

This is an Open Access document downloaded from ORCA, Cardiff University's institutional repository:<https://orca.cardiff.ac.uk/id/eprint/161370/>

This is the author's version of a work that was submitted to / accepted for publication.

Citation for final published version:

Zipper, Sam, Befus, Kevin M., Reinecke, Robert, Zamrsky, Daniel, Gleeson, Tom, Ruzzante, Sacha, Jordan, Kristen, Compare, Kyle, Kretschmer, Daniel, Cuthbert, Mark, Castronova, Anthony M., Wagener, Thorsten and Bierkens, Marc F.P. 2023. GroMoPo: A groundwater model portal for findable, accessible, interoperable, and reusable (FAIR) modeling. *Groundwater* 61 (6), pp. 764-767. 10.1111/gwat.13343

Publishers page: <http://dx.doi.org/10.1111/gwat.13343>

Please note:

Changes made as a result of publishing processes such as copy-editing, formatting and page numbers may not be reflected in this version. For the definitive version of this publication, please refer to the published source. You are advised to consult the publisher's version if you wish to cite this paper.

This version is being made available in accordance with publisher policies. See <http://orca.cf.ac.uk/policies.html> for usage policies. Copyright and moral rights for publications made available in ORCA are retained by the copyright holders.



Technology spotlight/

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

Sam Zipper

Kansas Geological Survey, University of Kansas, 1930 Constant Ave, Lawrence KS, 66047, USA; 785-864-0364; samzipper@ku.edu

Kevin M. Befus

Department of Geosciences, University of Arkansas, Fayetteville, AR USA

Robert Reinecke

Institute of Geography, University of Mainz, Mainz, Germany

Daniel Zamrsky

Department of Physical Geography, Utrecht University, Utrecht, The Netherlands

Tom Gleeson

Department of Civil Engineering, University of Victoria, Canada

Sacha Ruzzante

Department of Civil Engineering, University of Victoria, Canada

Kristen Jordan

Kansas Geological Survey, University of Kansas, Lawrence KS, USA

Kyle Compare

Department of Earth, Ocean & Atmospheric Science, Florida State University, Tallahassee, FL, USA

Daniel Kretschmer

Institute of Geography, University of Mainz, Mainz, Germany and Institute of Environmental Sciences and Geography, University of Potsdam, Germany

Mark Cuthbert

School of Earth & Environmental Sciences, Cardiff University, UK

Anthony M. Castronova

Consortium of Universities for the Advancement of Hydrologic Sciences, Inc (CUAHSI), Arlington, MA, USA

Thorsten Wagener

Institute of Environmental Sciences and Geography, University of Potsdam, Germany

Marc F.P. Bierkens

Department of Physical Geography, Utrecht University, Utrecht, The Netherlands and Deltares,
Unit Subsurface and Groundwater Systems, Utrecht, The Netherlands

Conflict of interest: None

Key words: groundwater models, open science, MODFLOW, reproducible research, numerical modeling, computational methods

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 (Hut, 2022). 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 Supporting Information), but almost none of these models are fully FAIR.

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 1). 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 km².

To add data to GroMoPo, there is a separate ‘Submit Model’ page with a data entry form. 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 its 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.

[INSERT FIGURE 1 HERE]

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.

[INSERT FIGURE 2 HERE]

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 functionality, 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!

Acknowledgments

GroMoPo development was supported by the Consortium of Universities for the Advancement of Hydrologic Sciences, Inc. (CUAHSI) through a HydroInformatics Innovation Fellowship to SZ along with assistance from Veronica Sosa-Gonzalez and Austin Raney. Most importantly, we want to thank all the groundwater modelers who have contributed effort, energy, and understanding to creating these useful tools.

Supporting Information

Additional Supporting Information may be found in the online version of the article, including details on the groundwater model search process and research questions enabled by GroMoPo. Supporting information is generally *not* peer-reviewed.

