Representing uncertainty using diverse model ensembles: A test case in an alpine karst system

Chloé Fandel*[1], Nico Goldscheider[2], Ty Ferré[1], Zhao Chen[2]

cfandel@email.arizona.edu, nico.goldscheider@kit.edu, ty@hwr.arizona.edu, chen.zhao@gmx.de

1. University of Arizona, Dept. of Hydrology & Atmospheric Sciences
2. Karlsruhe Institute of Technology, Institut für Angewandte Geowissenschaften

Problem

Karst aquifers are difficult to model because flow through conduits, rather than pore spaces, leads to high structural uncertainty[1]. Existing models rely either on detailed conduit maps, or on averaged parameters approximating a porous medium. Neither approach is adequate for most karst systems, where conduits are unmapped, yet flow patterns are fundamentally different from those in porous media.

We are testing a new approach to modeling karst based on **generating a large model ensemble from minimal data**, then **adjusting the ensemble based on model performance**. This adjusted ensemble can then be used to project future behavior under different conditions.

Study site

The Gottesacker-Schwarzwassertal karst system (German-Austrian Alps) is a long-term study site with complex hydrogeology (fig. 1). The primary karstifiable unit in the 35 km^2 watershed is the ~100-m-thick Schrattenkalk limestone, which is strongly folded and fractured. Karst conduits drain the system into three major outlets: an estavelle (QE), the Aubach spring (QA), and the Sagebach spring (QS)[2]. Over 25 years of pre-existing data are available for this site, including geologic maps, tracer test data, cave maps, and results from previous modeling efforts (which we use as our base model)[3].

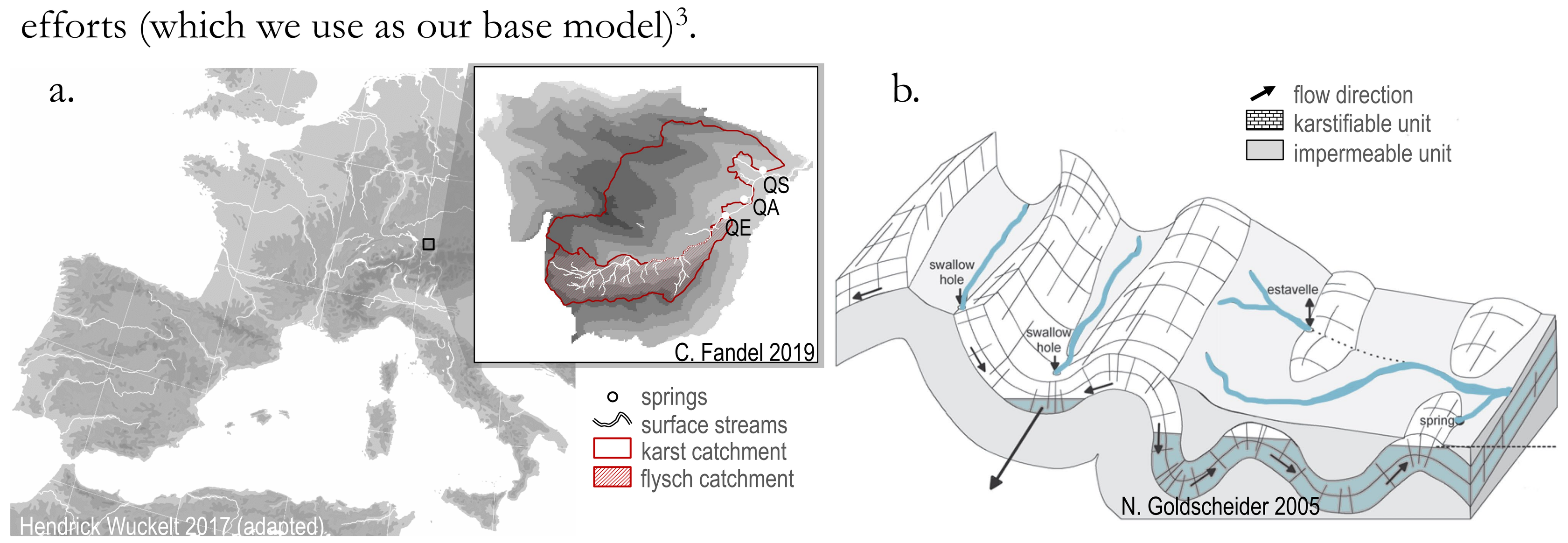

Figure 1: Site location

a. Location of the Gottesacker-Schwarzwassertal karst system, in the German-Austrian Alps.

b. Schematic diagram of the hydrogeology of the system: karst groundwater flows along the synclinal axes, which drain into a deeper zone where flowpaths can cut across the folds before emerging at springs.

