GroMoPo: A Groundwater Model Portal for Findable, Accessible, Interoperable, and Reusable (FAIR) modeling

Authors: Sam Zipper[1], Kevin M. Befus[2], Robert Reinecke[3], Daniel Zamrsky[4], Tom Gleeson[5], Sacha Ruzzante[5], Kristen Jordan[1], Kyle Compare[6], Daniel Kretschmer[3,7], Mark Cuthbert[8], Anthony M. Castronova[9], Thorsten Wagener[7], Marc F.P. Bierkens[4,10]

Author affiliations:
1. Kansas Geological Survey, University of Kansas, Lawrence KS, USA
2. Department of Geosciences, University of Arkansas, Fayetteville, AR USA
3. Institute of Geography, University of Mainz, Mainz, Germany
4. Department of Physical Geography, Utrecht University, Utrecht, The Netherlands
5. Department of Civil Engineering, University of Victoria, Canada
6. Department of Earth, Ocean & Atmospheric Science, Florida State University, Tallahassee, FL, USA
7. Institute of Environmental Sciences and Geography, University of Potsdam, Germany
8. School of Earth & Environmental Sciences, Cardiff University, UK
9. Consortium of Universities for the Advancement of Hydrologic Sciences, Inc
10. Deltares, Unit Subsurface and Groundwater Systems, Utrecht, The Netherlands

Author ORCID IDs:
SZ: 0000-0002-8735-5757
KMB: 0000-0001-7553-4195
RR: 0000-0001-5699-8584
DZ: 0000-0001-6046-688X
TG: 0000-0001-9493-7707
SR: 0000-0003-4569-0183
KJ: 0000-0002-7491-7490
KC: 0000-0001-6655-8195
DK: 0000-0003-0115-1268
MC: 0000-0001-6721-022X
TC: 0000-0002-1341-5681
TW: 0000-0003-3881-5849
MB: 0000-0002-7411-6562

1. Problem: Data is increasingly FAIR, but groundwater models are not

Groundwater systems are threatened worldwide by stressors including climate change, land use/land cover change, contamination, and water use (Gleeson et al. 2020). In many locations, numerical groundwater models have been developed to understand how these stressors and other processes impact water resources, to develop suitable management strategies, and to gain scientific insights about the drivers of change in groundwater quantity and quality. These groundwater models and their simulations are an incredible source of groundwater knowledge due to the many activities involved in model creation. Building a model requires developing one or more conceptual (or perceptual) models of dominant processes affecting groundwater system behavior (Enemark et al., 2019); synthesizing diverse datasets describing hydrostratigraphy, hydrology, climate, and human activities; and developing a mathematical representation of the groundwater system that can reproduce diverse observational data and guide management decisions (Hill and Tiedeman 2006; Wagener et al. 2021).

Effectively harnessing the knowledge embedded in groundwater models can help address humanity's groundwater sustainability challenges from local to global scales. Because the model-building process includes subjective choices and decisions based on regional expert experience, a groundwater model includes knowledge not captured by available datasets, and a synthesis of best understanding of how water resources would respond to stress. Extending the use of groundwater modeling efforts beyond the single or handful of studies they were originally designed for requires that models be FAIR - Findable, Accessible, Interoperable, and Reusable (Stall et al. 2017). FAIR models would enable meta-analyses and intercomparisons, promote more robust and consistent documentation, and avoid duplication of efforts through enhanced discoverability (Reinecke et al. 2022), acknowledging that re-use of models outside their original design purpose requires careful consideration of the transferability to other purposes (Doherty and Moore 2020). Strides have been made by funding agencies and journals, and FAIR data are now required for many grants/publications, rapidly becoming a community standard (Hall et al. 2022).

While data has become more FAIR, in our experience, the sharing of groundwater models is lagging behind in the academic community and rarely meets these standards (with some organizations, like the US Geological Survey, the Geological Survey of Denmark and Greenland, and the consortium of the Dutch Hydrological Instrument as notable exceptions). We speculate that there are multiple interconnected reasons for this, including that: (i) many models are developed for site-specific investigations or without a scientific research focus, for example, those developed for environmental assessment projects, and therefore are never published in the peer-reviewed literature; (ii) models may also contain proprietary intellectual property and/or private information (Zipper et al. 2019); (iii) models often require large input/output files that are challenging to archive; (iv) some numerical models require proprietary software (Zipper et al. 2022); (v) incentive structures in the academic system are not designed for common-good activities such as model sharing (Verbeke 2023); and (vi) those models that do get published are challenging to find due to the ever-increasing rate of publication (Stein et al. 2022). In sum, we

estimate that globally between 330 and 540 journal articles describing groundwater models are published (findable) every year (see Supplemental Information), but almost none of these models are fully FAIR.

