and download data sets.

The GGP will have two primary modes of operation, monitoring and prediction, both of which can be used for scientific inquiry as well as water management operations. The monitoring mode constitutes the continuous integration of a global groundwater model with in situ and remotely sensed observations using data assimilation approaches, focused on the most important variables and metrics. This will lead to full model-data reciprocity, in which observations inform and correct model states and fluxes (and possibly model parameter values and parameterizations). The model, in turn, fills in information gaps, and provides uncertainty estimates. Model evaluation is also a key component of monitoring mode. Gleeson et al. (2021) provide a comprehensive plan for model evaluation involving comparisons to observations, comparisons between models and expert judgment

The monitoring system provides an analysis of the past, and near real-time best estimate of the current state of the groundwater system. Spanning a long time period that should extend up to several decades of the past, this groundwater monitoring system enables calculation of anomaly correlation indices, which can be used in seasonal and decadal groundwater forecasts. Further, the groundwater monitoring datasets (including raw data and model results) can be used in a multi-nested modeling system to define boundary conditions for spatially- and temporally refined groundwater modeling applications at the regional and watershed scales. Finally, the continental to global groundwater monitoring system will provide physically- and spatially consistent extrapolation of groundwater changes in storage, fluxes and states over regions where observational groundwater data are sparse. This in turn can be used to design improved monitoring networks reflecting the hydrogeological complexities of the region of interest.

Results from the groundwater monitoring model will serve as initial condition for the probabilistic groundwater prediction mode applying the same modeling framework. The challenge of the prediction system will be to provide consistent short, intermediate and long term (interannual) predictions of water resources at the global scale including uncertainty estimates and scenario exploration. Probabilistic predictions will need to account for major sources of uncertainty such as those related to atmospheric forcings, model structural errors, vadose zone and aquifer hydraulic parameter distributions, vegetation and land use distributions, fluxes between groundwater and surface water, and human water use. Seasonal or interannual groundwater predictions face the challenge of requiring large ensemble sizes of the forcing data to account for atmospheric uncertainty adequately. In this case, anthropogenic water use information is required at the grid cell level, which should also be treated as an uncertain parameter further increasing the ensemble size. This becomes especially burdensome in the extension of the predictions into projections at climate timescales, because the uncertainty and computational requirements increase further. In the groundwater prediction system, the forcing data ensemble, high performance computing environment, and post-processing and analyses workflow must all be made available in a quasi-operational setting in order to ease the rapid dissemination of groundwater forecast products beyond the scientific community. For example, predictions would be most useful on a daily or weekly basis with a lead time of multiple weeks.

The applications of the proposed framework are numerous, here we provide a sample of potential beneficial uses. (a) The groundwater monitoring system would produce a true reflection of current and historical groundwater states, which would make analyses of future anomalies and trends of various states and fluxes possible in a global context. (b) The groundwater prediction system could serve as modeling kernel for seasonal groundwater monitoring, which has important implications for the implementation of large-scale transboundary water management strategies. Similarly, (c) groundwater predictions will provide additional and crucial information for the implementation of early warning systems for the management of natural hazards (e.g., droughts, floods), and in the context of food security. Currently, groundwater status is not included in those emergency management services (mapping and warning components) maintained through dedicated institutional programs (e.g., Copernicus at the European level; https://emergency.copernicus.eu), or the European Drought Observatory, although groundwater is often used as an alternative resource during drought. (d) Applying global change scenarios and story lines, and hypothesizing different human water use trajectories, projections of the groundwater system will be able to be performed in unprecedented ways using the groundwater monitoring results as initial conditions including the aforementioned uncertainties. (e) Results from the groundwater prediction will be of interest for addressing outstanding scientific questions related to global groundwater trends, propagation of sea level changes into the continental interior. (f) Results will also provide valuable information on connections between groundwater and global food production; for example, delineating regions and quantifying the populations affected by groundwater changes, and detection of the effect of changes in the groundwater availability on the global food trade.

4. Challenges and Requirements for Continental to Global Modeling and Monitoring

A successful Global Groundwater Platform must overcome significant conceptual, technical and data gaps for continental to global groundwater representations, which have persisted for quite some time. A global system must address the huge diversity of hydrogeologic systems that are partly to fully interconnected on the sub-continental scale and that need to be adequately represented while still providing reliable mass fluxes at resolutions on the order of 10–100s of meters relevant for scientists and stakeholders. The subsurface poses unique challenges relative to other earth system components, given the sparsity of observations and the broad range of spatial and temporal scales that must be considered. This limits the utility of purely data-driven empirical approaches and necessitates close integration of observations with physically constrained models. Here we outline some of the major outstanding challenges and requirements that must be addressed for the primary system components (a) global hydrogeologic model, (b) in situ observations, (c) groundwater flow model, and (d) cyberinfrastructure.

4.1. Global Hydrogeologic Model

Groundwater models require spatially continuous and consistent datasets of the hydrogeologic properties that control the movement of water through the subsurface. To generate a global model that is locally relevant one must also consider how the effective or representative properties such as hydraulic conductivity (K) values may change with the spatial scale, or resolution, of the model. Generating a continental to global hydrogeologic model has been proposed previously (e.g., Bierkens, 2015; Gleeson et al., 2021) and the task of defining subsurface parameters and structures is challenging for several reasons:

1. Hydrologic heterogeneity occurs at every spatial scale from sub-centimeters to thousands of kilometers covering an extremely wide range of structures, geometries and properties in 3D. Examples include fractured hard rock, alluvial and karst aquifers; tectonic faults connecting aquifer layers; preferential flow paths along buried river channels and tidal creeks, as well as the heterogeneity of the vadose zone that is interconnected with groundwater (Kim et al., 1997; Vereecken et al., 2019).
2. The identification of hydrogeologic heterogeneity structure and physical properties is difficult because it requires subsurface borehole and geophysical data that are often scarce.
3. Additionally, while the averaging volume of these measurements is highly variable, in the context of global groundwater modeling, in situ measurements constitute point values that cannot be easily transferred to a coarse computational grid.
4. Non-invasive methods, such as ground-penetrating radar and seismic methods provide only structural information, but can be useful in the interpolation of hydraulic property values from in situ measurements.

While these challenges may seem intractable, there are appropriate regional strategies to address them. Based on foundations discussed in Appendix A in Supporting Information S1 (Overview of the groundwater system) and Appendix B in Supporting Information S1 (Hydrogeology—subsurface representations), one can deconstruct the subsurface characterization problem into feasible steps that leverage regional geologic information and our knowledge of groundwater flow phenomena. In this workflow, an underlying objective is to produce a hydrogeologic model of not just the aquifers, but also of the non-aquifer (lower permeability) regions that also influence soil moisture and land-climate coupling. In other words, as groundwater is ubiquitous in the subsurface, global or continental groundwater models must aim to represent all of the groundwater systems and not just those commonly regarded as aquifers. Within the aquifer systems, it is also important to appropriately represent the degree of confinement under which the groundwater systems occur as explained in Appendix A.1 in Supporting Information S1.

