Karlsruhe Institute of Technology

Dear Editor, dear Reviewers,

we would like to thank you for your time and the constructive comments, which truly helped to improve the quality of the manuscript. Please find our detailed replies on the comments below. We hope that we answer all your remarks.

Our replies to the reviewer’s comments are highlighted in blue. To highlight the nature of our replies we use a traffic light system indicating agreement with the reviewer marked in green, partial agreement in yellow, and objections in red.

Reviewers' and Editors' comments:

Reviewer #1:

The present article utilises persistent homology (PH) to estimate the permeability of a single fracture (12 by 45 cm length) in sandstone from high-resolution scans of the fracture surfaces. Results are compared to permeability estimations from numerical simulations and from measurements using an air permeameter. Results are interesting because they validate the use of PH as a method for permeability estimation. However, there are significant issues that I believe should be addressed before this work could be considered for publication.

1. The manuscript states that its goal is to address the influence of roughness on fracture permeability, but no parameters of the fracture roughness are provided. I strongly recommend including a roughness quantification for the fracture in the paper (e.g. roughness exponent from power spectral analysis).

We agree. There are already existing values for the Hurst exponent of the fracture surfaces, which were determined by Gutjahr et al. (2022). We therefore add this information as follows (L101-105): “Furthermore, the findings of Gutjahr et al. (2022), Hale et al. (2020) and Hale and Blum (2022) are crucial, since they performed investigations on fracture permeability on exactly the same fracture. Gutjahr et al. (2022) investigated on the roughness of the fracture and calculated the Hurst exponent for different angles. The medians of all Hurst exponents in x-direction and in y-direction are 0.48 and 0.42, respectively.”

In addition, we discuss the Hurst exponent anisotropy briefly in context with the anisotropy of permeability (L245-249):
“The study of Gutjahr et al. (2022) shows that, in addition to the anisotropy of the permeabilities, a slight anisotropy of the roughness can be observed. Analogous to the permeability, the Hurst exponent in x-direction is higher (Hx = 0.48) than in y-direction (Hy = 0.42). It is noteworthy that the ratio of the Hurst exponents (Hx/Hy) is 1.1 and thus corresponds well with the determined ratios for permeabilities. This is reasonable, as increased roughness tends to result in more distinct flow channels with larger mechanical apertures. Consequently, this leads to increased permeability.”

However, this study was designed to primarily investigate the general functionality of persistent homology for permeability estimation of a single fracture. This was to be investigated by examining the anisotropy in the x- and y-directions as well as the resolution dependency. We rephrase the sentences in our objective section (L88-90):
“The focus is on the anisotropy of permeability in different flow directions as well as the influence of

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resolution on permeability. Thus, three data set of the same fracture are prepared, which have different resolutions (50 µm, 100 µm and 200 µm).”

We also add a comment in out conclusions section to show that the actual influence of roughness is a crucial issue, which should be addressed in future work (L345-346):
“Furthermore, the influence of roughness on the flow behaviour and the permeability distribution across the fracture should be investigated.”

2. In addition, the method of PH should be described more rigorously, and the discussion makes some questionable comparisons. Please find below my detailed comments.

We agree with the comment on the description of PH. Hence, we elaborated our description of persistent homology in section 2.3 as follows (L133-L194):

“We apply the permeability estimation method proposed by Suzuki et al. (2021), which uses persistent homology (PH) to extract information about the flow channels from image data. The first step is to convert the fracture information prepared in Section 2.2 into a 3D binarized image datasets.

Three-dimensional image construction of the bedding joint and the surrounding sandstone block was generated. The image construction is a series of binary cross-sectional images of the x-z-planes along the y-axis. The size of the image area is 115 mm × 8.4 mm × 3,922 mm. Three data sets with different resolutions were generated to investigate the effect of varying resolution on permeability estimation. The first data set was created with a low resolution of 200 µm in all spatial directions. The dataset contains 578 × 1,962 × 42 voxels. The second data set was generated with a medium resolution of 100 µm in each spatial direction. The dataset contains 1,154 × 3,922 × 84 voxels. In the third data set, the resolution was again reduced by half to 50 µm in all spatial directions. The dataset contains 2,308 × 7,844 × 169 voxels. The fracture was considered to be fully permeable with no low permeable filling or sealing. Since the matrix permeability is eight orders of magnitude lower than the fracture permeability, the matrix was considered to be fully impermeable (Cheng et al., 2020; Hassanzadegan et al., 2012). Thus, each image contains the permeable fracture in white colors (binary value = 1) and the impermeable matrix in black colors (binary value = 0).