2. Solution: A community-driven Groundwater Model Portal (GroMoPo)

To promote the FAIR dissemination of groundwater models, we developed an open-source Groundwater Model Portal (GroMoPo; www.gromopo.org) We envision GroMoPo as a community-driven resource for sharing and finding existing numerical groundwater models and information about those models. By developing this resource, we provide a tool for the groundwater community to harness the knowledge embedded in groundwater models and move towards FAIR modeling practices.

On its main page, GroMoPo includes a map display that allows users to explore a growing compilation of groundwater models around the world (Figure 1a). Polygons denote the locations of known groundwater models based on either the active extent of the model or a bounding box based on the model coordinates. Overlapping models are clustered to improve viewability at low zoom levels. Clicking on a model extent provides a pop-up box with model metadata including the model authors, publication details, spatial scale, year of development, and other information. Currently, the GroMoPo database has 487 models that span 103 countries, 65% of which are built using U.S. Geological Survey MODFLOW code and 76% covering a domain smaller than 10,000 km^2.

To add data to GroMoPo, there is a separate 'Submit Model' page with a data entry form (Figure 1b). The entry form has a limited number of required fields such as publication name, model location, authors, model platform, and model characteristics. There are additional optional fields that allow the user to include more information, for example related to model boundary conditions. For FAIR data storage and retrieval, GroMoPo is linked to the CUAHSI HydroShare repository (https://www.hydroshare.org/) via a resource submission with a 'GroMoPo' tag. This resource is immediately available in HydroShare, but has a flag indicating the submitted information has not yet been verified. Once a GroMoPo community volunteer checks the resource, the model is flagged as verified. Approximately weekly, a HydroShare Python API script compiles all tagged GroMoPo resources as a single HydroShare resource (http://www.hydroshare.org/resource/114b76f89d1c41c38e0e235443c7544c) and uses this to populate the GroMoPo map. GroMoPo is distinct from repositories such as HydroShare in that it's role is to collect and share model metadata for searching and discoverability purposes, rather than storing model input/output files. For long-term storage of model files, users are encouraged to deposit model input and output files in a repository such as HydroShare and link these to their GroMoPo entry for complete reproducibility, though GroMoPo can also connect with other model storage locations such as institutional websites.
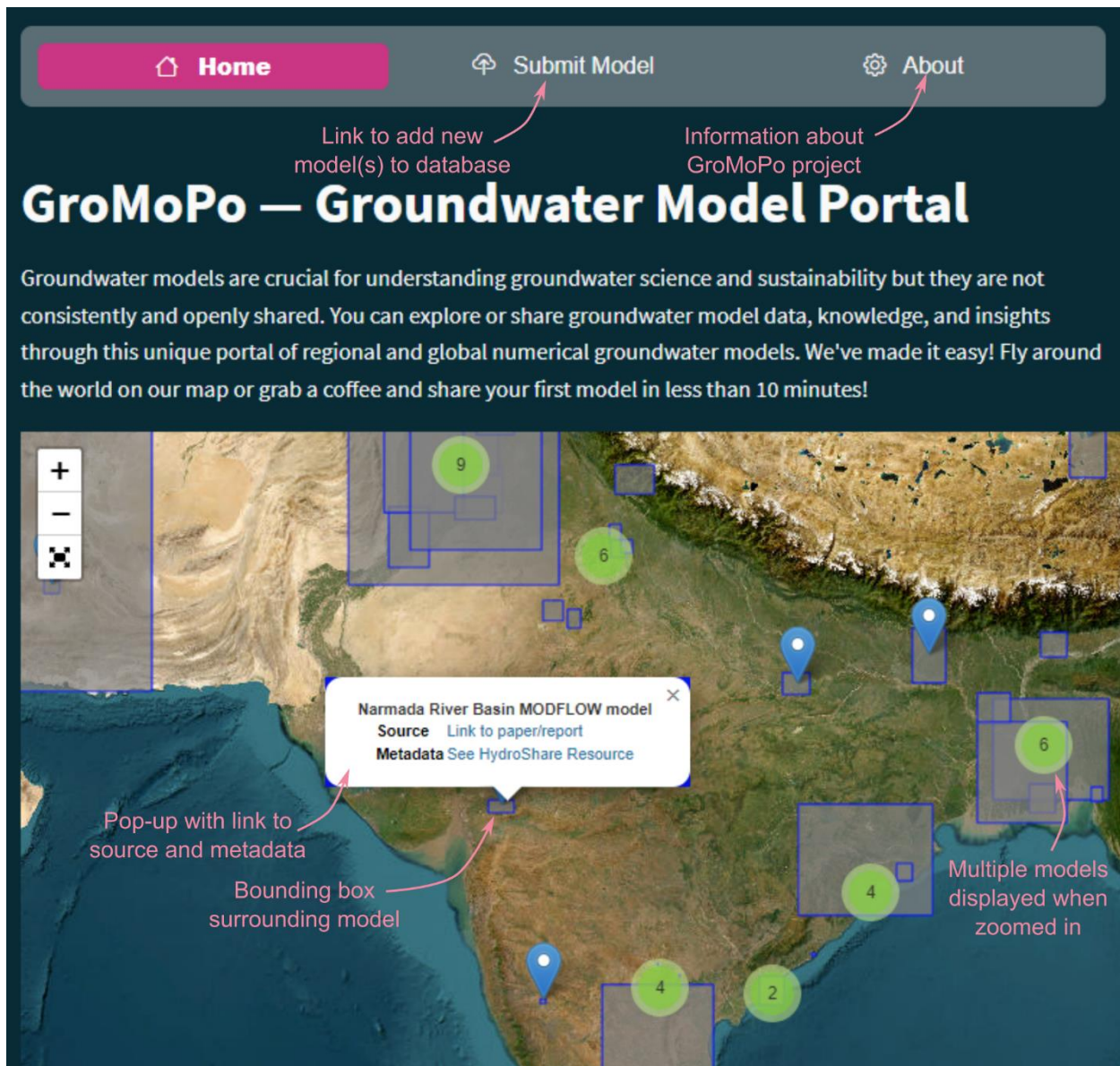
Figure 1. Screenshot of web app zoomed in to Northern India and surrounding region.