The need for global groundwater modeling should spur efforts to integrate hydrogeologic data worldwide to create a global groundwater atlas. The objective should be to create a global database containing a 3D description of hydrostratigraphy and hydrogeologic properties globally. The information is currently dispersed institutionally and geographically. It is not even clear how to define a universal metadata standard including a consistent definition of hydrostratigraphic properties, structural and geometrical elements, resolutions, and spatial extents. In large areas, even basic geologic information is missing and must be deduced from secondary information.

The envisioned hydrogeologic framework must fulfill a number of requirements to be useful to the groundwater modeling community:

1. It must be internally consistent. Hydrogeologic units, boundaries and associated hydraulic parameter values must be based on a globally consistent 3D hydrogeologic framework.
2. It should adopt consistent metadata standards that follow existing best practices and be continuously updated with incoming information. This will require community governance (development and sustainability plan) including revision control and release cycles.
3. The data structure must be designed such that the information can be readily applied to models based on different discretization schemes and resolution. To accomplish this, it is envisioned that the generation of the hydrogeologic framework should be accompanied by the development of ad-hoc and parameter-dependent upscaling techniques for different model configurations.
4. Groundwater modelers must be able to spatially expand and reduce the hydrogeologic framework model in a straightforward manner and easily update as new data is released. For example, the groundwater and overlying vadose zone need to be coupled to the land surface, which would require a seamless link to global soil and vegetation maps and related properties. The envisioned hydrostratigraphic framework is considered a living model which is continuously improved and updated in groundwater models.
5. The framework should be consistent with existing and reliable regional models in order to lend confidence in the global implementation. To achieve this there will need to be clear processes for regional modelers to contribute to the global framework within the version-controlled system.

4.2. In Situ Observation Network and Remote Sensing

Apart from global remote sensing data sets, there is currently no global data center or resource that compiles and manages transient hydraulic head observations, which could be used in the configuration and validation of global models. Borehole measurements (e.g., groundwater levels and piezometric heads, temperatures, hydrogeochemical variables) and observations remain dispersed between local, regional, national and international public and private institutions. Existing datasets are still missing many observations which are not easily accessible. In addition, data quality varies greatly with respect to metadata, measured values, and geographic coverage. Procedures for consistent quality assurance and quality control across data sources are lacking. Furthermore, our current datasets are static, and we lack a coherent global approach that can incorporate new observations as they are generated.

Except in the best instrumented basins, changes in groundwater storage are often poorly constrained due to limited observations. In disturbed groundwater systems, the two largest fluxes are typically abstraction from wells and recharge. The former is often not measured, and the latter is not directly observable. Consistent continental to global data sets of actual water abstraction by agriculture, industry and drinking water providers generally do not exist. In many places, pumping wells are ungauged, although there are exceptions at the regional scale. For example, in Europe and parts of the United States, abstraction rates are managed, but in a very diverse fashion based on communal, state and national laws and guidelines. Still, in large parts of the world groundwater abstraction rates remain unregulated and unmonitored. Experience has shown, however, that data on crop-water demand and surface water deliveries to irrigated lands can be used to reasonably estimate groundwater pumping, especially at the regional scale.

In addition to uncertainty and limitations in groundwater observations, uncertainty in the (boundary) fluxes and sources and sinks that drive the groundwater flow models is a significant concern. For example, while methods of estimating evapotranspiration (ET) have improved and potential ET can be determined fairly well with meteorological information, actual ET is much more challenging. The uncertainty associated with ET estimates of native or unirrigated landscapes can be larger than the estimated recharge rate in arid landscapes where recharge is small. In irrigated crop landscapes, actual ET is closer to potential and can sometimes be better determined as a result of decades of crop ET measurements. Also, in irrigated systems recharge from applied irrigation water is generally large enough to be less impacted by actual ET errors. However, it should be noted that there are still many challenges in irrigated landscapes. For example, in some cases actual ET can be significantly larger than potential ET due advection (de Bruin & Trigo, 2019). Also, as noted above, we often lack information on groundwater pumping which is critical water supply for irrigation in many locations.

Previous studies also suggest that groundwater discharge along the continental boundary may constitute a significant part of the continental mass balance in certain regions (Konikow, 2011) and conversely that coastal groundwater resources may be threatened by sea level rise (Befus et al., 2020). Yet the size flux across the land-ocean interface remains highly uncertain (Luijendijk et al., 2019); virtually no measurements are available to constrain this flux in continental to global models in a meaningful way. Currently, in large scale models, simple Dirichlet boundary conditions are commonly applied, which may result in a potential under- or overestimation over large spatial scales (Refer to Appendix C in Supporting Information S1 for more information on boundary conditions).

There has been great progress in remote sensing in recent years including the GRACE satellite mission that can be used to estimate terrestrial storage changes (described further in Section 5). Still, there are significant challenges with this data too. GRACE requires other observations to separate out groundwater storage changes from other storage reservoirs and in situ observations remain very important. Additionally, it has limited spatial resolution and we require wells and models to provide more local information at scales less than 400 km.

Groundwater is a sparsely observed system, therefore its critically important that the proposed Global Groundwater Platform makes the best use of the observations that we do have and help support expansion of monitoring. We envision an observation platform that can expand as we increase the accessibility and consistency of global monitoring datasets. To accomplish this, we need:

1. Consistent metadata standards for groundwater observations.
2. The ability to automatically import observations including ongoing transient observations.
3. Direct access to observation networks for other components of the physical system (such as streamflow and ET) that can be used to help constrain the groundwater system models.
4. Observations of agricultural systems, industrial and municipal systems that can be used to estimate groundwater abstraction. This may include pumping observations where available but given the limited observations should also include, crop type mapping, crop water demand, surface water irrigation estimates, irrigation efficiency estimates and municipal water demand estimates.

4.3. Groundwater Flow Model

The observations we have are not sufficient to fully define the groundwater system without the help of models. Groundwater states and fluxes (prerequisites for local storage change calculations) can be observed locally using well observations of groundwater levels or piezometric heads, or stream baseflow measurements. However, it is difficult to upscale aquifer storage changes from point observations due to (a) the sparsity of point observations; (b) lateral heterogeneity in aquifer properties and human activities that makes spatial interpolation difficult; and (c) the complex relationship between storage changes and changes in deep and shallow groundwater levels in layered systems that may have both confined and unconfined conditions. Furthermore, the location of existing groundwater monitoring stations is based on practical considerations (e.g., locations where wells are already drilled for water supply) rather than scientific criteria assuring the hydrogeological representativeness of the measured information. It should also be emphasized that many of the observations from wells are from stratified sedimentary basins, in which semi-confined conditions prevail, and as such the observations in these wells provide piezometric head values and not the water table. Thus, these observations cannot provide information on storage or fluxes directly unless they are put in the context of a 3D groundwater model that accounts for the hydrodynamic interplay between shallow and deep portions of the groundwater systems. A Global Groundwater

Platform is required to provide spatially and temporally coherent estimates of states and fluxes that are otherwise unobservable, and to enable predictions.

