Improving understanding of groundwater flow in an alpine karst system by reconstructing its geologic history using conduit network model ensembles

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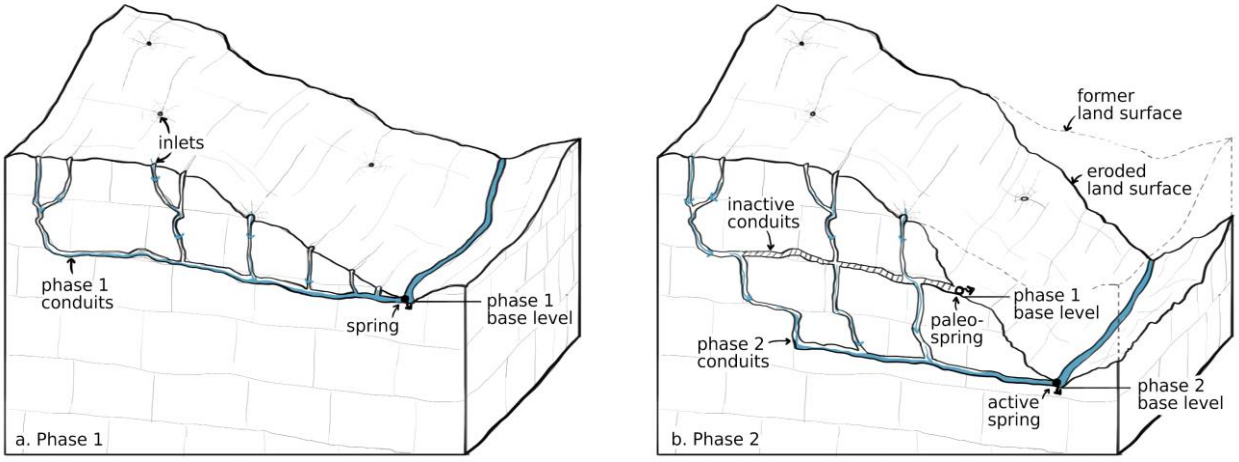
Abstract. Reconstructing the geologic history of a karst area can advance understanding of the system's present-day hydrogeologic functioning, and help predict the location of unexplored conduits. This study tests competing hypotheses describing past conditions controlling cave formation in an alpine karst catchment, by comparing an ensemble of modelled networks to the observed network map. The catchment, the Gottesacker karst system (Germany/Austria), is drained by three major springs and a paleo-spring, and includes the partially explored Hölloch cave, which consists of an active section whose formation is well-understood, and an inactive section whose formation is the subject of debate. Two hypotheses for the formation of the inactive section are: 1) glaciation obscured the three present-day springs, leaving only the paleo-spring, or 2) the lowest of the three major springs (Sägebach) is comparatively young, so its subcatchment previously drained to the paleo-spring. These hypotheses were tested using the pyKasso Python library (built on anisotropic fast marching methods) to generate two ensembles of networks, one representing each scenario. Each ensemble was then compared to the known cave map. The simulated networks generated under Hypothesis 2 match the observed cave map more closely than those generated under Hypothesis 1. This supports the conclusion that the Sägebach spring is young, and suggests that the cave likely continues southwards. Finally, this study extends the applicability of model ensemble methods from situations where the geologic setting is known but the network is unknown, to situations where the network is known but the geologic evolution is not.

1 Introduction

Mapping subsurface cave and conduit networks in karst systems provides crucial information for water resource management, hazard prevention, archaeological research, and the protection of important ecological and cultural sites. Even small-diameter conduits play an important role in groundwater flow. However, mapping conduit networks is a challenging task (Trimmis, 2018, Sellers and Chamberlain, 1998). Conduits can extend far below the surface, and speleologists attempting to explore them may experience dangers such as flash floods, falling rocks, hypothermia, and disorientation. Even in well-explored systems,

the full network is impossible to map, because small-diameter conduits (<0.5 m) are inaccessible to humans and difficult to detect by geophysical methods (Jaquet and Jeannin, 1994).

Understanding the speleogenetic processes driving cave formation and the geologic history of an area can help guide cave exploration, data collection, and groundwater resource management. Karst systems commonly evolve over time in several phases, during which different climate and geologic conditions control which parts of the system (e.g. diffuse recharge zones, focused inlets, outlets, conduits) are actively transmitting flow. Conduits or springs that see active flow during one phase of karstification may go dry when conditions change. Although these older parts of the system may become inactive, they are still open and can be reactivated during extreme flow events or when climate conditions shift again (Audra and Palmer, 2011) ~~(Figure 1)~~. An experienced geologist may be able to reconstruct how the karst system functioned in the past, and therefore predict the likely locations of presently inactive conduits. These predictions can sometimes be tested through targeted exploration of the locations where caves are suspected to exist. Some hypothesized conduits, however, may be inaccessible, making it impossible to confirm or refute their existence through exploration. In other cases, several different historical scenarios may appear equally plausible, making it difficult to determine how the system evolved. As a result, geologic intuition alone may not be sufficient to fully understand a karst area. This can lead to knowledge gaps or misconceptions that limit the reliability of future simulations of the system's behavior under projected climate or land use scenarios that differ from present-day conditions.



~~**Figure 1: Schematic illustration of two-phase karstification due to a drop in base level. (a) Phase 1: conduits form, connecting the active recharge zone to the active spring at base level. (b) Phase 2: as the base level drops due to erosion, the former spring and part of the phase 1 conduit system become inactive (they no longer transmit flow), replaced by new conduits and a lower-elevation spring. This is only one of numerous scenarios that can lead to karst systems composed of both active and inactive conduits and springs. Concept after Audra and Palmer (2011).**~~

2 Approach

This study presents a model-based approach to ~~reconstructing~~ identifying the geologic processes ~~driving~~ influencing cave formation. A real karst system was used as a test site, for which detailed cave maps are available in parts of the conduit network. While some portions of the explored cave system are very active, containing an accessible cave stream with open-channel flow that connects to a major karst spring, other portions of the explored system are now inactive, and are thought to have formed when past conditions were different from the present configuration of the system. However, two different explanations are possible: 1) glaciation obscured all of the present-day springs, leaving only the paleo-spring as the primary drainage point for the entire karst system, or 2) the lowest of the major present-day springs is significantly younger than the others, so the paleo-spring and the two uppermost springs jointly drained the aquifer system.

These competing hypotheses were tested using a computationally efficient karst network model to generate probability maps of possible conduit locations under each of the proposed past scenarios. The simulated conduit networks under each scenario were then compared with the mapped portion of the inactive cave system, to determine which scenario best matched the observed network. Finally, the analysis was extended to propose possible locations of the unmapped parts of the system.

3 Field site: Gottesacker

The modeling approach demonstrated in this study was tested on the complex, extensively studied Gottesacker karst system in the German/Austrian Alps, described in Goldscheider (2005). This 35 km^2 catchment consists of a series of plunging synclines and anticlines draining to the Schwarzwasser valley, which cuts roughly perpendicularly across the fold axes (Figure 1~~2~~). The karst aquifer lies north and northwest of the valley in a limestone unit widely exposed at the surface. It is locally overlain by sandstone and younger units, and underlain by non-karstifiable marl and older units.

This karst system is also the site of one of the longest caves in Germany, the 12 km Hölloch cave in the Mahdtal valley, which has been the subject of avid exploration and of several books and documentary films since the early 1900s (Höhlenverein Sonthofen, 2006). The local caving club has created and shared a detailed map of the explored portion of the cave. The northern part of the cave (trending SE) is active and contains a cave stream, while the southern part (trending NNW) is inactive and does not have any continuous underground drainage or cave streams.

Three major springs drain the system: an estavelle (QE, elevation 1120 m a.s.l.), the Aubach spring (QA, elevation 1080 m a.s.l.), and the Sägebach spring (QS, elevation 1035 m a.s.l.). The estavelle acts as swallow hole during low-flow conditions but acts as a spring during high-flow conditions. A paleo-spring (QO, elevation 1190 m a.s.l.) partway up the Mahdtal valley, near Höflealpe, remains dry for timespans of years to decades. In 2005, QO~~, and was only recently observed to become~~ temporarily re-activated, ~~under~~ during extreme high flow conditions (Figure 2). This is the only recorded flow event ever observed at this spring. QO is located at a geological contact between the karstified limestone aquifer and overlying low-permeability formations (sandstone and marl). Upstream from QO, the karstified limestone is exposed at the land surface, so