Modeling approach

To generate the initial model ensemble, we set aside almost all the available data and used only basic geologic information: point locations of contacts between units, strike & dip points, and the orientation of major fracture families.

We linked three existing modeling softwares with a custom Python script (available on GitHub):

- **GemPy**[4], for 3D geologic structure (fig. 2a);
- the **Stochastic Karst Simulator**[5] (SKS), for conduit network evolution (fig. 2b);
- the **Storm Water Management Model**[6] (SWMM), for flow through conduits (fig. 2c).

Each step required making conceptual assumptions and assigning parameter values, which differed for each individual model in the ensemble. Each model can therefore be thought of as a hypothesis of the system's structure and parameters. We recorded the choices made for each model, and visualized the relatedness of models with a **tree structure** (fig. 3).

We then compared model-predicted spring discharge to observed spring discharge and calculated error metrics for each model.

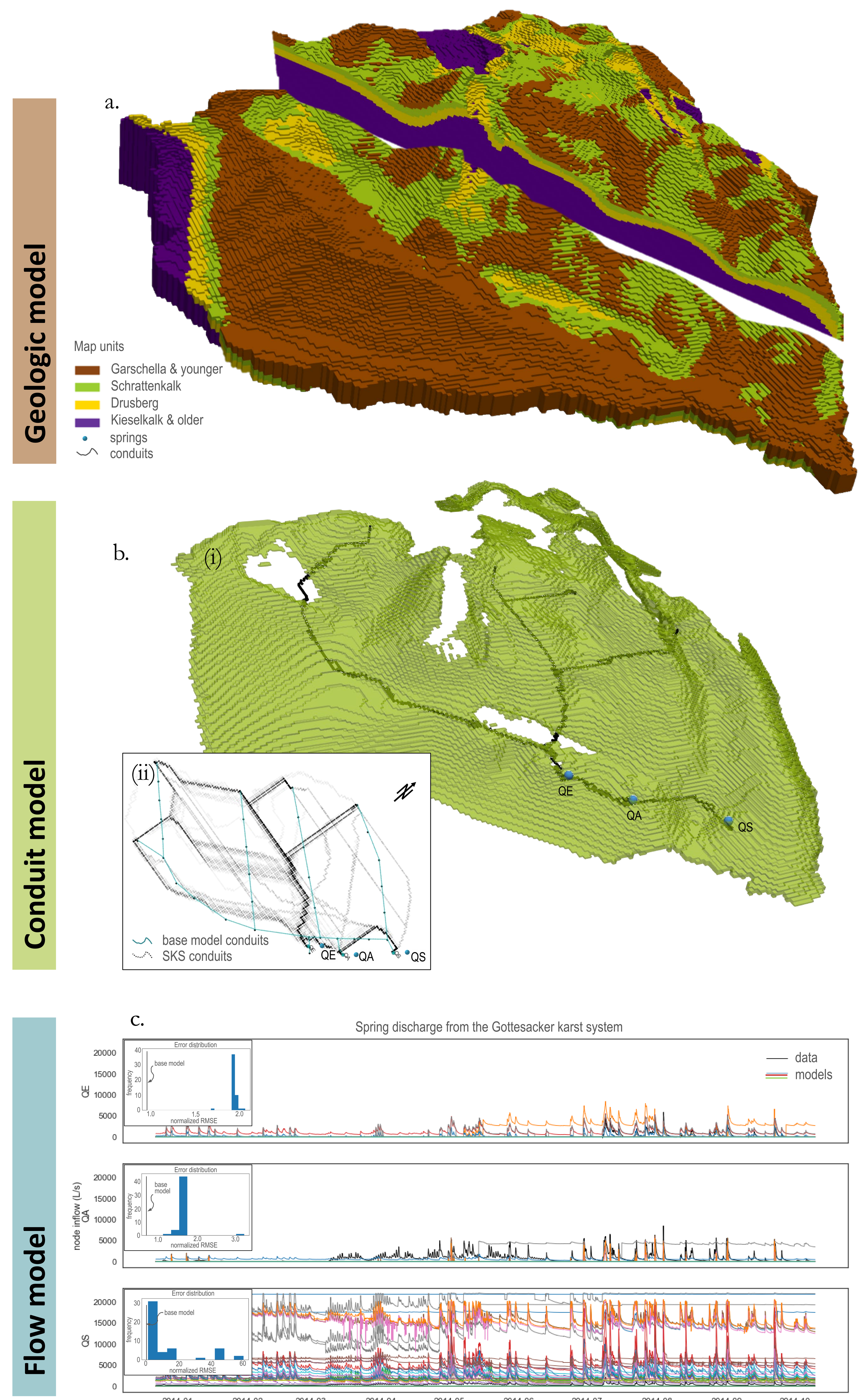

Figure 2: Modeling process

a. One realization of a 3D geologic block model of the system, created in GemPy[4].

b. (i) One realization of a conduit network, generated by the Stochastic Karst Simulator[5].

(ii) Heatmap of fifty conduit network realizations (gray), compared to the network used in the base model of the site[3] (blue).

c. Fifty predictions of spring discharge behavior (one per conduit network) with randomly-assigned flow parameters, returned by the Storm Water Management Model[6].

Choices	Order	Values to choose from
Allow branching conduits	1	yes, no
Fracture dataset	2	Goldscheider 2005, Fandel 2019
Number of fracture families	3	2, 3, 4
Fracture dominance (frac K / matrix K)	3	1, 5, 10, 20, 40, 60, 70, 80, 100
Include allogenic flysch inflow	5	yes, no