To build a reliable global groundwater modeling system, the hydrogeology framework described above will need to be transferred into a globally consistent numerical framework for groundwater flow modeling. This framework must be able to efficiently exploit current and future high-performance computing technologies to support the required spatial resolution, data assimilation and ensemble simulations without exceeding computational resources (further discussed in the following section). Because there are no true global groundwater circulations comparable to those for the atmosphere and ocean, individual models may be constructed up to the continental scale that could be maintained and applied across different groups and high-performance computing centers. This approach requires, however, careful consideration of the potential impact of varying hardware and software (e.g., compiler) configurations influencing the simulation results that is the global numerical consistency and (bitwise) reproducibility.

To be most useful the groundwater flow model should be able to represent subsurface fluxes and storage at high spatial resolution. Here we suggest 10s to 100s of meter lateral resolution, which is sufficient to resolve hillslope processes. Some applications of the model may not require such high resolution. For example, coupling with lower resolution Global Earth System models might be achieved with lower spatial resolution. However, previous research has emphasized the value of high resolution models to accurately capture hydrologic processes such as groundwater-surface water interactions, small surface water bodies and stream networks, as well as to provide information at the spatial scales that water managers need (Bierkens et al., 2015; Wood et al., 2011).

Furthermore, to accurately capture the full terrestrial hydrologic cycle and to provide accurate predictions moving forward, the proposed groundwater modeling framework must connect to the rest of the hydrologic system. Groundwater flow models will need to be extended toward the land surface in a continuum approach. For example, using Richards' equation to close the water cycle mathematically at the lower boundary. This is important in honoring the non-linear connection of the free, moving water table with the vadose zone that is essential in arriving at accurate dynamics and exchange fluxes (recharge and capillary rise) and capturing all relevant time scales.

Already there are several established approaches for integrated hydrologic modeling (see Section 5 for more details). Integrated models and groundwater models may be coupled to land surface models, to improve the hydrologic representation. Land surface models may be coupled to groundwater and integrated hydrologic models to relax simplifying assumption with regard to the upper boundary condition (Kollet et al., 2018; Kollet & Maxwell, 2006; Maxwell & Condon, 2016; Maxwell et al., 2007, 2015). However, in both approaches, the key exchange flux, groundwater recharge, is ultimately dominated by the precipitation, applied irrigation water, actual ET and soil hydraulic properties. This provides a significant challenge because the error in actual ET estimates are seldom small relative to the magnitude of recharge, and in fact may exceed the magnitude of recharge for non-irrigated lands. Additionally, focused recharge, a very important process in dryland regions, is often not represented well in models, because it requires a spatially explicit interaction between surface water and groundwater allowing surface runoff to infiltrate into the aquifer further downstream in a river basin. Ignoring this process leads to underestimations in recharge and groundwater levels. The plausibility of estimated recharge rates therefore is not supported or reinforced by the surface hydrologic budget, but rather, by how well the underlying groundwater model that is consistent with the regional system hydrogeology is able to reproduce the observed spatio-temporal fluctuations in head and computed discharge to the surface (e.g., stream baseflow, springflow, discharge to agricultural drains).

An additional challenge for any flow model is the representation of human systems. Humans strongly alter the entire hydrologic cycle and the need to represent human activity in global hydrological models has been widely recognized. In fact, one of the purposes of global groundwater modeling is to better understand future availability of groundwater and its sustainability under climate change that will not only affect precipitation and recharge, but also the demand for groundwater by humans and ecosystems, including agriculture. Numerous global or continental-scale studies have incorporated human impacts into global hydrological models (Alcamo et al., 2003; Döll et al., 2012; Haddeland et al., 2006; Hanasaki et al., 2008; Pokhrel et al., 2012; Rost et al., 2008; van Beek et al., 2011; Voisin et al., 2013; Wada et al., 2010; Wisser et al., 2010). However, most of these models take the water balance approach to calculate exchanges between surface water and groundwater but not directly simulating groundwater processes (i.e., groundwater fluxes and heads). Such models do not simulate groundwater level declines due groundwater pumping and, hence, cannot estimate changes in groundwater storage, explicitly. While this is valuable for some global applications the envisioned global groundwater model will need to incorporate human activities into process-based groundwater simulations.

Finally, we highlight the importance of model calibration, data assimilation and uncertainty as part of any simulation platform. The models may initially be relatively crude and poor predictors of changes in groundwater storage and water fluxes across the land surface and water table, but can improve through progressive incorporation of better data and hydrostratigraphic characterizations, in combination with careful cross-checking with already established, calibrated models. To the casual observer, uncertainty in the three largest groundwater fluxes (discharge, pumping, and recharge), combined with the fact that changes in groundwater storage are seldom directly measured, might appear to render groundwater simulation unconstrained or even ill-posed. On the contrary, however, we are able to build groundwater models and integrated hydrologic models that represent the hydrologic system sufficiently well to support problem solving and water resources management decision making. Accurate groundwater models are developed by relying on a variety of measurements such as hydraulic head, streamflow, spring flow, water chemistry, and aquifer properties, as well as characterization of the physical structure or architecture of the aquifer-aquitard system. Model representation of the subsurface hydrogeology can also provide an important constraint on the uncertainties stemming from large surface fluxes including evapotranspiration and precipitation. Still, given large uncertainty in subsurface parameters and geometry, most groundwater models depend heavily on calibration. It is outside the scope of this paper to suggest specific approaches for model calibration and parameter estimation, however additional details on existing approaches are provided in Appendix C in Supporting Information S1.

While there are many approaches that can be taken in model development and implementation we envision the following key requirements for the global groundwater flow model:

1. The flow model must be able to capture three-dimensional fluxes and storage states in the subsurface at multiple spatial resolutions depending on the application.
2. The groundwater model should be extended to the land surface or be easily coupled to land surface and atmospheric models in order to capture focused recharge and discharge to surface water bodies.
3. It should integrate human activities that influence the groundwater system such as pumping and irrigation.
4. The model must be sufficiently deep to capture the hydraulic connections between shallow and deep fresh groundwater systems. Most of the world's groundwater pumping comes from deep aquifer systems. Deeper groundwater systems can influence not only the water table and land surface processes, but also the availability of groundwater for extraction by wells.
5. The modeling platform should be designed to be compatible with the observation network to facilitate direct data assimilation and model evaluation.

4.4. Computational Platform Development

In practice, modeling groundwater flow (including data assimilation/inversion and uncertainty quantification) at spatial and temporal scales, and resolutions that are relevant for the scientific and water management communities, is computationally expensive. Moving from watershed to continental and global scales will easily result in more than 10^9 cells and increase the computational problem by orders of magnitude. Global high-resolution models will require thousands of cores for computation and generate petabytes of output. Addressing computational and data challenges will be critical to successful global modeling efforts. Massive parallel computing technologies will be essential in achieving this goal, requiring major software innovations in the hydrogeologic community.