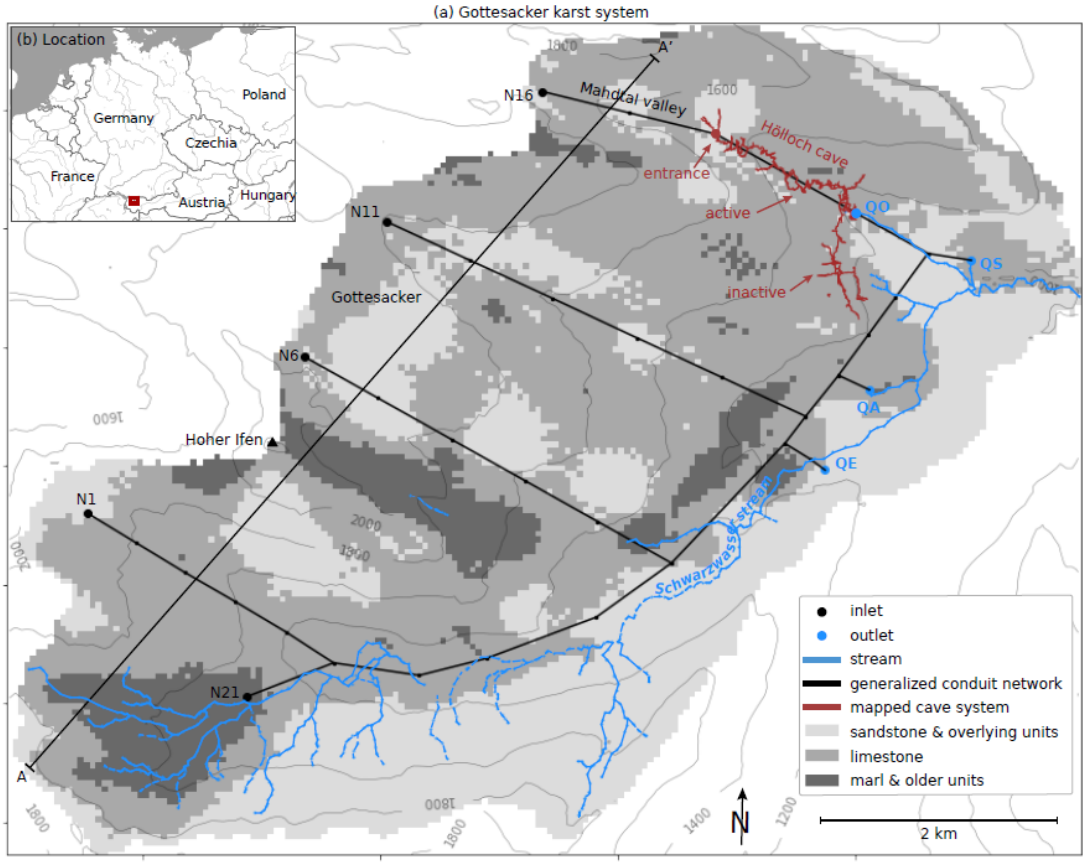
precipition infiltrates rapidly and does not generate any significant surface flow. However, since QO is located directly above and is connected to the cave stream in the conduit system beneath it, any surface water that does exceed the infiltration capacity of the karst or is injected at QO would reach the cave stream and flow to Sägebach spring (QS).

Downstream of QO, the overlying sandstone and marl in the core of the syncline confine the karst aquifer, which drains to the Sägebach spring (QS). QO can therefore act as an overflow when the discharge capacity of QS is exceeded, and large-scale backflooding occurs, as observed in 2005. In this lower part of the area, extending into the Schwarzwasser valley, the karst aquifer was (and partly still is) confined by overlying low-permeability sandstone and marl and by widespread moraine deposits.

South of the main Schwarzwasser valley, non-karstifiable flysch and marl lithology prevents conduit development, and drainage occurs instead through a network or surface streams. Several other geologic units and small springs are present, but for the purposes of conduit modeling, the geology was represented using a simplified model focused on delineating the boundaries of the karstifiable limestone unit.

The general configuration of the conduit network (referred to in the rest of this paper as the *expected network*) was originally defined by Chen and Goldscheider (2014), and refined by Chen et al. (2018), based on geologic mapping by Wagner (1950), predominant fracture orientations documented by Cramer (1959), several decades of speleological investigations by the regional caving club (Höhlenverein Sonthofen), 18 quantitative multi-tracer tests by Goldscheider (2005), Göppert and Goldscheider (2008), and Sinreich et al. (2002), and hydrogeological field observations by Goldscheider (2005). ~~Numerous previous tracer studies (Goldscheider, 2005, Goeppert and Goldscheider, 2008, Goeppert et al., 2020) have yielded a good understanding of the general configuration of the conduit network, which h~~ Anticlinal axes act as groundwater divides sectioning the region into sub-basins, each drained by a major conduit following synclinal axes. These conduits merge into a primary conduit that parallels the surface stream in the Schwarzwasser valley. This network map has been used successfully for several previous groundwater flow modeling efforts (Chen and Goldscheider, 2014, Chen et al., 2017, Chen et al., 2018, Fandel et al., 2021, Fandel et al., 2022). ~~The major karst conduits were determined to follow synclinal axes before merging into a primary conduit that parallels the surface stream in the Schwarzwasser valley~~.

~~This karst system is also the site of one of the longest caves in Germany, the 12 km Hölloch cave in the Mahdtal valley, which has been the subject of avid exploration and of several books and documentary films since the early 1900s (Höhlenverein Sonthofen, 2006). The local caving club has created and shared a detailed map of the explored portion of the cave. The northern part of the cave (trending SE) is active and contains a cave stream, while the southern part (trending NNW) is inactive and does not have any continuous underground drainage or cave streams.~~


(a) Gottesacker karst system
(b) Location
Poland
Germany
Czechia
France
Austria
Hungary
A'
N16
Mahdtal valley
Hölloch cave
entrance
active
inactive
QO
QS
QA
QE
N11
Gottesacker
N6
Hoher Ifen
N1
N21
A
Schwarzwasser stream
inlet
outlet
stream
generalized conduit network
mapped cave system
sandstone & overlying units
limestone
marl & older units
N
2 km
(c) Schematic cross-section A-A' (not to scale)
A
A'
Hoher Ifen
Gottesacker
Mahdtal valley
Schwarzwasser valley
flow direction

115

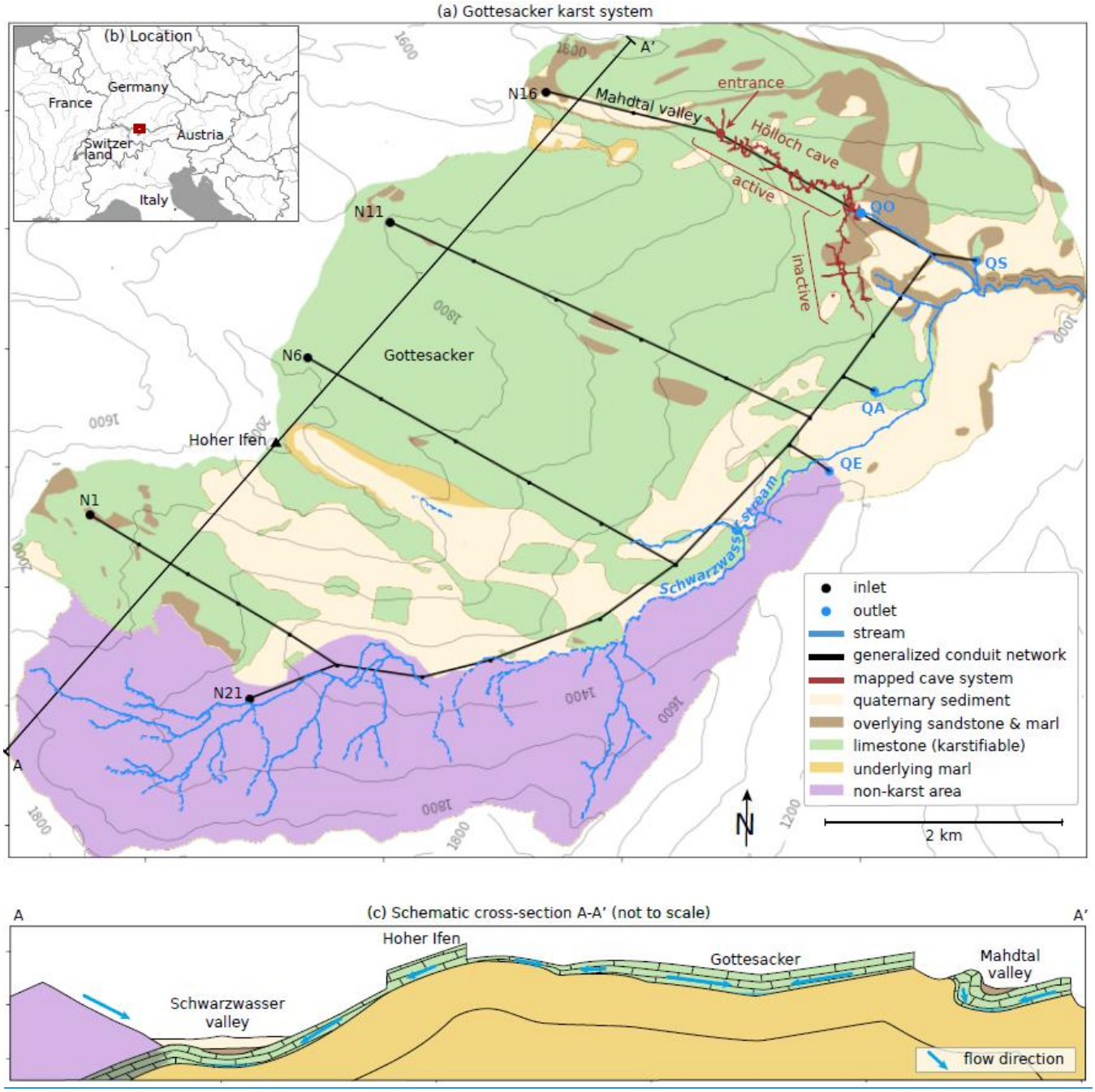


Figure 12: Overview of the Gottesacker karst system. (a) Simplified geologic ~~model~~ map ~~discretized into 50 m x 50 m pixels~~after Fandel et al. (2021). The karst aquifer is located in the limestone unit, and drains to the three springs in the lower part of the system (QE, QA, QS). The paleo-spring (QO) is only active during extreme high-flow conditions. All springs flow into the Schwarzwasser stream, shown in blue. Several small tributaries also feed the stream from the south. ~~Note: the sandstone patches are overrepresented spatially due to minor superficial modeling artifacts, which are not significant for the purposes of this study (see Fandel et al. 2021 for a detailed geologic map).~~ Outlets correspond to mapped karst springs after Goldscheider (2005). Expected c~~C~~onduit network

and inlet names ~~are model representations~~ after Chen et al. (2018) (b) Location within Europe. Basemap: ESRI. (c) Schematic cross-section along line A-A', adapted from Goldscheider (2005).