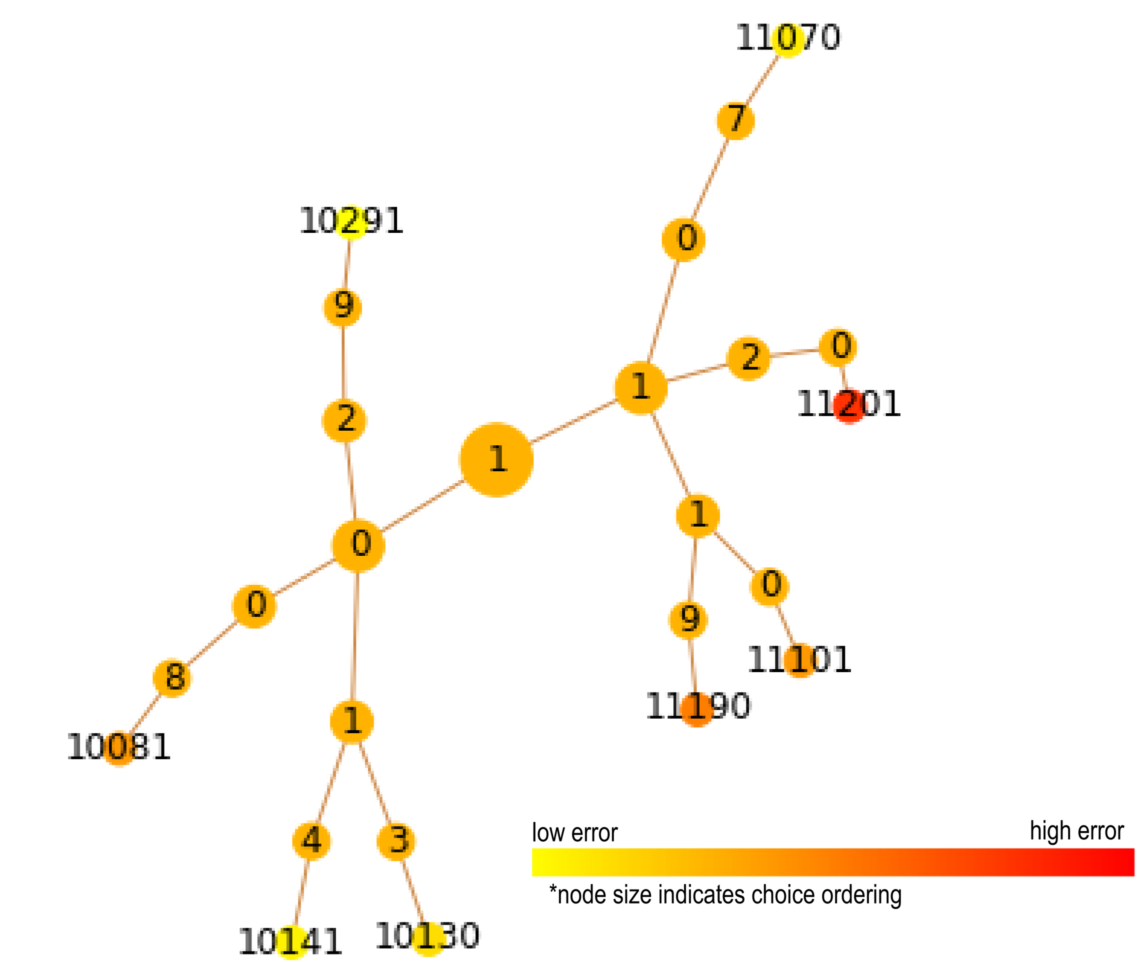

Figure 4: Model tree

Tree structure for the SKS portion of a mini model ensemble of only eight models. Each node represents a conceptual choice, with the last node on each branch corresponding to one conduit model in the ensemble. The ID string of each model records the series of choices that generated that particular model (listed in the table). A randomly-chosen set of SWMM parameters are then assigned to each conduit model. The color of the endmost nodes indicates how well that model's spring discharge predictions fit the data.

Next steps

The initial ensemble can be weighted to reflect the likelihood that each conduit network will simulate observed spring discharge behavior.

We plan to weight the ensemble using a Monte Carlo Tree Search[7], which balances exploring model space with exploiting good-fit models. Each network in the initial ensemble is run once with randomly-assigned SWMM flow parameters, and ranked by likelihood of reproducing observed spring discharge. The probability of a conduit model being selected and run again with a new set of random parameters is based on its initial likelihood. After each new run, the likelihoods of the entire ensemble are updated. At the end of the tree search process, the ensemble can be used to generate likelihood-weighted predictions of system behavior.

Questions

- Are conceptual modeling decisions fundamentally different than parameter value choices?
- Is the Monte Carlo tree search method the most appropriate/efficient way to search model space?
- Currently, many models in the ensemble are not behavioral. What strategies could increase the percentage of behavioral models?