Arguably, the groundwater community has been slow overall in the adoption of High Performance Computing (HPC) technologies in comparison to the atmosphere and ocean science communities, which have been driven strongly by the operational forecasting centers very early in the HPC age (e.g., the German Weather Service opened its first in-house HPC center in 1966 housing a CDC 3400 [super-]computer). To date only a small number of groundwater flow models exist that have been designed initially to use efficiently parallel computing resources. These parallel-computing models have been applied in proof-of-concept studies, large-scale flow and also reactive transport modeling, and groundwater-to-atmosphere simulation studies. However, the lack of widespread technology adoption is of major concern, as (a) model resolution is always increasing and (b) parallel

Table 1
Grid Cell Numbers, Storage Requirements (for One Double-Precision Variable) and Potential Compute Core Counts for a One Layer of a Global Groundwater Flow Model

Resolution	10 km	1 km	100 m	10 m
Number of grid cells	1.4E + 06	1.4E + 08	1.4E + 10	1.4E + 12
GB storage per time step	1.0E–02	1.0E + 00	1.0E + 02	1.0E + 04
Number of compute cores	1.4E + 01	1.4E + 03	1.4E + 05	1.4E + 07

Note. The total ice-free continental area is estimated at approximately 140 Mio km^2.

hardware technologies are evolving at an increasing speed, leading to a continuously increasing gap between hydrogeologic modeling and next generation parallel hardware infrastructures.

Traditionally, groundwater modeling software has been programmed in a monolithic way with the computational kernel and all additional code infrastructure are part of a single software. This approach makes the code compact for the user. However, new heterogeneous computing hardware and storage architectures based on very rapid development cycles do not lend themselves to the traditional approach because new hardware types require considerable adjustments of the code base. The key is to facilitate the porting of complex codes across hardware architectures, while maintaining performance (i.e., performance portability) (Lawrence et al., 2018). Currently, only a small number of groundwater flow model codes exist that are suitable for global groundwater modeling and performance portability in the future.

Global groundwater modeling and groundwater prediction is already possible with current HPC technologies. However, processor performance gains have essentially saturated and stopped following Moore's law, mainly because of power limitations. This has already led to a paradigm shift in the architecture of supercomputers, moving away from being purely cluster-based (large number of interconnected PCs) toward heterogeneous designs consisting of combinations of clusters and accelerators/boosters (mainly graphical processing units, GPUs). As a result, the landscape of parallel geoscientific software development will be changing considerably toward more hybrid parallel development strategies that are performance portable and scalable (Lawrence et al., 2018), and groundwater models will need to adapt quickly to these changes. In this context, other geoscience disciplines like the weather and climate communities have started outlining plausible roadmaps on how to rapidly adapt codes to available hardware (Lawrence et al., 2018). The groundwater community should make similar efforts and preferably in cooperation with these communities.

Table 1 provides an estimate of the number of grid cells, storage requirements and potential compute core counts based on previous experience with the parallel groundwater software ParFlow (Burstedde et al., 2018; Kollet et al., 2010). This assumes a groundwater flow model covering ice-free continental areas of the world, roughly 140 M km^2. Numbers provided are for different spatial resolutions of one model layer assuming a rectilinear, equidistant grid without local grid refinement. The number of compute cores were estimated assuming a problem size of 10^5 grid cells per core, which resulted in reasonable scaling on a massively parallel supercomputer (Burstedde et al., 2018). Numbers for a multilayer model can be obtained by multiplying the estimates in Table 1 by the number of model layers. Thus, a ten-layer global groundwater model at 1 km resolution leads to 1.4×10^9 grid cells, 10 GB of storage for one double-precision variable per time step (without compression), and a requirement of about 14,000 compute cores.

These numbers suggest that a global groundwater model is feasible in standard supercomputer environments today even in data assimilation mode assuming reasonable ensemble sizes on the order 10^1. As noted above, because no global groundwater circulation exists, the global model can be implemented separately for different continents in a grid computing approach, which would further distribute the required resources. This approach should also enable a 100 m resolution hillslope resolving global model, which would increase the required resources by a factor of 100. Note, the data storage burden could be efficiently reduced by implementing lossless and lossy compression techniques as well as by adopting an online analysis approach and storing just the information needed to re-run the model (check pointing). Inverse modeling, which is still much more compute intensive than forward modeling, could be applied for smaller areas like large aquifer systems. The inversely estimated

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spatial distribution of aquifer parameters can be introduced in the continental to global scale model improving (for a smaller region) the characterization of aquifer parameters.

5. Current State of Tools and Datasets for Continental to Global Groundwater

While the challenges and needs outlined above are significant there has been great progress in recent years in large-scale modeling, monitoring and data analysis. Here we highlight some of the most promising existing tools and datasets that can be used as a starting point in addressing the needs of a global platform.

5.1. Global Hydrogeologic Model

5.1.1. Hydrogeology Datasets

One of the earlier efforts in hydrogeology to map global aquifer properties is the WHYMAP initiative lead by the BGR (German Federal Institute for Geosciences and Natural Resources) and UNESCO (Richts et al., 2011). The product is a vector map, produced in 2004 and updated in 2008, of the extent of the major aquifers in the world classified into three categories: major groundwater basins; aquifers with complex hydrogeological structure; and local and shallow aquifers. Recharge (in mm/year) was also mapped, which, together with the aquifer type, reflects the aquifers' productivity and groundwater renewal rate.

More useful for the parameterization of large-scale groundwater models are global lithology maps, because they can provide estimates of parameters like hydraulic conductivity and porosity. Two well-known maps are by Dürr et al. (2005) and Hartmann and Moosdorf (2012). However, these maps only describe the lithology at the surface, without explicit 3D geometric information.

Information on the depth of the productive aquifers can be found by inspecting so-called depth-to-bedrock and sediment thickness maps. Several depth-to-bedrock maps exist, but what they represent differs and can be contradictory. The four most relevant maps are listed here. (a) The depth to bedrock map of Pelletier et al. (2016) estimates the thickness of the soils, underlying regolith layers (in uplands) and unconsolidated sediment stacks (in lowlands) to a maximum depth from land surface of 50 m. (b) Shangguan et al. (2017) produced a data set that targets the same properties, but is not limited to the 50 m maximum depth for the unconsolidated sedimentary deposits. The depth to bedrock maps are quite different from the sedimentary thickness estimates produced by the petroleum geology community. For instance, (c) Limberger et al. (2018) provide a map of sediment thickness based on seismic data where sediment thickness includes not only the unconsolidated (soft) sediments, but also the more consolidated sedimentary rocks, which are often of lower hydraulic conductivity and not represented in global groundwater models. Moreover, this data set only considers the larger sedimentary basins and not the shallow groundwater bearing layers in mountain areas. (d) Finally de Graaf et al. (2015), as part of an effort to build a global groundwater model, provide estimates of aquifer thickness of the larger sedimentary basins. The target variable of this data set is therefore quite similar to the sediment thickness of Limberger et al. (2018).