References

- Doherty, J., and C. Moore. 2020. Decision Support Modeling: Data Assimilation, Uncertainty Quantification, and Strategic Abstraction. *Groundwater* 58, no. 3: 327–37, <https://doi.org/10.1111/gwat.12969>.
- Enemark, T., Peeters, L.J.M., Mallants, D., Batelaan, O., 2019. Hydrogeological conceptual model building and testing: A review. *Journal of Hydrology*, no. 569: 310–329, <https://doi.org/10.1016/j.jhydrol.2018.12.007>
- Gleeson, T., L. Wang-Erlandsson, M. Porkka, S. C. Zipper, F. Jaramillo, D. Gerten, I. Fetzer, et al. 2020. Illuminating water cycle modifications and Earth system resilience in the Anthropocene. *Water Resources Research* 56, no. 4: e2019WR024957, <https://doi.org/10.1029/2019WR024957>.

- Hall, C. A., S. M. Saia, A. L. Popp, N. Dogulu, S. J. Schymanski, N. Drost, T. van Emmerik, and R. Hut. 2022. A hydrologist's guide to open science. *Hydrology and Earth System Sciences* 26, no. 3: 647–64, <https://doi.org/10.5194/hess-26-647-2022>.
- Hill, M. C., and C. R. Tiedeman. 2006. *Effective groundwater model calibration: with analysis of data, sensitivities, predictions, and uncertainty*. John Wiley & Sons.
- Huggins, X., T. Gleeson, J. Castilla-Rho, C. Holley, V. Re, and J. S. Famiglietti. 2023. Groundwater connections and sustainability in social-ecological systems. *Groundwater*, <https://doi.org/10.1111/gwat.13305>.
- Hut, R., 2022. FAIR Models. *Groundwater* 60, no. 3: 309–310. <https://doi.org/10.1111/gwat.13180>
- Reinecke, R., T. Trautmann, T. Wagener, and K. Schüler. 2022. The critical need to foster computational reproducibility. *Environmental Research Letters*, <https://doi.org/10.1088/1748-9326/ac5cf8>.
- Stein, L., S. K. Mukkavilli, and T. Wagener. 2022. Lifelines for a drowning science - improving findability and synthesis of hydrologic publications. *Hydrological Processes* 36, no. 11: e14742, <https://doi.org/10.1002/hyp.14742>.
- Verbeke, R. 2023. FAIR and Open Data requires proper incentives and a shift in academic culture. *Nature Water* 1, no. 1: 7–9, <https://doi.org/10.1038/s44221-022-00012-1>.
- Wagener, T., T. Gleeson, G. Coxon, A. Hartmann, N. Howden, F. Pianosi, M. Rahman, R. Rosolem, L. Stein, and R. Woods. 2021. On doing hydrology with dragons: Realizing the value of perceptual models and knowledge accumulation. *WIREs Water* 8, no. 6: e1550, <https://doi.org/10.1002/wat2.1550>.
- Zipper, S. C., W. H. Farmer, A. Brookfield, H. Ajami, H. W. Reeves, C. Wardropper, J. C.

Hammond, T. Gleeson, and J. M. Deines. 2022. Quantifying Streamflow Depletion from Groundwater Pumping: A Practical Review of Past and Emerging Approaches for Water Management. *JAWRA Journal of the American Water Resources Association* 58, no. 2: 289–312, <https://doi.org/10.1111/1752-1688.12998>.

Zipper, S. C., K. Stack Whitney, J. M. Deines, K. M. Befus, U. Bhatia, S. J. Albers, J. Beecher, et al. 2019. Balancing Open Science and Data Privacy in the Water Sciences. *Water Resources Research* 55, no. 7: 5202–11, <https://doi.org/10.1029/2019WR025080>.