We envision GroMoPo as a resource developed and maintained by the groundwater modeling community with both contributions from, and benefits to, diverse groups (Figure 2). As the core of GroMoPo is a database of groundwater models, **groundwater modelers** are the primary contributor of model metadata to the database. Anticipated benefits to model creators include increased visibility and discoverability of their efforts, a better ability to find other models from similar hydrogeological settings for guidance and to evaluate transferability, and an ability to determine if groundwater models have already been created for a region of interest to serve as a starting point for developing models in new or related areas. For **educators**, GroMoPo provides a resource to find models for instructional purposes and in-class examples allowing students to explore the diverse approaches used for representing groundwater systems around the world. These educators, in turn, could contribute to the broader use of GroMoPo by sharing their

lesson plans on a platform such as HydroLearn that use the database for other members of the groundwater community. For **researchers outside the groundwater community**, GroMoPo would provide a community-curated platform to find models and groundwater information for specific regions under investigation, which would allow them to better incorporate local hydrogeological conditions into their work. For example, ecologists working on groundwater-dependent ecosystems may require information about local groundwater conditions and sources, and by linking these studies to models through GroMoPo we can elevate the diverse connection between groundwater science and other disciplines in both the physical and social sciences (Huggins et al., 2023).

More broadly, the **groundwater community** as a whole (including modelers, field investigators, data scientists, and the many other roles in our discipline) will benefit from GroMoPo through the opportunities it presents for improved groundwater understanding and science. For example, GroMoPo would enable a field investigator to discover existing groundwater models of a region to identify areas with poorly understood hydrogeological conditions to prioritize data collection during a field investigation. Conversely, meta-analysis and synthesis of the GroMoPo database would allow groundwater modelers to gain a better understanding of current groundwater modeling practices, strengths, and weaknesses. Additionally, as the GroMoPo database continues to grow, it will help spotlight the current scope, distribution, and characteristics of groundwater models, both emphasizing the worldwide importance of groundwater science as well as revealing understudied conditions and regions that merit future research. In sum, this will create new short-term and long-term scientific research trajectories (Table S1) that will help the community better understand current groundwater modeling approaches, areas for needed improvement, and ways to serve society.
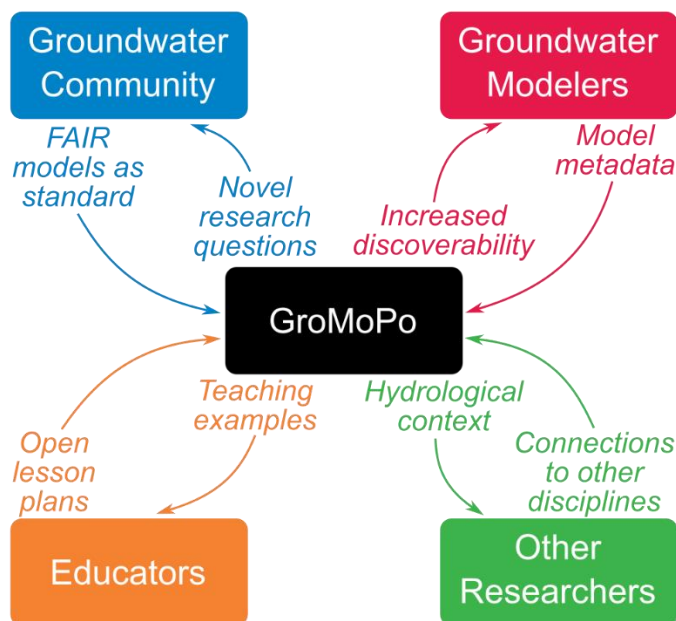