A few global estimates of hydraulic properties of the subsurface have been developed. (a) Permeability and porosity of the upper 50 m were derived by Gleeson et al. (2014) and Huscroft et al. (2018) based on the lithology map of Hartmann and Moosdorf (2012) and estimated permeabilities and porosities from reported U.S. groundwater studies. (b) de Graaf et al. (2017) extended the aquifer depth data set of de Graaf et al. (2015) to a two-layer global hydrogeological model including the confining layers or characteristics within many of the global aquifer systems. Transmissivities and storage coefficients were derived from Gleeson et al. (2014) and calibrated based on observed groundwater data. Additionally, the GEWEX global soilwat initiative is working to survey soil properties used in global land surface models and build global soil parameter datasets.

It should be noted that most existing datasets are two-dimensional: no consistent 3D lithologic, hydrogeologic or hydrofacies data set exists at the global scale. Within most sedimentary basins, data that could be used to extend the listed datasets into the vertical dimension exists but are not assembled and/or not readily accessible. This is another area in which the global modeling effort could be used to encourage international cooperation. Conversely, in upland and mountainous areas in which fractured rocks dominate, much less data exist for the 3D spatial patterns in aquifer conditions and properties.

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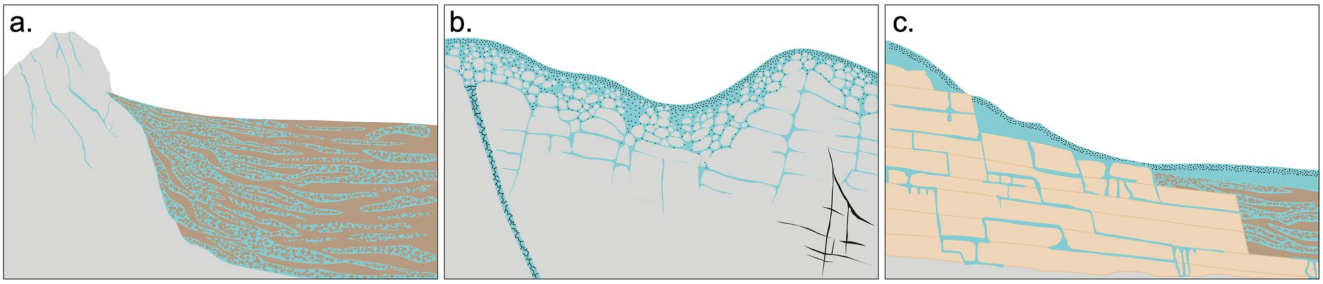

Figure 3. Conceptual illustrations of the three major hydrogeologic system types (a) clastic sedimentary basins (CSB), (b) low-K hard-rock systems (LKHR), and (c) high-K hard-rock or cavernous (karst) systems (HKHR).

5.1.2. Approaches for Model Parameterization and Addressing Heterogeneity at Scale

Regardless of the challenges of multi-scale heterogeneity, there are numerous examples of moderately to very successful regional groundwater models, many of which have been shown to represent groundwater systems while sufficiently honoring measured parameters, heads and fluxes (e.g., Belitz & Phillips, 1995; Faunt, 2009; Sahs, 2018; Texas Water Development Board, 2020). Many successful approaches circumvent the local-scale heterogeneity and upscaling challenges by using a deductive rather than inductive approach. In the inductive approach to model building, one would attempt to collect as many local-scale measurements of parameters (e.g., hydraulic conductivity or transmissivity) and induce the upscaled equivalent parameters by theoretical means or calibration. In the deductive approach, one starts at the more regional scales by leveraging geologic characterization and the pumping-test-based estimates of parameters that are already representative of integral average properties, commonly at scales as extensive as 10^2–10^3 m. Importantly, in the deductive approach the geologic stratigraphy, or more specifically, the hydrostratigraphy in which both stratigraphy and hydrogeology are integrated, together with structure (e.g., basin boundaries, faulting) are used to form the conceptual model of the occurrence of groundwater, including the locations and geometries of aquifers and aquitards. Once this hydrostratigraphic framework is delineated, the aquifer/aquitard properties can, at minimum be inferred from knowledge of the rock types (e.g., Senger & Fogg, 1987), or, more ideally, be estimated through joint analysis of the geologic and hydrogeologic data (Faunt, 2009; Fogg, 1986; Texas Water Development Board, 2020).

The above-mentioned "deconstruction" of the problem can proceed by using geologic characterizations to categorize the groundwater systems into three or more basic types within which similar modeling strategies and assumptions can be applied (see Appendix B.2 in Supporting Information S1 for more information). Here we highlight three major groundwater system types shown in Figure 3: *clastic sedimentary basins, low-K hard-rock* systems*,* and *high-K hard-rock or cavernous (karst)* systems (CSB, LKHR, and HKHR). The CSBs, which could include glacio-fluvial deposits of the mid-to-upper latitudes, are the most studied and modeled of groundwater systems, so they already have numerous hydrogeologic data sets and working groundwater flow models. Because of all the work on the CSBs, these can help serve as "reservoirs" of information for benchmarking the continental-scale models. Within each system type, one must further exploit any regional geologic characterizations on the subsurface structure and stratigraphy to define the hydrogeologic system framework, including locations of aquifers and aquitards in 3D. This framework together with hydrogeologic data on groundwater level fluctuations and porous media parameters can further be used to identify where the groundwater is under unconfined, semi-confined and confined conditions. This aspect on degree of confinement will be particularly essential for relating changes in groundwater levels to changes in storage (see Appendix. B.2 in Supporting Information S1) without creating significant errors.

The LKHR groundwater systems typify most uplands or mountainous areas and pose some of the most serious challenges to development of representative groundwater models at both local and regional scales. All the data upon which we rely to build and calibrate models in the CSB systems is typically lacking in the uplands and mountains. Moreover, unlike in the case of CSBs, the fracture-rock system hydraulic parameters are much more difficult to estimate based purely on geologic information. Nevertheless, the commonly high topographic relief in LKHRs can produce strong, definable driving forces (Appendix A.1 in Supporting Information S1), which together with data on stream baseflow, spring flows, and lake elevations (as manifestations of the water table), can be used to constrain the LKHR groundwater models. There is much ongoing research on groundwater in LKHRs, and it needs to further expand and accelerate in support of global groundwater modeling needs. Of particular importance is the nature of the hydrogeologic transition from the uplands to the lowlands which is commonly referred to as the "mountain front" (Wilson & Guan, 2004). If hydrogeologic properties of the mountain fronts are not adequately estimated, the high hydraulic potential (head) in the mountains will tend to swamp out the lowlands in any continental-scale model, as exemplified in Reinecke et al. (2019). Future research on not only mountain hydrology, but also mountain-front recharge should be a high priority.

Many of the HKHR systems are similar to the CSB in that because they were long ago discovered as major aquifer systems, they already contain relatively abundant data and some calibrated groundwater models (e.g., the Edwards aquifer, Texas; Columbia River basalt deposits of Washington, Oregon and Idaho).