PH analysis was then performed using HomCloud (Obayashi et al. 2022). Since HomCloud can only handle a maximum data volume of 1021^3 voxels in a single analysis run, the data sets were divided into several subpackages, which were processed separately (Figure 2). The dataset with low resolution (200 µm/pixel) has 578 × 1,962 × 42 voxels and were split into 2 divisions in y-direction. Thus, 2 subpackages were created for the data set with low resolution, each of which contained 578 × 981 × 42 voxels. The x-direction and y-direction for the dataset were not necessary because the length of one side of the image was < 1021 pixels. The dataset with middle resolution (100 µm/pixel) has 1,154 × 3,922 × 84 voxels and were split into 2 divisions in x-direction and 4 divisions in y-direction. The dataset was divided into 8 subpackages with an average of 577 × 981 × 84 voxels each. The dataset with high resolution (50 µm/pixel) has 1,154 × 3,922 × 84 voxels and were split into 3 divisions in x-direction and 8 divisions in y-direction. The data set was divided into 24 subpackages with an average of 769 × 981 × 169 voxels each.

PH analysis was then performed for each subpackage. HomCloud allows to extract topological features; a 3D object can consist of three different topological features. First, 0-dimensional topological features characterise connected components such as impermeable, solid matrices without voids. Structures such as fractures or connected pores are recognized as 1-dimensional (1D) topological features. Finally, 2-dimensional (2D) topological features are represented by enclosed pores not connecting to other flow channels. Since only fractures connected between an inlet and an outlet of the domain can serve as potential flow channels, this study focuses on the analysis of 1D topological features.

In HomCloud, a process called Filtration is performed to detect 1D topological features from image data. For simplicity, an example of a two-dimensional image is shown in Figure 3. In the binary image, the black areas are the rock matrix (binary value = 0), while the white areas are the void space (binary value = 1). During the filtration, the black pixels are thinned or thickened by one pixel from the boundary between the white and black pixels. The process is considered as time variation, and the initial image is assumed to be time 0 (t = 0). The time change in the negative direction is to make the black pixels thin, and the time change in the positive direction is to make the black pixels thick. The images are stored at each time. Continuing this operation, if the pixels continue to be thinned (time change in the negative direction), the image becomes all white. If time is advanced in the positive direction from the all-white state, a channel (i.e., 1D topological feature) appears at certain times, and if time is continuously advanced in the positive direction, the channel disappears further. Note that the channel (1D topological feature) here is the connected shape from left to right, surrounded by black pixels. These times are called birth (b) and death (d), respectively. This method is named “persistent homology” because it attempts to see how persistent topological features are. While other topological data analysis extracts only topological features, the advantage of PH is that by utilizing birth-death information, one can obtain not only topological features but also the geometric information on length.

In HomCloud, the output is a Persistence Diagram representing a frequency distribution of the number of birth and death pairs as shown in step II of Figure 2. From the definitions of birth and death, the presence of a flow channel (1D topological feature) in an image means that birth-time is negative and death-time is positive. Thus, the number of such pairs (b < 0 < d) can be considered the number of flow channels in the image. In addition, in the case of the process of thickening the black area as shown in Figure 3, the fracture is closed from both sides (see the image “t = d”). Therefore, the doubling of death and multiplying by the resolution of the image can be taken as the smallest aperture of the channel. Thus, from HomCloud, the frequency distribution of the number of channels present in the image and their minimum aperture widths can be obtained. It is important to note that the 1D topological features evaluated in PH include the aforementioned left-to-right connected shapes surrounded by black pixels, as well as the void ring structures that are not connected to the outside. How to remove such structures is described in Suzuki et al. (2021). It should also be noted that if the channels are connected like a ladder, PH may detect a large number of channels.