Figure 2: Two views of the paleo-spring (QO) re-activating during extreme high-flow conditions in 2005. This is the only observed flow event at this spring, which is completely dry most of the time. Photos by N. Goldscheider.

4 Hypotheses

Two different hypotheses are currently under consideration to explain the formation of the inactive part of the Hölloch cave system:

Hypothesis 1: The Schwarzwasser valley was covered by a glacier, overlying the karstifiable units up to the elevation of the paleo-spring (QO), which was the primary spring draining the entire system.

Geologic evidence: Widespread moraines and other geomorphologic evidence indicate the presence and extent of the main glacier in the Schwarzwasser valley, ~~-~~which covered all of locations of present-day valley springs (QE, QA, QS) and filled the valley up to an elevation just below the paleo-spring (QO), located approximately 200 m above the valley floor. The glacier appears to have filled the rest of the valley with roughly the same thickness of ice, creating a boundary just below and parallel to the inactive portion of the mapped conduits. There is clear geomorphologic evidence that the entrance shaft of the Hölloch cave was formed by sinking glacial meltwater, and was an active inlet during and after glaciation. The streambed created by meltwater flowing down the valley is still visible, and still channels temporary surface flows during snowmelt or intense

rainfall. End moraines further up the Mahdtal valley indicate the presence of a local glacier in the upper part of this valley, as well as in the upper part of the valley located in the breached syncline northeast of Hoher Ifen.

Hypothesis 2: Low-permeability sedimentary formations covered the Sägebach spring (QS), so the paleo-spring (QO) drained the Mahdtal valley and connected to the Aubach spring (QA), which was at the time the lowest spring in the system.

Geologic evidence: Field evidence indicates that the~~The~~ Sägebach spring (QS) is much younger than the Aubach spring (QA), but it is difficult to estimate the exact age difference. QA is located in a large ~~narrow~~gorge (hundreds of meters long and tens of meters deep), with many open fractures and cavities and a cave entrance. It is in the middle of a zone of exposed and highly karstified limestone. It does not appear to have an upper limit of discharge, and looks like a very well-developed, older outlet for the karst aquifer system. QS, on the other hand, is located along a fault, in a short, narrow, and shallow gorge. The karstified limestone is only very locally exposed and is surrounded and overlain by younger, less permeable units (sandstone, marl, and glacial moraine deposits). QS has limited discharge, causing back-flooding when the discharge capacity of the spring is exceeded. This geologic setting suggests very young (probably post-glacial) exposure by erosion of the confining layers along the fault.

~~depression at a fault, where the top of the karst aquifer limestone unit is exposed only very locally, and is surrounded and overlain by low-permeability sandstone and marl. This geologic setting suggests very young (probably post-glacial) exposure by erosion along the fault. By comparison, the other springs (QE and QA are located in fully exposed karst limestone, indicating that they have been in existence for a longer time.~~

Both of these scenarios are supported by field observations, so the question is not whether they occurred, but whether they were determinant for the formation of the now-inactive portion of the cave network. ~~A third possibility also exists, in which some combination of the above scenarios occurred, with glaciation and low-permeability sediments covering the valley and the Sägebach spring (QS), then the glacier retreating before the Sägebach spring was uncovered. Since both hypotheses are supported by geologic evidence, it is quite likely that all of these geologic events occurred, but there remains the question of which events had the strongest influence on cave formation, which d~~This depends both on the temporal order and on the duration of the different processes at work.

5 Method: Anisotropic fast marching to generate probability maps

To test these hypotheses, many possible network configurations were modelled using anisotropic fast marching methods, implemented in the Python karst modelling package pyKasso (Fandel et al., 2022). Anisotropic fast marching algorithms calculate the optimal path from one point to another through a medium, in which the ease of travel varies both spatially and directionally. Karst conduits can be simulated using this type of algorithm based on the assumption that a conduit represents

the fastest path from an inlet (such as a doline or swallow hole) to an outlet (a spring). The travel medium represents the geologic setting, in which some rock units are more soluble than others (i.e. easier for conduits to travel through). Conduits are also assumed to form preferentially in certain orientations: in the direction of the maximum downward hydraulic gradient, and/or along the dip direction of bedding planes (Audra and Palmer, 2015; Dreybrodt et al., 2005; Palmer, 1991). The user can specify which plane should influence conduit orientation. For shallow, unsaturated karst systems with an impermeable basal unit such as the example presented here, the hydraulic gradient roughly coincides with the topographic gradient, which is significantly simpler to calculategradient of the lower contact between the karstifiable unit and the underlying non-karstifiable unit is the dominant influence, . In this study, the topographic gradient was therefore used as a proxy for the hydraulic gradient. because water recharging downwards from the land surface encounters a low-permeability barrier and subsequently flows laterally along this low-permeability surface (Filipponi, 2009).

Stochasticity can be introduced to the simulations through the generation of a unique fracture network for each model realization, based on the statistical distribution of fracture families observed in the field. The statistical metrics describing the fracture network are the density, the minimum and maximum strike, and the minimum and maximum length. For a table of fracture statistics, see Fandel et. al. (2022). Fractures are assumed to be easier for conduits to travel through than the surrounding rock.

Additional controls on the configuration of the simulated network are possible by iterating over multiple phases of karst development, and over multiple outlets. The conduits leading to each outlet can be simulated in separate iterations, to represent springs of different ages. Existing conduits are easier to travel through than the surrounding rock, and therefore attract younger conduits forming in later iterations, resulting in a branching network structure commonly observed in real karst systems. The inlets to the system can also be divided into groups and assigned to separate outlets, representing different subcatchments within the larger system. All these aspects can be controlled in a deterministic or stochastic manner depending on the available information for a given site (see Fandel et al., 2022 for a full explanation of possible variations).

The primary advantages of fast marching methods are their low data requirements and their computational efficiency compared to other conduit network models. These characteristics allow the rapid simulation of hundreds of network realizations for a single site (for this study, 100 simulations ran in under two minutes on a laptop with a 2.7 GHz dual-core i7 processor and 16 GB RAM). However, this approach does not represent the actual physical and chemical processes driving speleogenesis. Unlike more complex speleogenetic models, each individual pyKasso model realization, because it is based on very little information, is unlikely to capture the true network configuration. Instead, this method is more appropriate for rapidly exploring various scenarios and generating probability maps: visual representations of a model ensemble indicating the likelihood of a simulated conduit being present at any given location.

5.1 Quality check: accuracy of network simulations

To represent the Gottesacker karst system with pyKasso, For the medium through which conduits form was bounded using, a three-dimensional geologic model, was created using the Python package GemPy (de la Varga et al., 2019). For a detailed

description of the geologic model, see Fandel et al. (2021). ~~To avoid edge effects, the initial geologic model extends beyond the study area, and was then cropped to the catchment boundaries.~~ For use with pyKasso (currently only available in 2D), the ~~3D model was sliced using the surface topography, because, in most of the study area, the karstifiable unit is exposed at the land surface~~3D extent of the karstifiable limestone unit was projected onto a 2D plane. The resulting 2D geologic map has a resolution of 181 x 141 cells, with 50 m x 50 m pixels (Figure 3b & c). ~~This is not fine enough to capture the detailed layout of the Hölloch cave, but is suitable for representing the general location and orientation of conduits.~~

This resolution was chosen because it is detailed enough to represent the criteria used to test the hypotheses under consideration in this study (the general location and orientation of conduits), but coarse enough to maintain the fast computation times needed to run hundreds of simulations. A model with 5 m x 5 m pixels was originally tested, but was discarded because it significantly increased the computation time (nearly 50 minutes compared to less than 2 minutes to run 100 simulations) without significantly increasing the degree of confidence with which the study questions could be answered.