- Precipitation inputs are calculated from only a few rain gages, but the strong elevation gradient suggests that precipitation is highly spatially variable. How could precipitation be spatially distributed?

References

1. Hartmann *et al.* 2014. Karst water resources in a changing world: Review of hydrological modeling approaches. *Reviews of Geophysics* **52**, 218–242
2. Goldscheider 2005. Fold structure and underground drainage pattern in the alpine karst system Hochifen-Gottesacker. *Eclogae Geologicae Helvetiae* **98**, 1–17
3. Chen & Goldscheider 2014. Modeling spatially and temporally varied hydraulic behavior of a folded karst system with dominant conduit drainage at catchment scale, Hochifen–Gottesacker, Alps. *Journal of Hydrology* **514**, 41–52
4. de la Varga *et al.* 2019. GemPy 1.0: open-source stochastic geological modeling and inversion. *Geoscientific Model Development* **12,** 1–32
5. Borghi *et al.* 2016. Can one identify karst conduit networks geometry and properties from hydraulic and tracer test data? *Advances in Water Resources* **90**, 99–115
6. Rossman 2015. Storm Water Management Model User's Manual Version 5.1. U.S. Environmental Protection Agency. EPA-600/R-14/413b
7. Silver et al. 2016. Mastering the game of Go with deep neural networks and tree search. *Nature* **529**, 484-489

Acknowledgements

Thank you to everyone in the KIT Dept. of Applied Geosciences for hosting me for a one-year research stay, and to Prof. Wolfgang Nowak & his research group for suggesting the Monte Carlo Tree Search approach.

THE UNIVERSITY OF ARIZONA

Karlsruher Institut für Technologie

Deutscher Akademischer Austausch Dienst
German Academic Exchange Service

Find the code here:
GitHub
https://github.com/cfandel/gottesacker