Suzuki et al. (2021) assumed that the channels have parallel-plate geometries and that they are parallel to each other. The permeability is estimated based on the power law as follows:

$$\boldsymbol{K = \sum_{i=1}^{N} \frac{w_i h_i^3}{12A}} \tag{1}$$

A is the surface area of the cross section of the medium and N is the number of flow channels. wi is the depth of flow channel i and hi is the aperture of the flow channel i. As mentioned above, the number of flow channels N was estimated from the number of birth-death pairs and the aperture hi was estimated as 2d_i δ in PH analysis, in which di is the death of the flow channel i and δ is the resolution of the images. The average of the depth of flow channel w¯is determined by the cross-sectional area of the image (Suzuki et al., 2021). Thus, the above equation can be converted to the parameters from PH and image analysis.”

We partially agree with the comment about questionable comparisons. The comparisons presented in this study are used to show that persistent homology is used for permeability assessment in single fractures in addition to porous media and fracture networks. In addition, the general trend is to be shown that persistent homology slightly overestimates the reference value. It is by no means intended to draw conclusions that single fractures in sandstone behave exactly as 3D-printed fracture networks.

3. I have made some language suggestions that the authors can decide whether to incorporate or not, but the manuscript would greatly benefit from thorough language editing.

We agree and implemented the language suggestions. A detailed list of the implemented changes can be found below. The line numbers refer to the revised manuscript and may differ slightly from the unrevised ones.

Abstract:
L11: the topological method **of** persistent homology
L12: the permeability **of** fracture networks
L13: **on** was deleted

Introduction:
L32: to study **how fluid flow is** influenced
L35: cheap**,**
L47-49: **rephrased**: Flow-through experiments allow to investigate direct fluid flow through fractures. The flow distribution and preferred flow paths can be predicted by replicating the fracture geometry in transparent materials.
L49: to determine **the** permeability
L50: **Air permeameters allow** to measure **the** permeability …
L51-53: rephrased: In addition, it is also possible to obtain a zonal observation of the permeability, since several measurements have to be conducted along an fracture outcrop due to the measurement method (Hale et al., 2020).
L63: **removed:** however
L66: without experiment**s** and numerical simulation**s.**
L69-70: **rephrased:** …, but adequate use of machine learning requires deep technical understanding, rigorous testing and sufficient amounts of training data.
L71: **from** big data
L72-73: **rephrased**: TDA is an analysis method that focuses on the structure of data within the field of algebraic topology, demonstrating particular strengths in handling data types such as images, complex structures, and networks.
L73-77: **rephrased**: TDA can capture the structure of the data in a rough sense and characterize the features of connectivity and holes, therefore, ignoring noises in data and extracting important information, independent of coordinate system and number of dimensions. Persistent homology (PH), one of the most used TDAs, can capture changes and continuity of topological features by tracking algebraic descriptions called homology.
L76: **rephrased:** most used (see comments of reviewer #2)
L77: **removed:** already
L79: …**, and** biology
L79-80: **rephrased:** In geosciences, this approach has only been applied in the past decade to characterize porous rocks and to determine their permeability
L84-85: **rephrased**: In these small-scale (millimeter to centimeter scale) studies the effect of fracture roughness was not particularly investigated

L88: **removed**: hence

Methods:
L96: with a **length** of 120 mm
L97-98: **rephrased:** Previous studies have already characterized relevant hydro-mechanical properties of Flechtinger sandstone such as …
L100-111: In fact, this is an incorrect statement of our side. The range of matrix permeability is rather 0.1-1 mD, which is based on the measured values of 0.17-0.36 mD by Hassanzadegan et al. (2012) and the statement of Cheng et al. (2020) that the permeability is in the range of 10^{-18} m^2. This was adjusted accordingly.