Figure 2. GroMoPo anticipated contributions from (inwards arrows) and benefits to (outwards arrows) different groups.

3. Future: Where could the community go from here?

The vision laid out above is ambitious but necessary to advance groundwater science to FAIR status and more effectively integrate with fields outside our disciplinary boundaries. To achieve these goals, the groundwater community needs to set and enforce an expectation that models will be open and reproducible (Figure 2). This can be done by diverse mechanisms, but will likely include sharing requirements enforced by journals, institutions, and funding agencies (Verbeke 2023). This requirement does not need to be onerous: GroMoPo data entry is designed to take less than 15 minutes yet provide immense value collectively. Additionally, it will require the incorporation of a much larger database of existing groundwater models, some of which are already in organizational databases, for example with various geological surveys. The 487 models currently included in GroMoPo were identified through a keyword search on Web of Science. During this timeframe, an additional 330-540 potential model publications were published (see SI), indicating that potential groundwater models are being published at a rate of 1-2 per day - far exceeding the abilities of any one person or team to incorporate into GroMoPo. Additionally, the current version of GroMoPo remains in development with future priorities including improved model search and filtering processes, improved map funtionality, and migrating to community hosting platforms. Harnessing the collective knowledge of our community that is embedded in groundwater models will require a true community effort and we hope that you, the reader, will pitch in. Please visit us on the web (www.gromopo.org) to join the effort!

4. Acknowledgments

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5. Department of Civil Engineering, University of Victoria, Canada
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8. School of Earth & Environmental Sciences, Cardiff University, UK
9. Consortium of Universities for the Advancement of Hydrologic Sciences, Inc. (CUAHSI), Arlington MA, USA
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Groundwater model search process: The Web of Science search was conducted on title, abstract, author keyword, and Keywords Plus® fields using 52 search strings separated by OR operators. The terms included variations of "groundwater model," "hydrogeologic model," "groundwater * transport model," "saltwater intrusion model," "numerical model + groundwater", "finite (difference|element|volume) model + groundwater," "aquifer model," and 24 groundwater modeling software names. The search terms and up-to-date results can be viewed (with a Web of Science subscription) here. As of February 8, 2023, this search identified 17,773 records. The 100 latest records were screened, and 37 were deemed relevant (they described groundwater models). We thus estimate that $37 \pm 9\%$ of the records identified by this search are relevant. An average of 1170 records are found for the past 5 years (2018 - 2022), suggesting that between 330 and 540 models are published yearly.

Research questions enabled by GroMoPo

Table S1. A non-exhaustive list of potential near-term and long-term research questions that are enabled by a robust groundwater model database.

Near-term research questions	Long-term research questions
☆ How do current models span different hydrogeologic environments, geologies, calibration/evaluation targets, model codes, purposes, and other variables?	☆ How does the depth distribution of the water table vary at different model scales and different environments?
☆ Which groundwater depletion hotspots are covered in regional models?	☆ How do the groundwater-surface water fluxes compare at different model scales and different environments?
☆ How do socioeconomic conditions affect the density of groundwater models and type of science questions addressed?	☆ Can integration of regional model knowledge improve continental to global estimates of transmissivity, recharge, specific yield, storativity, and other parameters?
☆ What socio-environmental variables predict the presence/absence of a groundwater model?	☆ What is the relationship between groundwater regulation and model availability?
☆ How does the density and types of observational data affect the likelihood of a groundwater model being developed there?	☆ What subjective information has been added by modelers' and where has this information been particularly valuable?
☆ How well do global hydrostratigraphic datasets agree with regional model inputs?	☆ Where do local-regional and continental-global models agree and disagree, and why?
☆ Why do people make groundwater models and how does this differ regionally?	☆ How has the complexity (processes involved, characterization of heterogeneity) and dimension (resolution) of groundwater models developed over the years and how does this relate to model accuracy and type of questions answered?
☆ How do models in transboundary aquifers differ depending on political unit?	
☆ What percent of groundwater models are FAIR?	
☆ How does the proportion of FAIR models vary regionally?	