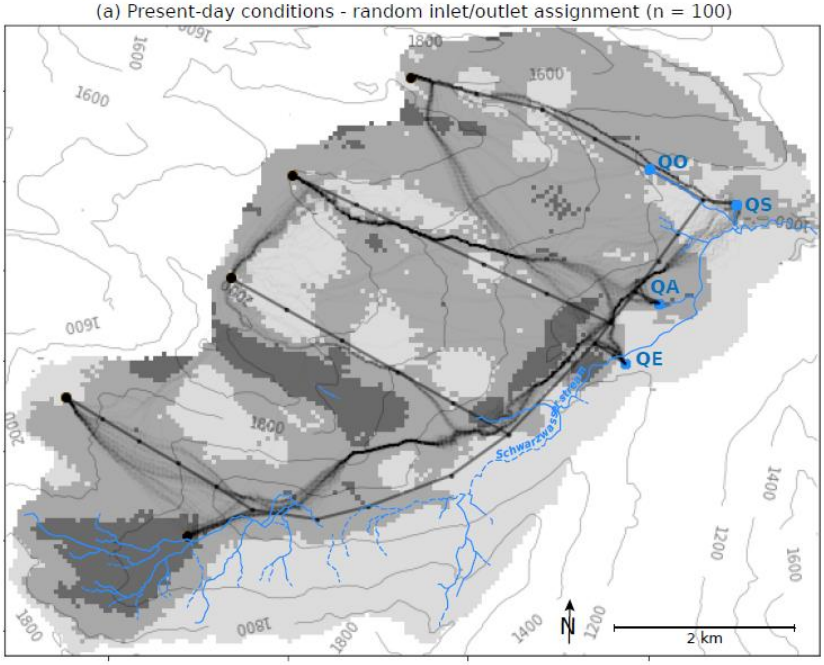
The gradient driving the preferred orientation of conduit formation was calculated from the surface of the contact between the base of the karstifiable limestone and the less-permeable underlying marl. Previous work by Filipponi (2009) demonstrated that in the stratigraphic sequence present at this study site, where the Schrattenkalk limestone is the primary karstifiable unit, conduits form preferentially along the lower contact between the Schrattenkalk and the underlying Drusberg marl, parallel to bedding planes.

O~~o~~utlet coordinates were assigned based on mapped spring locations (Goldscheider, 2005). I~~and i~~nlet coordinates and inlet/outlet pairings were assigned based on locations and springshed boundaries inferred from tracer test evidence and geologic structure in previous flow modeling efforts ~~by~~ (Chen and Goldscheider, 2014). ~~For the medium through which conduits form, a three-dimensional geologic model was created using the Python package GemPy (de la Varga et al., 2019). For a detailed description of the geologic model, see Fandel et al. (2021). To avoid edge effects, the initial geologic model extends beyond the study area, and was then cropped to the catchment boundaries. For use with pyKasso (currently only available in 2D), the 3D model was sliced using the surface topography, because, in most of the study area, the karstifiable unit is exposed at the land surface. The resulting 2D geologic map has a resolution of 181 x 141 cells, with 50 m x 50 m pixels. This is not fine enough to capture the detailed layout of the Hölloch cave, but is suitable for representing the general location and orientation of conduits.~~

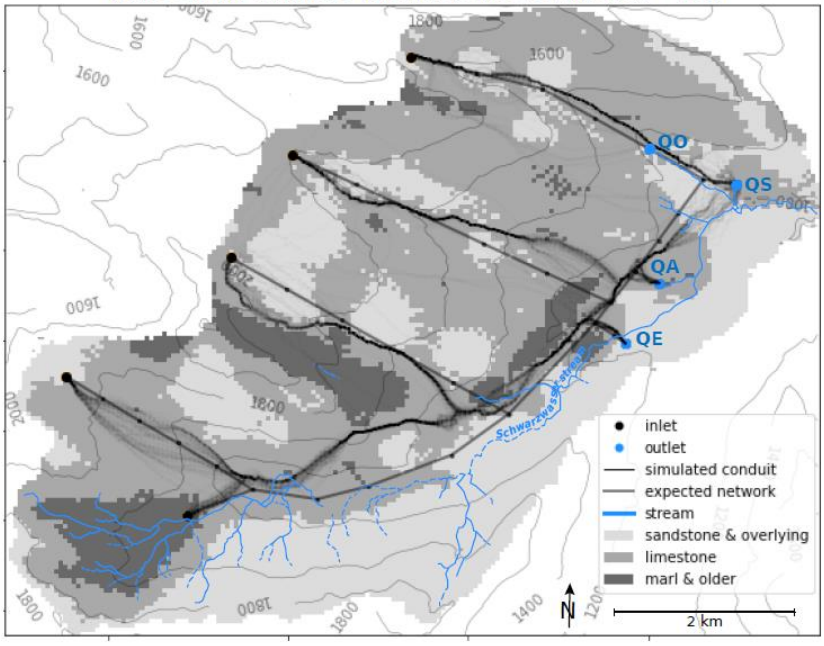
~~A pyKasso-generated ensemble of 100 realizations with the simplified inputs described above, random inlet/outlet assignments, and random spring ordering yielded a probability map in which many of the likely conduits roughly follow expected paths (Figure 3a). However, some simulated conduit paths were highly geologically improbable (e.g. conduits climbing up and over anticlines). These are largely attributable to the random inlet/outlet pairings, which sometimes assign an inlet to an outlet located in a different subcatchment, thereby forcing unrealistic model behaviors.~~ For a full description of the original conduit model parameters, results, and limitations, see Fandel et al. (2022). The conduit model presented in this paper is modified from that in Fandel et al. (2022) in that it uses as input a 2D projection of the extent of the karstifiable unit (rather than a map of where the limestone crops out at the land surface), and the contact surface between limestone and marl (rather

than the land surface). ~~When the inlet/outlet assignments were fixed, th~~The resulting probability map of conduit locations closely matched the branching pattern of the expected network (Figure 3a~~3b~~), despite the limitations of using a low-resolution, simplified, 2D geologic model as the travel medium and the ~~land~~ contact surface gradient as a proxy for the hydraulic gradient. These results support placing confidence in the ability of pyKasso-generated ensembles to ~~simulate~~ provide information about the approximate ~~general~~ configuration of ~~real~~ karst conduit networks in this system. Displaying the ensemble of simulations on the same map also provides information about the probability of conduit occurrence in different zones of the study area: zones where most of the simulations generate conduits in the same general location and orientation suggest that the probability of a real conduit existing in that location and orientation is higher (e.g. conduits departing from inlet N16 in Figure 3a), while zones where there is a wide spread of simulated conduit locations and orientations indicate that lower confidence should be placed in model predictions for that part of the study area (e.g. conduits departing from inlet N6 in Figure 3a) ~~, particularly when the inlet/outlet assignments are fixed~~.

(a) Present-day conditions - random inlet/outlet assignment (n = 100)



(b) Present-day conditions - fixed inlet/outlet assignment (n = 100)