In addition, the following sentences were **rephrased**: Of particular interest for this study is the low matrix permeability of 0.1-1 mD (Cheng et al., 2020; Hassanzadegan et al., 2012). Furthermore, the findings of Gutjahr et al. (2022), Hale et al. (2020) and Hale and Blum (2022) are seminal, since they performed investigations on fracture permeability on exactly the same fracture. Gutjahr et al. (2022) investigated on the roughness of the fracture and calculated the Hurst exponent for different angles. The medians of all Hurst exponents in x-direction and in y-direction are 0.48 and 0.42, respectively. Hale et al. (2020) and Hale and Blum (2022) determined the average fracture permeability to be 5.6 × 10^{-10} m^2. In addition, they found that the center of the fracture is less permeable than the left and right side of the fracture (according to the front view of the sandstone block shown in Figure 1a). On the right side of the fracture, this can be explained by a barite vein intersecting the fracture, which was formed before the fracture opening. In the closer vicinity of the vein, the mechanical aperture is increased compared to central parts of the fracture. Comparing fracture and matrix permeabilities shows that the fracture permeability exceeds matrix permeability by more than eight orders of magnitude. Thus, the matrix permeability is considered negligible in this study.
L128: … was then determined **by** applying …
L143-143: **rephrased**: Since the matrix permeability is eight orders of magnitude lower than the fracture permeability, the matrix was considered to be fully impermeable.
L187: … **have** parallel-plate geometries …

L209-211: We **rephrased** the sentence, since the reviewer misunderstood the statement: This study uses both, existing air permeameter measurements from Hale et al. (2020) and measurements conducted in this study. In the study of Hale et al. (2020) experiments along the long edge (y-direction) of the fractured block were performed and the permeability in x-direction was measured.
L217: **Apart from** experimental …
L228: **removed**: These resulted in hydraulic apertures of 85 µm in x-direction (6.0 × 10 10 m^2) and 73 µm in y-direction (4.4 × 10 10 m^2), respectively.

Results and discussion:
L241: **rephrased**: Detailed examination of the individual fracture surfaces and the matched fracture shows
L250: We agree that this is confusing and **removed** the following two sentences: It can be seen that the permeability in the x-direction of the 50 µm resolved data set better matches the higher permeability of the 200 µm data set compared to the 100 µm data set. On the other hand, the permeability in the y-direction fits better to the lower permeability of the 100 µm data set.
L283: **rephrased**: at relatively lower permeabilities
L290-291: **rephrased**: In addition, it is also not surprising that the results of this study have permeability values closer to those of fracture networks rather than porous rocks.
L294-295: **rephrased**: … the same trend of permeabilities, **the majority of which** are overestimated slightly, …

Reviewer #2:

Before presenting my comments, I would like to point out that my experience relevant for reviewing this manuscript is in topology-based methods for estimating fracture network connectivity, and geological analysis of fracture networks. Perhaps experience in geomechanical simulations of fracture networks is also useful. I am, however, no expert specifically in Persistent Homology (PH), or in laboratory or numerical flow simulations for fracture permeability estimation. Thus, for some of the questions or comments, an explanation might suffice.

Summary and general comments
The manuscript presents a novel topology-based method, Persistent Homology (PH), to estimate single fracture permeability from high-resolution imagery. The study demonstrates this application of PH using a sandstone sample and compares the resulting permeability estimates to values obtained with established methods for permeability measurements (air permeameter and numerical simulations). The main result of the study is that it validates the proposed use of PH, as it provides similar values for permeability as the established methods. The presented data and results are certainly interesting and of fair to good scientific value.

However, there are several issues in the presented manuscript that require major revisions before the publication of the study would seem justified. From my point of view, the main issues are:

1. There is a strong mismatch between the stated focus of the study and the presented results. The authors write that "The focus is on the influence of roughness of the fracture surfaces on the flow behavior and the determination of the permeability distribution across a natural bedding plane fracture." Yet, the manuscript contains no quantitative data on roughness or any other comparison of permeability between fractures of varying roughness that would allow the intended assessment. Permeability distribution is also limited to a very brief presentation of permeability anisotropy, which is also not satisfactory if this is the focus of the study.