In the above-described, well-established approach for regional model building, uncertainty around the parameters and even the underlying conceptual models remains a stubborn challenge, but can be managed through careful model calibration and comparisons of measured and monitored groundwater levels, including the water table, and fluxes. In this regard, measured fluxes such as streamflow, baseflow, spring flow, and well pumping are most consequential for minimizing and managing model uncertainty (e.g., Hill & Tiedeman, 2006)

5.2. In Situ Observation Network and Remote Sensing

There are currently a few initiatives that collate groundwater level time series on continental to global scales. In North-America, the USGS maintains the National Water Information System (NWIS) containing 850,000 records. In Europe, the Groundwater Drought Initiative (Bloomfield et al., 2018) uses a collaborative approach. They work with national data holders and scientists in almost all countries combining data from national groundwater monitoring systems into a Europe-wide groundwater level data set. Cuthbert, Taylor, et al. (2019) have taken considerable effort to collate long-term groundwater level time series in Africa. Also, the International Groundwater Resources Assessment Center (IGRAC) has developed a Global Groundwater Information System (GGIS) which is an online platform for sharing groundwater data. All of the datasets mentioned required significant efforts to assemble and are a valuable step forward. However, they still remain limited in their spatial coverage. Even those areas with coverage have significant spatial and temporal gaps and suffer from short periods of record, limited meta-data, or low-quality observations. Additionally, not all these datasets are easily publicly accessible without coordination with the data set creators (although it should be noted that the IGRAC GGIS system is working to address sharing issues). International cooperation at a number of levels will be required to improve the available data. Global groundwater modeling can be used to elucidate valuable data and encourage the needed international cooperation.

Quite recently, attempts have been made to provide global water use estimates at relatively high spatial and temporal resolution (up to 0.1° at daily time steps). Examples include the products by Wada et al. (2016) and Siebert et al. (2010) which combine statistical data from public, agricultural and industry sources to calculate water demand based on land cover, soil information, and weather data. While approximate, these values are currently the best available for use in global groundwater models.

With respect to groundwater stores, remote sensing techniques provide new avenues for quantitative assessment. Most remote sensing products provide information on the vegetation layer (e.g., vegetation indices) or the first few centimeters of the vadose zone (e.g., SMOS or SMAP satellite derived products), which are useful for estimating groundwater recharge and evapotranspiration. GRACE (Gravity Recovery and Climate Experiment; Rodell et al. (2009, 2018) provides data on water storage over large areas, including water in the surface and subsurface. Rodell et al. (2018) provide a data set of water storage changes derived from the analysis products of the satellite mission GRACE and additional data products are available from Watkins et al. (2015) and Tellus (2012). This is the first global estimate of its kind and provides unprecedented large-scale quantification of storage changes. However, applications of GRACE are limited by its coarse spatial resolution (about 150,000 km^2 at midlatitudes). Also, GRACE only provides total storage changes (i.e., surface and subsurface), and additional analysis is needed to extract the subsurface component which can result in large errors (e.g., Brookfield et al., 2018; Van Loon et al., 2017). Another remote sensing approach is to use heat flow and temperatures as a tracer to estimate groundwater discharge (Anderson, 2005; Liu et al., 2016). These methods can be very sensitive to small-scale land surface processes such as evapotranspiration, sensible heat flux and soil heat flux, and applications to large scale simulations have not been developed.

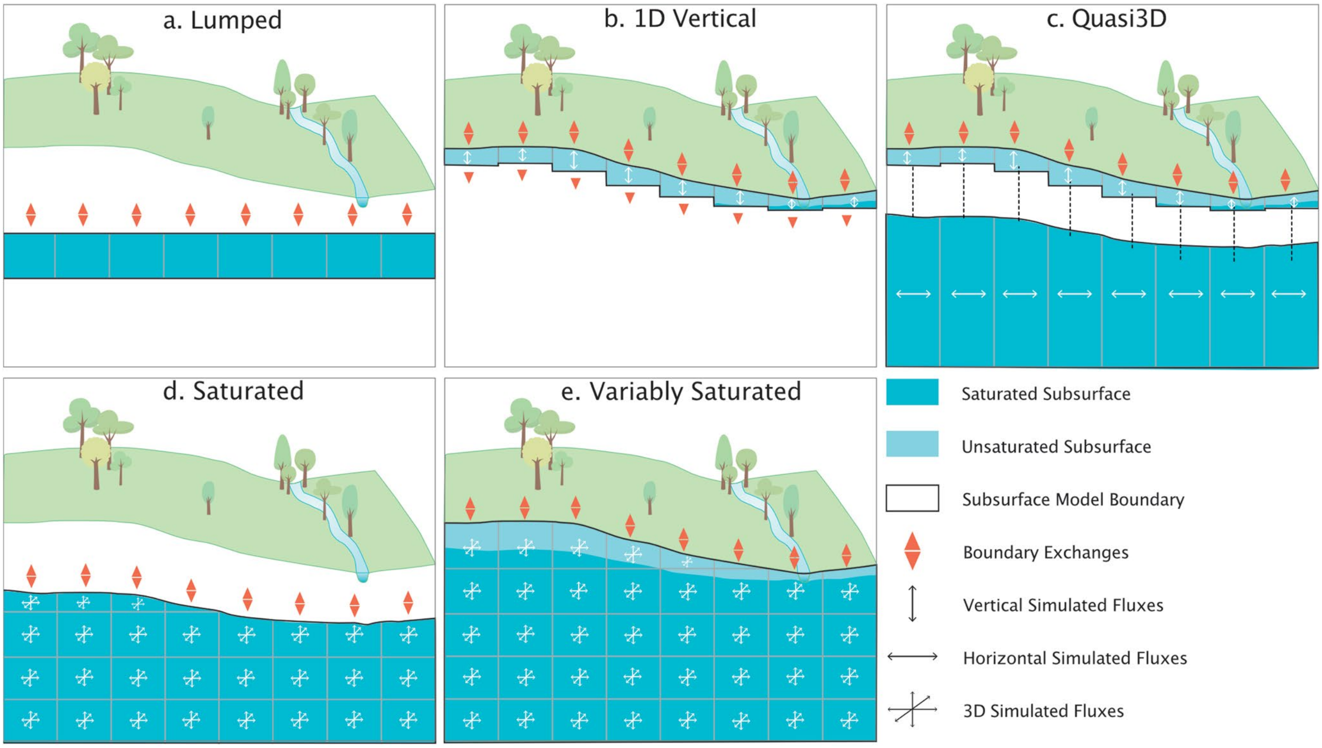

Figure 4. Conceptual illustration of the different approaches to groundwater simulation which are employed in continental to global scale models.

5.3. Groundwater Flow Model

Existing groundwater simulation approaches applied at the continental to global scale generally fall into four categories (illustrated in Figure 4):

1. **Steady state models:** Static groundwater configuration based on the long-term balance of recharge and discharge.
2. **Saturated flow models:** Saturated groundwater flow (i.e., from the water table down). Recharge from the land surface and exchanges with surface water bodies are included in these models primarily as upper boundary conditions.
3. **Quasi-3D models:** Commonly applied in land surface and earth systems models, these approaches simulate variably saturated vertical flow in the soil column combined with a dynamic water table lower boundary condition.
4. **Variably saturated flow models:** Variably saturated flow three-dimensional flow throughout the entire subsurface.