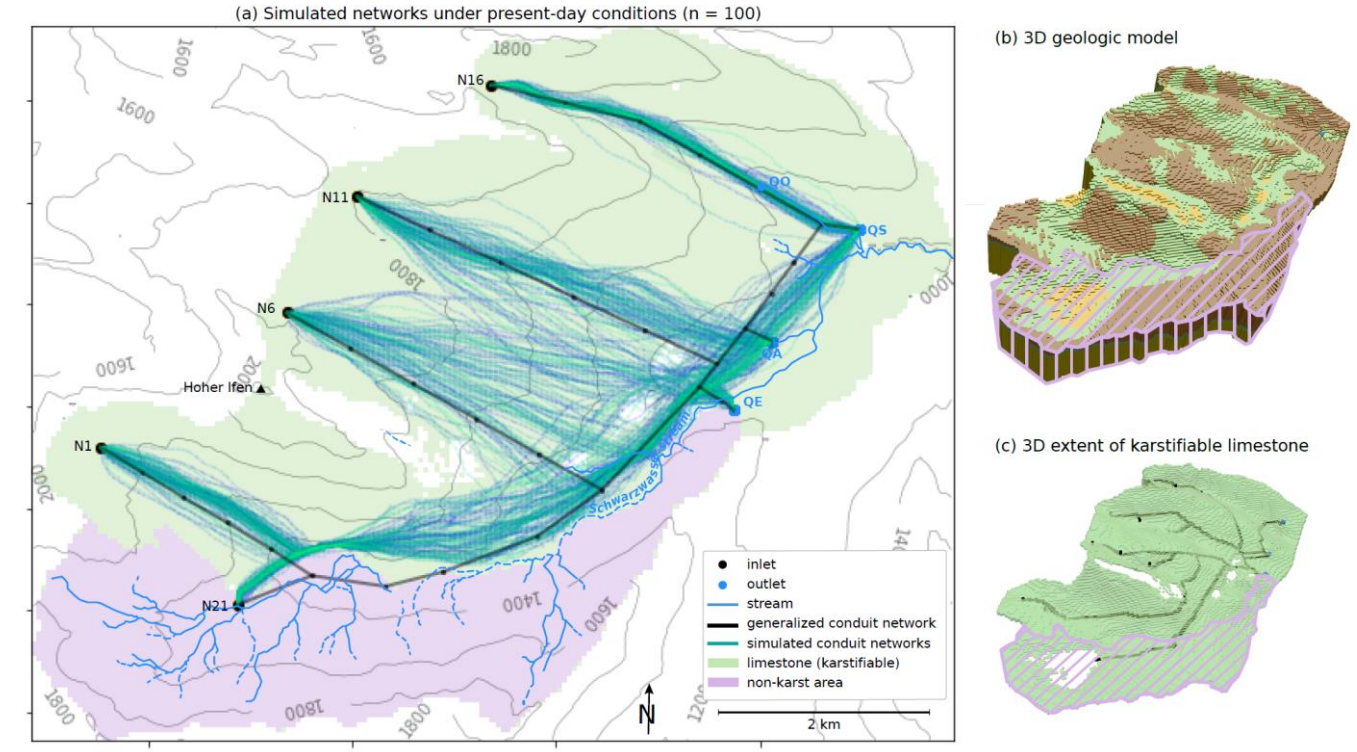


Figure 3: ~~**Probability maps of the conduit network**~~**Conduit simulations under present-day conditions. (a)** ~~**When the inlet/outlet pairings and the outlet iteration order are randomly shuffled, some simulated conduits follow expected paths while others take geologically improbable routes, such as crossing anticlines. (b)**~~ **One hundred simulations with** ~~**When the**~~ **inlet/outlet pairings** ~~**and the outlet iteration order are**~~ **fixed based on tracer test results (Goldscheider 2005)**~~**, only, and t**~~**. Stochasticity arises from the fracture network. The simulated conduits generally match the expected network configuration, but conduit location and orientation predictions are more certain some areas than others (e.g. high certainty departing from inlet N16, low certainty departing from inlet N6).** ~~**Adapted from Fandel et al. (2022).**~~**(b) 3D geologic model with overlay showing the non-karstifiable zone of flysch and other units. (c) 3D extent of karstifiable limestone unit only, used to create 2D projection used in (a).**

5.2 Hypothesis testing

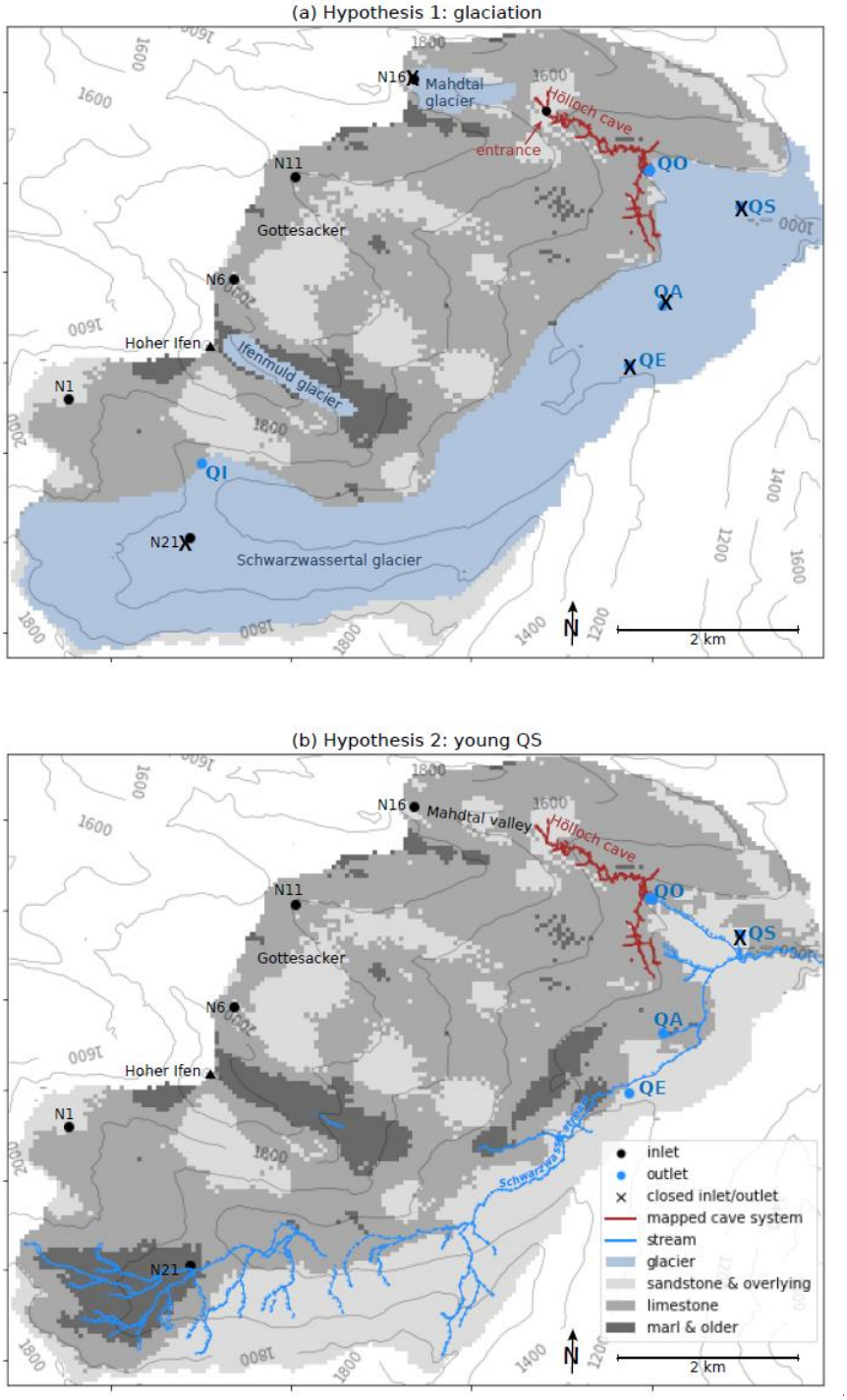
To test the two hypotheses for the past geologic conditions controlling conduit formation, 100 network realizations were run for each scenario using pyKasso, at the same model resolution previously used to simulate present-day conditions (50 m x 50 m cells).

To simulate Hypothesis 1 (glaciation closing all springs except QO), t~~the general extent of glaciation was first reconstructed by the authors, based on mapped glacial deposits and on the elevation of the paleo-spring (Figure 4a). The glacier was assumed to have filled the Schwarzwasser valley up to the level of the spring, located approximately 200 m above the valley floor, and to have covered the rest of the valley with roughly the same thickness of ice. Geomorphological evidence indicates that two smaller glaciers also existed in the northern part of the catchment, one in the upper portion of the Mahdtal valley and one in the breached syncline northeast of Hoher Ifen. T~~he model cells covered by the glacier were assigned a very high travel cost, discouraging conduits from crossing the glaciated area. The inlets and outlets covered by the main glacier and the two smaller

valley glaciers (inlets N21 and N16 and outlets QE, QA, and QS) were removed from the model, and inlet N16 was replaced with an inlet at the entrance to the Hölloch cave. Under this scenario, inlet N1 was separated from the rest of the karst system by the glacier, and was assumed to have drained to a paleo-spring near Ifersguntenalpe (QI). However, the extent of the glacier in this subcatchment is uncertain, so the focus of this simulation remains on the eastern portion of the karst network connected to the paleo-spring (QO), which drained all remaining inlets not covered by the glacier (Figure 4a).

To simulate Hypothesis 2 (QS is much younger than the other springs), the Sägebach spring was removed from the list of system outlets and replaced with the paleo-spring (Figure 4b). The existing inlets remained the same as the present-day configuration. Under this scenario, the Aubach spring (QA), which is lower in elevation than the paleo-spring, was assumed to have served as an "attractor" receiving flow from the entire system, including the Mahdtal valley. An additional inlet was therefore co-located with the paleo-spring and assigned to the Aubach spring ~~(Figure 4b)~~.

For both scenarios, the inlet/outlet pairings and iteration order were kept constant. A new fracture network was stochastically generated for each realization, using the same input statistics as the simulations of the present-day network. All other parameters were held constant.



~~Figure 4: Two competing hypotheses for past geological conditions controlling cave formation. (a) A glacier filled the Schwarzwasser valley, obscuring the karstifiable unit up to the elevation of the paleo-spring (QO). (b) Low-permeability sediments covered the Sägebach spring (QS), making the paleo-spring (QO) and the Aubach spring (QA) the primary outlets for the system. A third hypothesis (not shown) is that some combination of the above occurred.~~