We agree. Please also see our reply to comment #1 by Reviewer #1. This study was designed to investigate the general functionality of persistent homology for permeability estimation of a single fracture. This was to be investigated by examining the anisotropy in the x- and y-directions as well as the resolution dependency. We therefore rephrase the sentences in our objective section as follows (L88-90):
"The focus is on the anisotropy of permeability in different flow directions as well as the influence of resolution on permeability. Thus, three data set of the same fracture are prepared, which have different resolutions (50 µm, 100 µm and 200 µm)."

We also add a comment in out conclusions section to show that the actual influence of roughness is a crucial issue, which should be addressed in future work (L345-346):
"Furthermore, the influence of roughness on the flow behaviour and the permeability distribution across the fracture should be investigated further."

2. In part, the comparisons made with other studies in the results and discussion sections are difficult to justify, or they are not explained well enough. For instance, I had trouble seeing how absolute permeability values of a single fracture of a real sandstone can or should be

compared to permeabilities of fracture networks in an unspecified material (probably synthetic). The same applies to the comparison with trends of PH-derived permeability of porous media.

We partly agree. The comparisons presented in this study are used to show that persistent homology is used for permeability assessment in a single fracture in addition to porous media and discrete fracture networks. In addition, the general trend is to be shown that persistent homology slightly overestimates the reference value. It is by no means intended to draw conclusions that a single sandstone fractures (bedding plane) behaves exactly as 3D printed discrete fracture network (DFN). Nevertheless, we elaborated the section (L286-L296):
“Of particular interest for this study are the permeabilities of fracture networks, which are displayed as dark gray diamonds in Figure 5, since they are also based on fractured instead of porous material. In general, it can be identified that permeabilities of fracture networks are distributed closer around the 1:1 line compared to porous media values (light gray crosses) in Figure 5. In addition, it is also not surprising that the results of this study have permeability values closer to those of fracture networks rather than porous rocks. This is due to mechanical aperture of the individual fractures, which form a fracture network, being of a similar order of magnitude to the single fracture investigated here. Since the most values from fracture networks are results of the analysis of fracture networks with plane fracture surfaces in the study of Suzuki et al. (2021), it is possible to estimate the influence of surface roughness as well. The rough single fracture studied here shows the same trend of permeabilities, the majority of which are overestimated slightly, as the planar fracture networks addressed. This suggests only a minor influence of the roughness on the final result of the PH analysis. However, it should be considered that typically fracture surfaces have roughnesses of $H > 0.5$, whereas the roughness of the used fracture is slightly lower (Hx = 0.48 and Hy = 0.42).”

3. The authors conclusions on overestimation of permeability when using PH do not seem to convincingly match their own data. Note that is not necessarily a bad thing, because the presented permeability estimates match those from the other methods rather well.

We partly agree. The data shows that the experimentally or numerically determined reference p are slightly exceeded for the majority of the estimated permeabilities in this study (67 % of estimated permeabilities exceed their reference value). In fact, the overestimation of permeability is rather low compared to the other permeabilities presented. Since the same trend can be seen in the study of Suzuki et al. (2021), we have included the conclusion on overestimation of permeabilities in this study.

4. One interesting and perhaps critical feature in the sample, a barite vein, is qualitatively interpreted to have important influence on the fracture permeability. However, this feature is not mentioned in the sample description, nor is it described quantitatively.

We agree. Hence, the barite vein is now mentioned in the sample description as follows (section 2.1, L101-109):
“Furthermore, the findings of Hale et al. (2020) and Hale and Blum (2022) are crucial, since they performed investigations on fracture permeability on exactly the same fracture. They determined the average fracture permeability to be 5.6×10^{-10} m². In addition, they found that the centre of the fracture is less permeable than the left and right side of the fracture (according to the front view of the sandstone block shown in Figure 1a). On the right side of the fracture, this can be explained by a barite vein intersecting the fracture, which was formed before the fracture opening. In the closer vicinity of the vein, the mechanical aperture is increased and the roughness is lower compared to central parts of the fracture.”

5. Overall, I think that the rich high-resolution image data would allow for much more nuanced and quantitative analysis and discussion. The quality of the study would greatly benefit from including quantification of the fracture's properties (roughness, spatial variability) and combining that data with PH-derived permeability.