Each of these approaches has been applied with multiple modeling platforms and coupling strategies. In many cases the groundwater model is coupled or integrated with a land surface, vegetation or atmospheric model. It is outside the scope of this paper to explore in detail the myriad of earth systems model and coupling approaches. Rather here we focus specifically on the groundwater simulation portion of these models summarizing each of the general approaches including their strengths and weaknesses and the current state of their application at continental to global scales. For additional details on model capabilities and types we also refer the reader to Gleeson et al. (2021) who provide a classification table of large-scale groundwater models that includes a detailed breakdown of components and capabilities of different platforms.

For the purposes of this discussion we also exclude lumped groundwater storage approaches, because these are not directly simulating flow through the groundwater system in a physical way. Lumped mass balance approaches treat groundwater storage as a simple storage reservoir and parameterize exchanges in and out of storage based on surface water runoff diffuse recharge and groundwater pumping. This approach was typically applied in global hydrologic models which were originally designed to assess future water availability and human water usage. However, many of these platforms have developed groundwater modules that simulate transient groundwater flow directly in recent years (see Section 5.3.2).

Our intent here is to provide an overview of the progress that has been made in continental to global scale groundwater simulation with these approaches. For those new to groundwater modeling, additional details on model approaches can be found in Appendix C in Supporting Information S1.

5.3.1. Steady State Models

Steady state groundwater models provide an estimate of static groundwater configuration. They are derived using the long-term balance between groundwater recharge and discharge and represent a hydrologic equilibrium condition. They are useful for evaluating spatial patterns in groundwater depth and groundwater surface water interactions, and can provide initial conditions for transient simulations. Steady state simulations can be derived with any of the modeling approaches shown in Figure 4. We separate them out here as a special case, and cover transient simulations by modeling approach in the following subsections.

One of the first published efforts was the paper of (Fan et al., 2013) who presented a high-resolution global map of groundwater depth. The map is based on simulations with a steady state groundwater parameterization in a land surface model. Their model assumes saturated unconfined systems using the Dupuit-Forcheimer approximations of 2D flow (i.e., horizontal groundwater flow where discharge is proportional to aquifer thickness). For the hydrogeologic properties Fan et al. (2013) assumed exponential decay of permeability with depth based on surface permeability derived from (Gleeson et al., 2011) and topographic slope, and calibrated the rate of decay using observed groundwater data. This global groundwater level map is often treated as a data set, but we include it here because the mapping actually relies on a groundwater model.

Subsequently, de Graaf et al. (2015) built a global steady-state groundwater model at 6' resolution using MODFLOW and a previously developed aquifer depth model as input. Groundwater recharge and surface water levels needed to force the groundwater model were obtained from the global hydrological model PCR-GLOBWB (van Beek et al., 2011). This approach also assumes a single layer unconfined system and simulates saturated groundwater flow similar to Fan et al. (2013).

Maxwell et al. (2015) built a steady state groundwater model for the Continental United States (CONUS) at 1 km lateral resolution using the integrated hydrologic model ParFlow. This model differs from previous steady state simulations because the model uses Richards' equation to simulation 3D variably saturated flow. Additionally, the model had five vertical layers, capturing additional complexity in soil and geologic parameters. This model was used to evaluate patterns in groundwater residence time (Maxwell et al., 2016) and spatial drivers of groundwater configuration (Condon et al., 2015; Condon & Maxwell, 2015).

5.3.2. Saturated Flow Models

Transient saturated flow models use Darcy's law to simulate saturated groundwater flow (i.e., flow below the water table) dynamically. These approaches explicitly resolving lateral fluxes in the subsurface, and can therefore capture groundwater convergence and lateral redistribution of moisture in the subsurface not possible with groundwater storage models. MODFLOW is the most widely known and applied saturated groundwater flow model (Hughes et al., 2017). Because saturated flow models focus on the flow below the water table, they require parameterized exchanges or fluxes for groundwater recharge and discharge as boundary conditions. Increasingly, saturated flow models such as MODFLOW and GSFLOW incorporate these recharge and discharge processes using coupled modules instead of imposing them via boundary fluxes for example, Markstrom et al. (2008).

de Graaf et al. (2017) developed the first transient global MODFLOW model. This work builds from the steady state simulation presented in de Graaf et al. (2015) expanding to include a two-layer hydrogeological schematization (aquifers and confining layers) and a transient simulation of groundwater heads. de Graaf et al. (2017) used this model to assess global groundwater depletion as a result of groundwater over-abstraction. More recently a two-way coupled model version (between MODFLOW and PCR-GLOBWB) was used to globally estimate the effects of groundwater withdrawal on environmental streamflow (de Graaf et al., 2019). Additionally, Reinecke et al. (2019) developed another global saturated flow model called G^3M, developed specifically for the WaterGap global hydrology model. This model takes a gradient based approach similar to de Graaf et al. (2015) but uses its own groundwater flux model, as opposed to MODFLOW.

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5.3.3. Quasi-3D Approaches

Land surface models (LSMs) and earth systems models (ESMs) were designed to simulate fluxes from the land to the atmosphere. Here, Richards' equation is generally implemented vertically in a 1D isolated column with variable vertical discretization commonly increasing from top to bottom from 10^{-2} to 10^{0}m and extending only to shallow depth on the order of meters. This type of implementation is based on the assumption that over large lateral spatial scales of a computational grid cell on the order of 10^{-1} to 10^{2} km^{2}, lateral shallow flow can be neglected, and vertical flow can be effectively simulated by a 1D column representing the average dynamics over large spatial scales. Traditionally a free gravity drainage lower boundary condition was applied. However more recently there have been increasing efforts to include groundwater representation to this lower boundary. These approaches generally maintain 1D vertical exchanges through the soil column but replace the lower boundary condition with a single layer aquifer model to represent water table depth (e.g., Lo & Famiglietti, 2010, 2011; Niu et al., 2007).

Such methods have also been used to connect land surface model-based groundwater parameterizations into regional atmospheric models to interrogate potential feedbacks, mainly at the continental scale (Anyah et al., 2008; Barlage et al., 2015; Niu et al., 2007; Schlemmer et al., 2018; Seuffert et al., 2002; York et al., 2002). This is an active research area with a myriad of model platforms and coupling strategies. We refer the reader to Clark et al. (2015) and Fan et al. (2019) for a more detailed summary of modeling approaches in LSMs and ESMs. Still, there remain significant limitations to current approaches. Comparing different global models with various GRACE products, Scanlon et al. (2018) provided a quite sobering view of the skill of current land surface models incorporating groundwater parameterizations. They showed that land surface models generally under or overestimate storage changes and have difficulties in reproducing long-term storage trends. Note however, that none of the models included in the analysis of Scanlon et al. (2018) included a groundwater flow model.