Figures

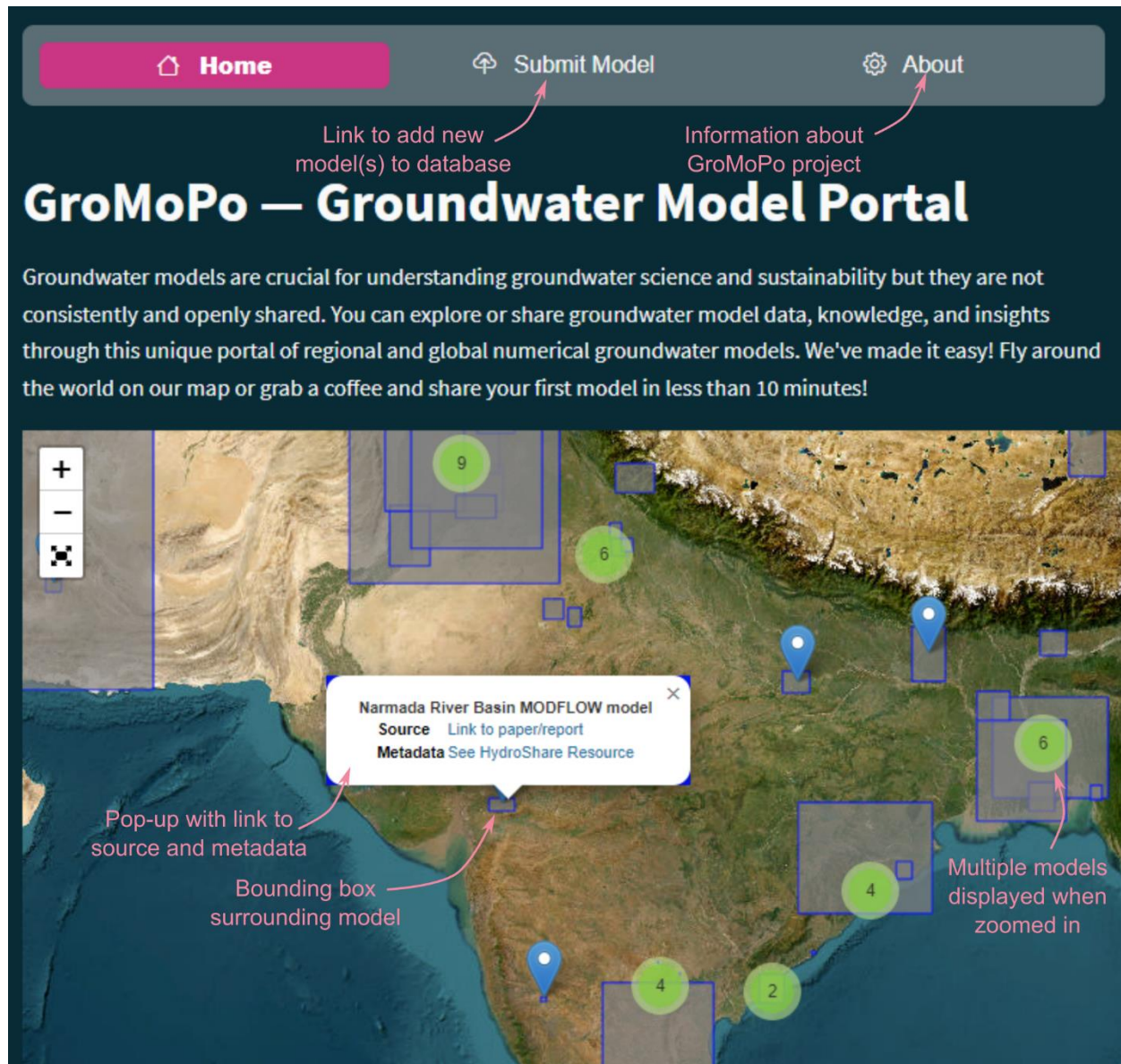


Figure 1. Screenshot of web app zoomed in to Northern India and surrounding region.

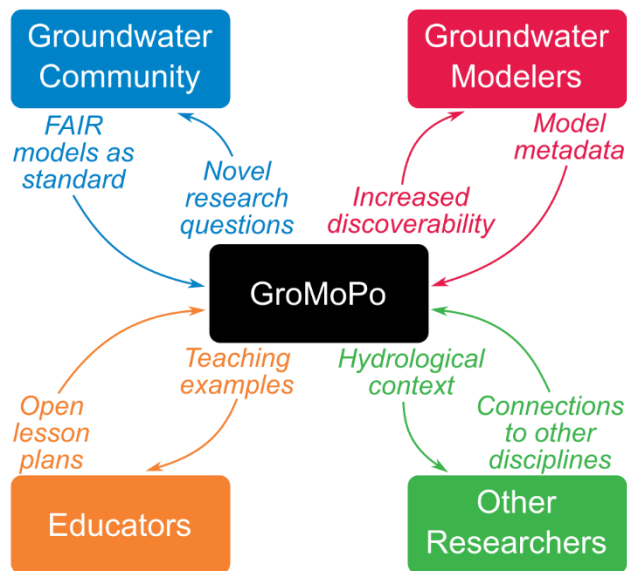


Figure 2. GroMoPo anticipated contributions from (inwards arrows) and benefits to (outwards arrows) different groups.