We partly agree. The primary aim of this study was to prove the general functionality of persistent homology for permeability estimation of single fractures. For this reason, this study is limited to the general trends and directionality of permeability. Certainly, a more detailed consideration of the permeability distribution in parts of the fracture would be possible based on the high-resolution scans. However, we see this as part of future work and therefore included the following paragraph in the "Conclusions" chapter (L347-349):
"In addition, a more detailed investigation of the permeabilities of different areas of this fracture could be performed on the basis of the high-resolution scans used here. This could also allow a potential scaling effect of the permeabilities to be analysed in more detail."

Regarding the inclusion of fracture properties such as roghness, please see our reply to comment #1 by Reviewer #1.

6. In addition to the scientific content, the authors might consider performing extensive language editing for conciseness and more clarity.

We agree and implemented the suggestions in our manuscript. The line numbers refer to the revised manuscript and may differ slightly from the unrevised ones:

Introduction:
L41-42: **rephrased:** Experimental methods provide more detailed results than empirical methods which use more simplified relations for fast practical application.
L59: **rephrased:** …, which would exceed technical possible conditions in laboratory experiments.
L61: **removed:** it has to be considered
L63: **removed:** however
L69-70: **rephrased:** …, but adequate use of machine learning requires deep technical understanding, rigorous testing and sufficient amounts of training data.
L71: **removed:** crucial
L76: **rephrased:** most used
L84-85: **rephrased**: In these small-scale (millimeter to centimeter scale) studies the effect of fracture roughness was not particularly investigated

Methods:
L101-111: In fact, this is an incorrect statement of our side. The range of matrix permeability is rather 0.1-1 mD, which is based on the measured values of 0.17-0.36 mD by Hassanzadegan et al. (2012) and the statement of Cheng et al. (2020) that the permeability is in the range of 10^{-18} m^2. This was adjusted accordingly.
In addition, the following sentences were **rephrased**: Of particular interest for this study is the low matrix permeability of 0.1-1 mD (Cheng et al., 2020; Hassanzadegan et al., 2012). Furthermore, the findings of Hale et al. (2020) and Hale and Blum (2022) are seminal, since they performed investigations on fracture permeability on exactly the same fracture. They determined the average fracture permeability to be 5.6 · 10-10 m^2. In addition, they found that the center of the fracture is less permeable than the left and right side of the fracture (according to the front view of the sandstone block shown in Figure 1a). On the right side of the fracture, this can be explained by a barite vein intersecting the fracture, which was formed before the fracture opening. In the closer vicinity of the vein,

the mechanical aperture is increased and the roughness is lower compared to central parts of the fracture. Comparing fracture and matrix permeabilities shows that the fracture permeability exceeds matrix permeability by more than eight orders of magnitude. Therefore, the matrix permeability is considered negligible in this study.
L142: The barite vein is not sealing the fracture, since it was created before the opening of the fracture. For clarification, we added this statement in L107-108.
L143-144: **rephrased**: Since the matrix permeability is eight orders of magnitude lower than the fracture permeability, the matrix was considered to be fully impermeable.
L164: black areas are **the rock matrix** …
L197: … is thickened (**cyan**) and thinned (**pink**)
L224-225: The following sentence was **added**: In equation 2, ah is the hydraulic aperture of the fracture, v is the fluid flow velocity, µ is the dynamic viscosity, L is the length of the fracture (in flow direction) and Δp is the hydraulic pressure gradient.
L228: Yes, the results were obtained by cubic law, but they were removed anyway (c.f comments to reviewer #1)

Results and discussion:
L242: We added the description of the barite vein in the methods (c.f. comment to L101-110)
L260: **removed**: Nevertheless
L285: … to the results of **Suzuki et al. (2021)**.
L29-2987: **rephrased**: Furthermore, the local cubic law, seems to be also valid for rough single fracture such as a bedding plane joint of a sandstone
L298-299: This is **overall in good agreement** with …
L299: **local** cubic law
L311: **In previous sections**, it is shown that …
L331: **removed**: This is particularly valid in the order of magnitude from 10^{-10} to 10^{-8} m².
L332: **removed**: However
L350: **removed**: However