5.3.4. Variably Saturated Flow Models

Similar to saturated flow models, variably saturated flow models (generally referred to as integrated models) can simulate lateral groundwater flow for confined, unconfined and semi-confined conditions and incorporate aquifer heterogeneity in three-dimensional space. The key difference with these approaches is that they simulate the entire subsurface (both above and below the water table) using Richards' equation to handle variably saturated flow. This approach is more robust for capturing groundwater recharge and dynamic interactions between groundwater, soil moisture and streamflow. However, it is also more computationally expensive than saturated flow approaches. There are a number of integrated groundwater models including CATHY (Paniconi & Wood, 1993), HydroGeosphere (Therrien & Sudicky, 1996), and ParFlow (Kollet & Maxwell, 2006).

There are no integrated global groundwater models at this point, but several continental scale models have been developed using ParFlow. Transient simulations have been developed at 1 km resolution for the Contiguous US building from the steady state ParFlow model (Maxwell et al., 2015) and coupling with the CLM land surface model. PF-CONUS has been used to study multi-scale groundwater-evapotranspiration feedbacks (Maxwell & Condon, 2016), hydrologic impacts of large scale groundwater depletions (Condon & Maxwell, 2019), and the role of groundwater in warming systems (Condon, Atchley, & Maxwell, 2020; Condon, Markovich, et al., 2020).

(Keune et al., 2016) constructed an integrated model for Europe coupling ParFlow to a land surface and atmospheric model. By incorporating an atmospheric model, they were able to directly investigate connections from the bedrock to the atmosphere. Keune et al. (2016, 2018) demonstrated the mitigating impact of groundwater on the 2003 heatwave and the systematic redistribution of water resources due to human water use. The European model by Keune et al. (2016) was also implemented in an experimental monitoring/forecasting system producing real-time predictions of water flows and stores of the critical zone from groundwater across the land surface into the atmosphere (Kollet et al., 2018). Zipper et al. (2019) also used this model to demonstrate the role of groundwater and land use changes on drought over Europe in an ensemble modeling approach.

6. The Path Forward

We envision a Global Groundwater Platform that will combine observations and models to provide spatially and temporally continuous and consistent groundwater monitoring and prediction. We argue that such a system is needed to address the critical gaps in our understanding and predictive capacity of the terrestrial hydrologic cycle outlined in Section 2. For example, fully coupled groundwater-to-atmosphere ensemble retrospective forecasts carried out using different configurations (e.g., hydrogeological settings) would represent a viable way to explore the underlying mechanisms that explain two-way feedbacks between global groundwater states and natural modes of variability such as ENSO, which are dominant sources of sub seasonal-to-seasonal predictability. The proposed framework will also provide the opportunity to assess the impact of long-debated issues in groundwater modeling (e.g., scaling with grid resolution and uncertainty characterization) on the quality of the atmospheric forecasts. Additionally, the sustainable management of groundwater resources is key to resolving future challenges of global food and energy security in a world subject to population growth and climate change. A consistent global groundwater framework is essential to global assessment of the effects of adaptation measures that are mostly local in nature. Ultimately, this platform can help unlock the potential of groundwater as a source of predictability in operational weather systems, and produce valuable information to a new and wider range of decisions related to the water management, agricultural, and energy sectors.

As outlined in Section 4 we have identified four key components for the Global Groundwater Platform. Here we re-iterate these components and the essential elements that will be needed for a successful GGP.

1. Hydrogeologic Model: We require a globally consistent hydrogeologic framework which can provide the necessary hydrologic parameters for groundwater simulation at multiple spatial scales. This model must be three dimensional providing consistent spatial information at depth and it must adhere to standard metadata formats. A successful platform will be easily updated and closely linked with the other parts of the platform to facilitate model inversion and calibration across different domains and for flexible model grid configurations.
2. Groundwater Observation Platform: A global groundwater level database needs to be established including all historic records available today and providing for automatic ingestion of ongoing temporal observations. This will require coordination with myriad of agencies currently collecting this data, both for data gathering and to ensure consistent metadata standards that can facilitate global analysis. In addition to direct groundwater observations the GGP will need direct connections to exiting observations networks for other parts of the physical system as well as human activities.
3. Groundwater Flow Model: To facilitate all of the goals outlined above the groundwater flow model must be able to capture three-dimensional flow in the subsurface at multiple spatial scales and resolutions. It should be connected to land surface and overland flow processes and must include both shallow and deep groundwater systems to encompass connections between shallow and deep groundwater systems as well as human pumping. The flow model must be able to incorporate human operations and should be designed to be closely connected with the observation platform and the hydrogeologic model.
4. Cyberinfrastructure: The first three components listed here will require significant computational power, data storage and analysis capabilities. The groundwater observation and monitoring system will require cyberinfrastructure for real time in automated groundwater level measurements, wireless data streams and automated quality control. The data streams must be connected via networks having the necessary carrying capacity and minimal latency to the supercomputer infrastructure where modeling and data assimilation is performed. In Section 4, we summarized some rough estimates of the demands of the groundwater modeling platform. There would be multiple approaches to building and managing this in a distributed fashion (e.g., splitting up continental models). However, significant community design will be needed to ensure a globally consistent and interoperable system and any successful approach will need to efficiently leverage modern HPC architectures and best software development practices.

The requirements outlined above may appear lofty; however, we would like to emphasize that significant progress has already been made in each of these areas. As outlined in Section 5, the interest in global groundwater simulation and observation has been increasing, and there are multiple ongoing efforts to expand our modeling and observation capabilities. There are community data collection efforts, such as the European Groundwater Drought Initiative (Bloomfield et al., 2018), and the IGRAC Global Groundwater Information System; as well as model intercomparison and development projects, such as WaterMIP (Haddeland et al., 2011), GEWEX-ISMC, and ISI-MIP (Warszawski et al., 2014). What is critically lacking in these efforts is an organized community effort to pull all of the required data and modeling elements together in a consistent platform. Many of these efforts remain siloed among communities, and as a result, synergies that can result from closer collaboration between the modeling and observation communities are missed. Additionally, because we lack consistent model and metadata standards, it remains difficult and time consuming to build community resources for model evaluation, and prediction. A framework for global groundwater model evaluation is proposed by Gleeson et al. (2021) to address some of these challenges. We also see a divergence in the modeling community that is building global models and many hydrogeologists and regional groundwater modelers. We need better connections across these groups so that the Global Groundwater Platform uses consistent research and best practices that have been established through decades of groundwater modeling at the local and regional scale.

We propose here that the GGP community needs to include not just global groundwater modelers working with land surface and atmospheric modelers, but also hydrogeologists, data holders, water managers, and software engineers. Ideally, we would have leaders and sub teams for each of the major platform components that can work together on design and integration. One of the first major requirements is to define metadata standards for both observations and the hydrogeology model. Additionally, we will need to work together to establish shared infrastructure that can be used to start constructing and managing the platform.

While the implementation of the technology requires considerable investments at the national and international level, the scientific, societal, and economic return of a Global Groundwater Platform is certainly higher. Commensurate technologies have been applied operationally for decades in the large atmospheric forecasting centers. We suggest that by 2022, when Groundwater is the theme of World Water Day, we will have set up the framework for a global groundwater monitoring and prediction system. This requires scientists, data holders, modelers, national and international organizations to collaborate and pull resources and data together.

Data Availability Statement

No new data are presented in this review paper.

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