6 Findings

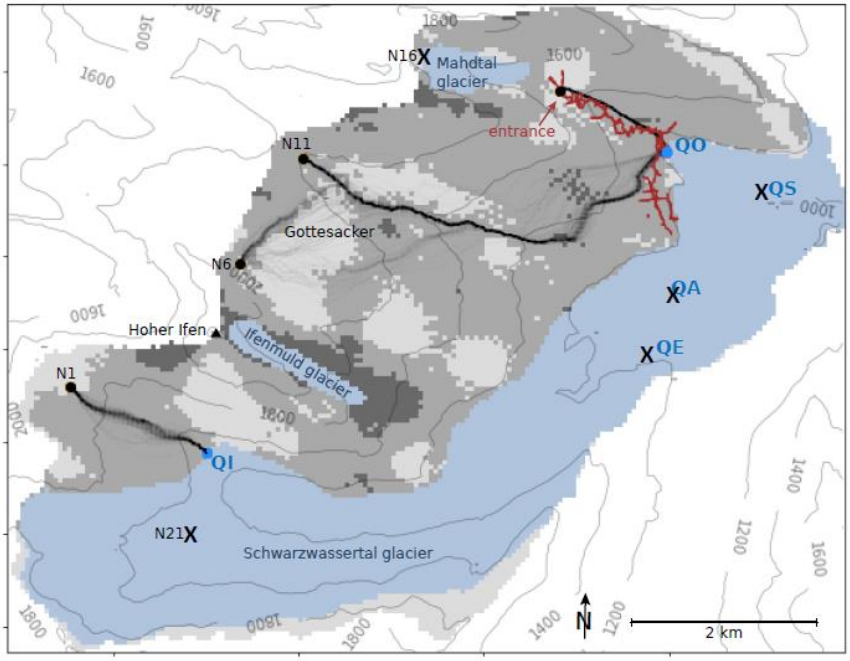
The modeled probability maps support Hypothesis 2 (a comparatively young QS) more than Hypothesis 1 (glaciation) (Figure 4). The simulated networks under Hypothesis 1 (glaciation) only matched the location and orientation of the mapped conduits in the active upper portion of the cave system, not in the inactive lower portion which is the focus of inquiry (Figure 4a). Of note, the spread of predicted conduit locations in this area includes a wide range of possible conduit locations northwest of the mapped cave system, but out of the 100 simulations, not a single one predicted conduits located along the axis of the actual cave system. These results support the conclusion that Hypothesis 1 has a low probability of explaining the formation of the inactive conduits.

The simulated networks matched the location and orientation of the mapped cave system better under Hypothesis 1, when the Sägebach spring was removed from the list of outlets and replaced with the paleo-spring. ~~In fact, t~~The orientation of the simulated conduits is tightly clustered and matches well, while the location of the simulated conduits is slightly to the east of the mapped conduits ~~lie in an envelope of possibilities visible in the probability map~~with more overlap in the southern portion (Figure 4b). ~~By comparison, the simulated networks under Hypothesis 1 (glaciation obscuring the valley bottom) only matched the location and orientation of the mapped conduits in the active upper portion of the cave system, not in the inactive lower portion which is the focus of inquiry (Figure 4a). These results support the conclusion that~~

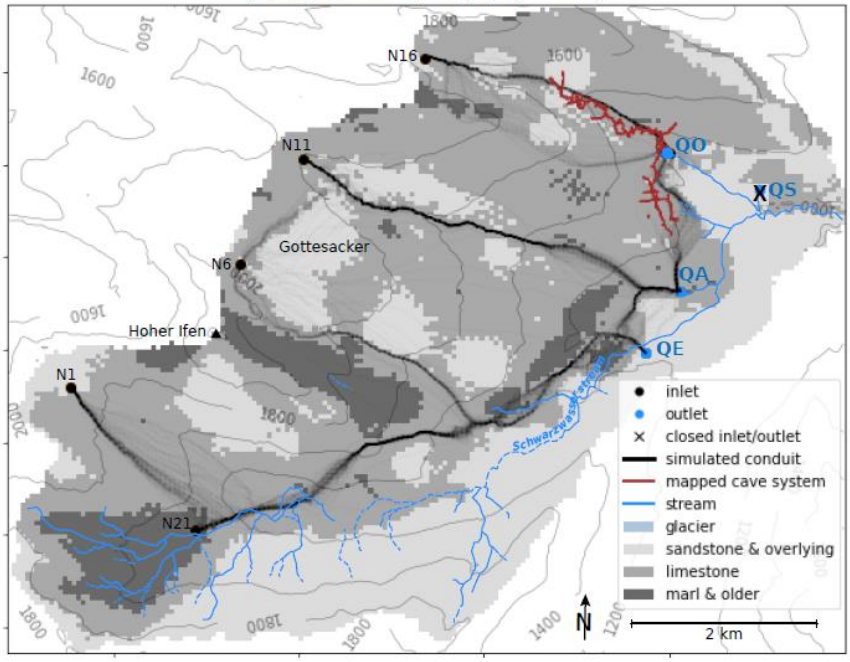
Under this scenario, in the present day, the partially-mapped inactive conduits should extend to make a connection from QO to QA. Because QO is at a higher elevation than QA, the general flow direction when these conduits were active would have been from QO towards QA, even if the inclination of some individual conduits is inverse. Although these conduits now are generally dry, it is possible that under extreme high-flow conditions, groundwater in the Mahdtal syncline overflows the southward bordering anticline and flows towards the Aubach spring (QA).

While these results indicate that Hypothesis 2 is ~~the~~ a ~~most~~ more likely representation of the past geologic conditions that led to the formation of the inactive portion of the Hölloch cave system that Hypothesis 1, other explanations cannot be ruled out. The primary contribution of the model results is that Hypothesis 1 can be ruled out as significantly less probable than originally expected based solely on tracer tests and hydrogeological intuition. ~~The Sägebach spring was likely covered by overlying non-karstifiable units until relatively recently, at which point the older conduits were abandoned in favor of the more direct present-day connections confirmed by tracer tests.~~

(a) Hypothesis 1: glaciation (n = 100)



(b) Hypothesis 2: young QS (n = 100)



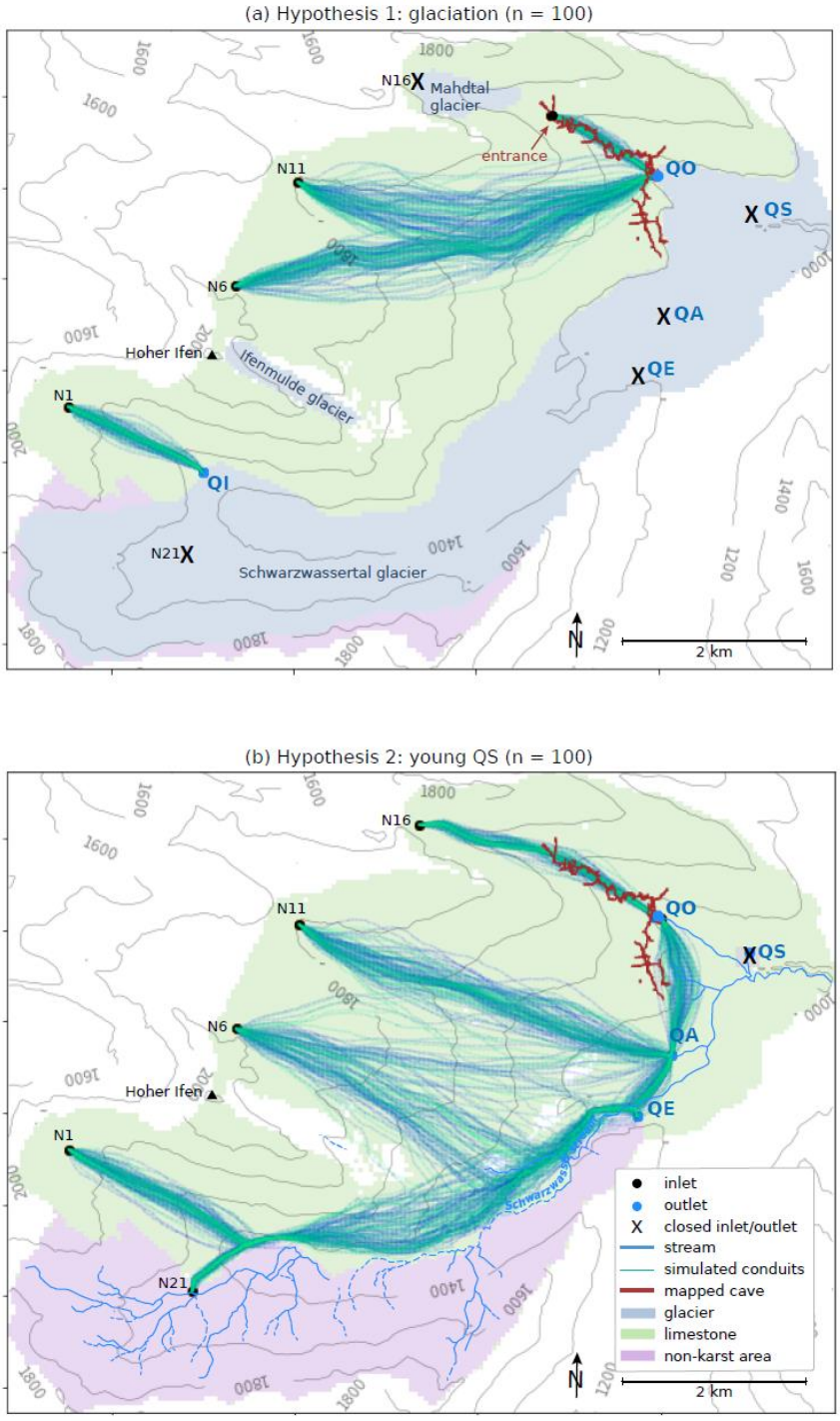


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Figure 4: Probability maps for 100 simulations under each hypothesis, compared to the observed cave map. (a) Hypothesis 1 ~~diverges from~~ yielded no networks matching the mapped cave system. (b) Hypothesis 2 ~~more closely matches~~yielded networks matching the orientation of the inactive cave network ~~than hypothesis 1~~, located slightly to the east of the mapped network. This~~, suggesting that the Sägebach spring is relatively young~~ suggests that hypothesis 2 is less probable than hypothesis 1.

7 Discussion

The model ensembles in this study clearly support one hypothesis over the other: the probability map for Hypothesis 1 shows a range of possibilities, but no conduits along the mapped portion of the inactive cave system, while the map for Hypothesis 2 shows a cluster of conduits suggesting that the inactive portion of the Hölloch cave continues southeast for several hundred meters before turning first southwest, then due south to connect to the Aubach spring (Figure 4b). This configuration is illustrated schematically in Figure 5.

These results suggest two additional ways that these hypotheses could be further tested by fieldwork:

1) Additional speleological explorations, focusing on the passages trending in the directions projected by the probability map – if the hypothesis is correct, these passages will continue rather than terminating in dead-ends. This information may be helpful in guiding future speleological exploration.

2) A tracer injection under extreme high flow conditions at the Hölloch cave entrance in the Mahdtal valley with sampling at the Sägebach spring (QS) and the Aubach spring (QA). When, under high flow conditions, the water level in the cave system is greater than the elevation of the Aubach spring (QA), the paleo-spring (QO) becomes active. Previous tracer tests under normal flow conditions found a connection only to the Sägebach spring, but under extreme high flow conditions, the normally inactive conduits projected to connect to the Aubach spring may reactivate. ~~Currently, no conduits have been found along the path expected if glaciation had controlled conduit formation.~~ Unfortunately, the logistical challenges of waiting for such an extreme event to occur and then achieving a high-quality tracer test on short notice are significant.

A third hypothesis is also possible, a combination of the two scenarios explored in this study: that an initial phase of conduit formation occurred dominated by the influence of the glacier covering the valley, another phase occurred after the glacier had retreated but before the Sägebach spring was exposed, and the most recent phase developed with all three major springs (QE, QA, and QS) active. If this were to have occurred, two sets of inactive conduits should be present, corresponding to the two past phases of karstification. Currently, no conduits have been found along the paths expected if glaciation had ~~controlled~~influenced conduit formation. However, exploration of the Hölloch system is incomplete. If future exploration reveals new conduits along the paths simulated under the glaciation scenario, this hypothesis of two-phase karstification could also be supported.

~~Another possible scenario that we did not explore in depth is that some combination of different springs were cyclically occluded then exposed over the course of several phases of glacial and inter-glacial periods (with some springs active during the inter-glacials but covered during the glaciations).~~

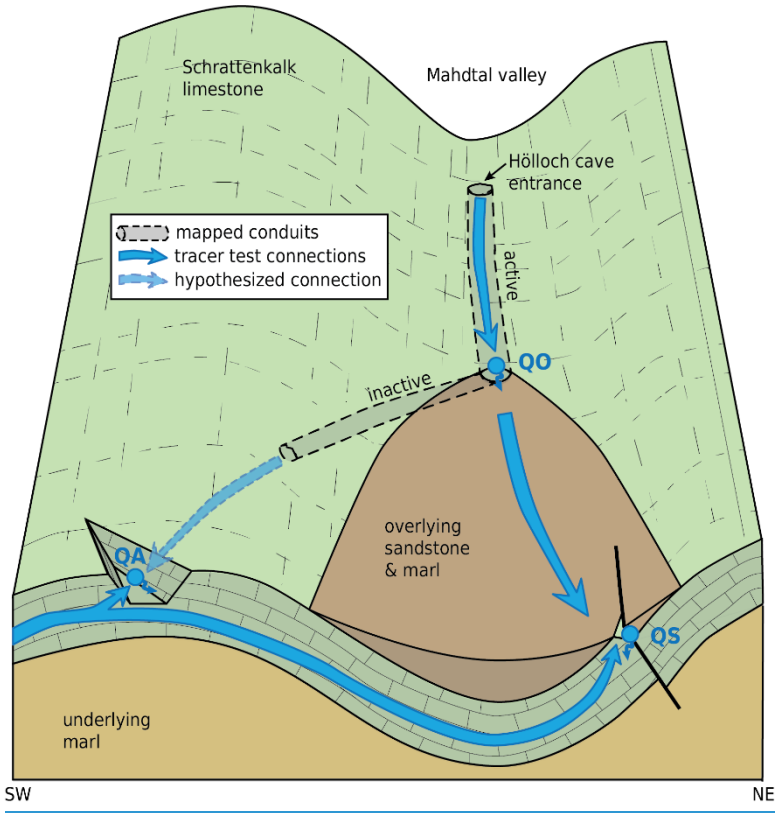

Figure 5: Schematic block diagram of the northeastern portion of the study site based on Hypothesis 2, showing the relationships between the subsurface conduit system and the points where it connects to the land surface. Surface water can enter the system through diffuse recharge where karstified limestone is exposed at the land surface, as well through concentrated point recharge through vertical shafts (e.g. the Hölloch cave entrance). Groundwater can exit the system at three springs: QA (large, well-developed), QS (limited discharge capacity), or QO (only during extreme high-flow conditions). The karst system is confined by overlying impermeable sediments in the lower part of the Mahdtal valley. An active cave stream flows through subsurface conduits from the Hölloch entrance towards QO. Flow connections from the entrance to QS, from QO to QS, and from QA to QS, have been demonstrated by tracer tests. Inactive conduits to the southwest of QO have been partially explored. Modeling results suggest that these conduits continue, connecting QO and QA

While the model results provide insight into this area's geologic past, some questions and limitations remain. In both scenarios, the underlying geologic model is a limitation. A 2D geologic map simplifies the complex three-dimensional reality. ~~In this example, patches of sandstone appear in the middle of the Gottesacker plateau when in fact, almost the entire plateau consists of exposed limestone (Figure 6). This is because the upper contact between the limestone and the overlying sandstone closely coincides with the land surface, so when the 3D model is sliced using the surface topography, cells near the contact are frequently mis-assigned. This results in conduits curving around or crossing fold axes in geologically implausible ways to avoid patches of hard-to-traverse geologic units in 2D, when in fact in 3D the conduit paths should be able to pass unobstructed beneath the shallow sandstone (particularly for the conduits departing from inlet N6). These issues could be resolved with a 3D geologic model (currently in development for pyKasso).~~ However, a preliminary test using a development 3D version of

pyKasso, with the 3D geologic model as input, yielded conduit maps that did not appear significantly different from the 2D version used in this paper. ~~the hypothesis testing presented here focuses on a small area within the catchment (the lower part of the Hölloch cave), in which the geologic model is fairly representative, with few slicing artifacts, so this is not a major issue for the purposes of this study.~~

Another question arises from the observation that, although the simulated conduits under Hypothesis 2 (a young QS) are much more similar to the inactive portion of the Hölloch cave than under Hypothesis 1 (glaciation), they do not exactly match the mapped cave system. The simulated conduits tend to lie slightly to the east of the mapped conduits, skirting the edge of the overlying sandstone unit. This is likely ~~a limitation of the model's ability and our simplified assumptions to predict exact conduit locations rather than general orientations and connections~~due to our simplification of the geology – in reality, the karstifiable limestone in this part of the system is covered by non-karstifiable sandstone, marl, and quaternary sediments. These overlying units may have made it more difficult for conduits to develop beneath them, encouraging conduit development along their northwestern boundary. However, ~~it~~the mismatch may also indicate a conceptual gap in our understanding of the system. A few examples of factors not considered in this study that could affect conduit formation include:

1) The presence of an unmapped tectonic feature with higher or lower conduit-forming propensity than the surrounding rock. This would attract or repel conduits in the model.

~~2) A difference between the shape of the land surface topography and the topography of the base of the karstifiable limestone unit. The conduits in this study are generated under the assumption that the land surface and the base of the limestone unit are parallel, so if they are in reality not parallel, there would be some error in the anisotropy field.~~

3) An eastward (downgradient) shift in the location of the contact between the karstifiable limestone and the thin overlying sandstone unit as the sandstone erodes over time. The modeled conduits in this specific location tend to follow the contact, so the real conduits being slightly westward of the modeled conduits could be explained if the contact were previously also slightly westward of its current location.

4) More phases of karstification than hypothesized could have occurred, in various orders, resulting in a conduit network that is partially but not fully explained by the hypotheses presented here.

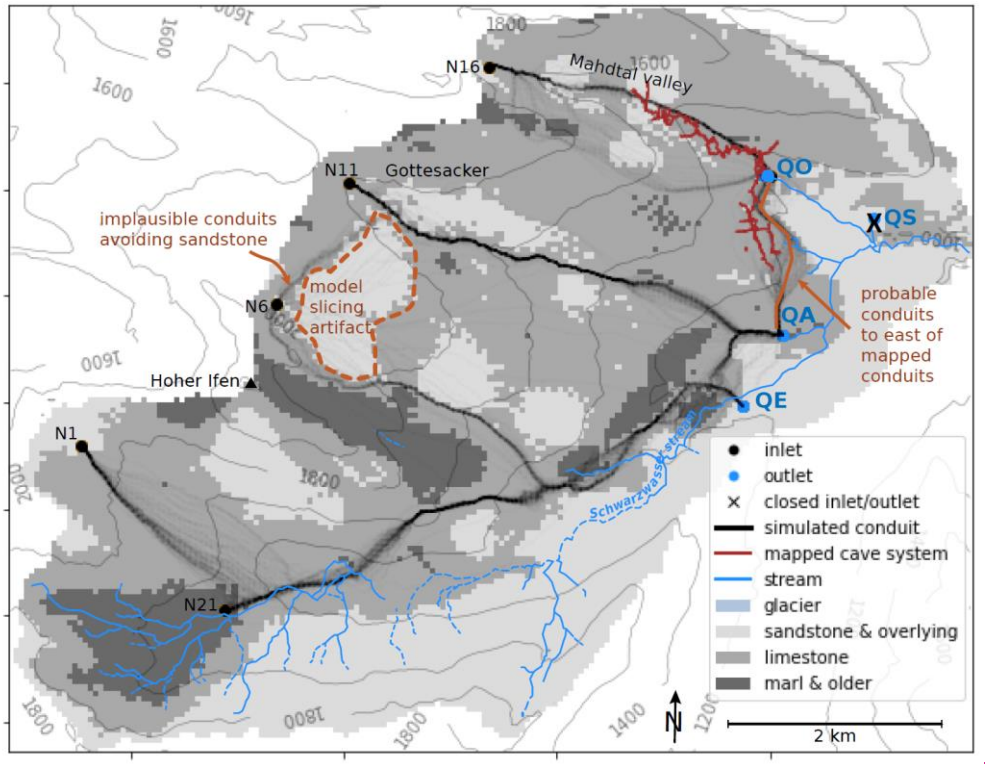

Figure 6: Inaccuracies in the simulated conduit networks, highlighting limitations of the anisotropic fast marching approach.

7.1 Applicability to other situations

The advantages of the approach presented in this study are that it requires very little data (inlet and outlet coordinates, fracture distribution statistics, and a geologic map), and is computationally efficient. This allows for rapid exploration of different scenarios and quick hypothesis testing.

The disadvantages of this approach are that the probability maps produced by running multiple model realizations must be interpreted with care. They represent the probability of a conduit simulation being present within the framework of the set of assumptions and available (often incomplete) data used to construct the model. If the underlying model inputs and assumptions are flawed or incomplete, the resulting ensemble of simulated networks may fail to capture the actual network configuration. There are several particularly significant assumptions that could influence the model results: that the system has distinct inlets with known locations rather than diffuse recharge across a general area, that a simplified 2D geologic model can adequately represent the subsurface geologic structure, and that the topographic gradient is an adequate proxy for the hydraulic gradient. These assumptions are taken to be valid in the well-studied Gottesacker system, because the shallow karstifiable unit is generally exposed at the land surface, its structure roughly paralleling the topography. The close fit between the expected conduit network as determined from tracer tests and the simulated networks in the present-day scenario model ensemble further supports the validity of the anisotropic fast marching approach for this system, and increases our confidence in the historical

~~simulations. However, these assumptions may not be appropriate in other karst systems, and the simulated conduits represent only the general network configuration, not the detailed local structure of the conduits. It is therefore crucial when transferring this approach to other locations first to consider whether it is well-suited to the karst system in question, and second, to pair modeling efforts with supporting fieldwork in less well-studied sites.~~

8 Conclusion

This study demonstrates the application of anisotropic fast marching methods for rapid model ensemble generation to test competing hypotheses describing the past geologic conditions that controlled karst conduit evolution in a real catchment. It extends the applicability of these methods from situations where the goal is to generate a map of an unknown conduit network, to situations where the goal is to understand how an already-mapped conduit network was formed.

For the field site investigated in this study, the Gottesacker karst system, comparing the conduit network under different past scenarios (based on model-generated probability maps of conduit locations) to the actual conduit network (based on maps of the explored present-day cave system) allowed the identification of the past conditions with the greatest influence on cave development. The model results indicate that the most probable scenario is that the conduits of interest formed before the lowermost spring in the catchment came into existence, and drained to the other two major springs in the system (as opposed to conduit formation being dominantly influenced by glaciation occluding all three major present-day springs). The modeling results also enabled making recommendations to guide cave exploration efforts and future data collection that could further test the conduit formation hypotheses.

The strength of the anisotropic fast marching method is its comparatively low cost in terms of computational resources and quantity of initial input data required. This allows for rapid iteration and exploration of many different scenarios, which makes it especially well-suited for ensemble modeling. The model ensemble approach demonstrated in this study could be applied to other karst systems with mapped conduit networks, both to better understand the past geologic conditions that influenced the conduit network development, and to better target future mapping and data collection efforts to answer outstanding questions about the system. It also holds potential for exploring competing conceptual understandings of a karst system, and identifying possible conceptual gaps, both of which are significant sources of uncertainty in predicting karst systems' response to anthropogenic stresses.

Code availability

The code and supporting data used to generate the figures in this paper are presented in a Jupyter Notebook available in a public GitHub repository here:
https://github.com/randlab/pyKasso/blob/replace-fast-marching-with-HFM/notebooks/Fandel_et_al_2022_HESS.ipynb

Author contribution

NG developed the concept for the paper and the hypotheses, and provided data on the study site. FM, CF, and PR developed and debugged the pyKasso modeling package. CF implemented the model and performed the simulations. TF provided research supervision and guidance in the use of model ensemble approaches. CF created the figures and wrote the manuscript draft, and NG and PR reviewed and edited the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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References

Audra, P., and Palmer, A.N.: The pattern of caves: controls of epigenic speleogenesis. Géomorphologie Relief Process. Environ. 17, 359–378. https://doi.org/10.4000/geomorphologie.9571, 2011

Chen, Z., and Goldscheider, N.: Modeling spatially and temporally varied hydraulic behavior of a folded karst system with dominant conduit drainage at catchment scale, Hochifen–Gottesacker, Alps. J. Hydrol. 514, 41–52. https://doi.org/10.1016/j.jhydrol.2014.04.005, 2014.

Chen, Z., Hartmann, A., and Goldscheider, N.: A new approach to evaluate spatiotemporal dynamics of controlling parameters in distributed environmental models. Environ. Model. Softw. 87, 1–16. https://doi.org/10.1016/j.envsoft.2016.10.005, 2017.

Chen, Z., Hartmann, A., Wagener, T., and Goldscheider, N.: Dynamics of water fluxes and storages in an Alpine karst catchment under current and potential future climate conditions. Hydrol. Earth Syst. Sci. 22, 3807–3823. https://doi.org/10.5194/hess-22-3807-2018, 2018.

Cramer, K.: Die Geologie des Mahdtales und der Karst des Gottesackergebietes, Master thesis. TH Munich, Munich, Germany, 1959.

Fandel, C., Ferré, T., Chen, Z., Renard, P., and Goldscheider, N.: A model ensemble generator to explore structural uncertainty in karst systems with unmapped conduits. Hydrogeol. J. 29, 229–248. https://doi.org/10.1007/s10040-020-02227-6, 2021.

Fandel, C., Miville, F., Ferré, T.P.A., Goldscheider, N., and Renard, P.: The stochastic simulation of karst conduit network geometries using anisotropic fast marching, and its application to a geologically complex alpine karst system. Hydrogeol. J. https://doi.org/10.1007/s10040-022-02464-x, 2022.

Filipponi, M., Jeannin, P.-Y., Tacher, L.: Evidence of inception horizons in karst conduit networks. Geomorphology 106, 86–99. https://doi.org/10.1016/j.geomorph.2008.09.010, 2009.

Goeppert, N., and Goldscheider, N.: Solute and Colloid Transport in Karst Conduits under Low- and High-Flow Conditions. Ground Water 46, 61–68. https://doi.org/10.1111/j.1745-6584.2007.00373.x, 2008.

Goeppert, N., Goldscheider, N., and Berkowitz, B.: Experimental and modeling evidence of kilometer-scale anomalous tracer transport in an alpine karst aquifer. Water Res. 115755. https://doi.org/10.1016/j.watres.2020.115755, 2020.

Goldscheider, N.: Fold structure and underground drainage pattern in the alpine karst system Hochifen-Gottesacker. Eclogae Geol. Helvetiae 98, 1–17. https://doi.org/10.1007/s00015-005-1143-z, 2005.

Höhlenverein Sonthofen: Das Hölloch im Mahdtal – 100 Jahre Höhlenforschung im Kleinwalsertal, Sonthofen. Sonthofen, 2006.

Jaquet, O., and Jeannin, P.Y.: Modelling the Karstic Medium: A Geostatistical Approach, in: Armstrong, M., Dowd, P.A. (Eds.), Geostatistical Simulations, Quantitative Geology and Geostatistics. Springer Netherlands, Dordrecht, pp. 185–195. https://doi.org/10.1007/978-94-015-8267-4_15, 1994.

Sellers, W.I., and Chamberlain, A.T:. Ultrasonic Cave Mapping. J. Archaeol. Sci. 25, 867–873. https://doi.org/10.1006/jasc.1997.0232, 1998.

Trimmis, K.P.: Paperless mapping and cave archaeology: A review on the application of DistoX survey method in archaeological cave sites. J. Archaeol. Sci. Rep. 18, 399–407. https://doi.org/10.1016/j.jasrep.2018.01.022, 2018.