

Review History for "Modeling acoustic emissions in heterogeneous rocks during tensile fracture with the Discrete Element Method" *Robert A. Caulk* 2020

Summary

The paper was sent to three Reviewers: Dr. Vanessa Magnanimo, University of Twente (Reviewer 1), one anonymous reviewer (Reviewer 2), and Dr. Giovanni Grasselli, University of Toronto (Reviewer 3). The three reviewers remained anonymous during the entire revision process. After the reviewing process was completed, Reviewers 1 and 3 decided to disclose their identity.

In the first round of review, Reviewer 1 found the quality of the work insufficient for publication and recommended to decline the submission. Both Reviewer 2 and Reviewer 3 found the work suitable for publication, with only minor revisions to be made to the manuscript before it could be accepted. It is worth mentioning that Reviewer 2 pointed out to the Editors that this manuscript was very similar to a technical note by the same Author, available on Zenodo (an open-access repository developed under the European OpenAIRE program and operated by CERN). The Editor decided to ask the Author to submit a revised version taking into account the suggestions by the three Reviewers (major for Reviewer 1, minor for Reviewers 2 and 3), and also clarifying the issue with his technical note on Zenodo.

In the second round of review, Reviewer 2 recommended to accept the paper without any further modification. Reviewer 1 and 3 had still some reservations about the scientific value of the paper, and asked for further revision. Moreover, Reviewer 1 suggested that the existence of the technical note on Zenodo might be a reason not to accept the paper for publication in Open Geomechanics. The Editor decided to ask the Author to submit yet another revised version to address the technical remarks by Reviewers 1 and 3, while emphasising that **the existence of an unreviewed technical note on Zenodo by no means precludes the interest for Open Geomechanics to publish a similar (or even the same) work after peer review.** In this case, publication in Open Geomechanics does not make the work more accessible, but rather more credible – thanks to a (public) peer review process.

In the third and last round of review, Reviewers 1 and 3 have agreed on our position with respect to the technical note on Zenodo, and recommended to accept the manuscript without any further modifications. The Editor confirmed this decision.

Please note: In the Author's responses, quoted reviewer comments are in grey.

Review Round 1

Reviewer 1 (Vanessa Magnanimo)

The paper addresses the ability of a new experimental/numerical approach to predict acoustic emission related to fracture in rocks. The methodology involves a combination of digital image analysis to infer cracks heterogeneity in rock samples and Discrete Element simulations. Despite the relevance of the topic and the high potentiality of the approach, I find the quality of the work insufficient for publication in this journal. General and detailed comments are reported below.

General comments:

- There are too many acronyms and over-technical words that make the article impervious to read.
- It is not clear if the approach that combines image analysis to infer EILD and implementation of this distribution in DEM samples has been proposed in this paper for the first time or it has been proposed by the authors (or other authors) in a previous paper.
- It is unclear how the experimental procedure described in Sec. 3 is applied to the specific case in Sec. 4. Is the EILD distribution inferred from the experiments in (Zietlow and Labuz, 1998) and then applied to the DEM sample? How are the other parameters in Table1 defined? How is the size distribution of the DEM particles decided?
- I do not see a real match in the macroscopic response between experiments and DEM. In order to discuss about AE in "that specific" experimental sample, a proper calibration should be performed on the same rock either on the stressstrain response of the test or (better) via an independent experiment. This is missing in the present paper. Moreover, the validation phase is somehow confused with a parametric study on the influence of gamma on the materials response. The two aspects should be treated independently. After proper calibration, the response should be validated against experimental data and later the parametric study can be performed.
- There are often cross references to analysis in other papers (e.g., line 291-292). A paper cannot rely on information provided in different paper. Rather, it should be self-explaining.
- Many figures are not properly introduced or commented, e.g. Figs. 3, 9, 11, 12, and 13.

Minor comments:

- Eq. 2: there is a mismatch in the definition of kn.
- I would hesitate to relate kt/kn to the Poisson's ratio.
- Eq. 7: how are the friction and cohesion at contact calibrated?
- Eq. 8: how does theta_{int} enter in the equations? How is theta_{int} calibrated/validated?
- Is it plausible to assume that the grain strength follows EILD? Is this anyhow validated in this or previous works?
- I don't understand why the assumption of a Weibull distribution is needed if the actual edges size and distribution is obtained via image analysis.
- Line 170: gamma is not defined.
- The steps between Figs. 2, 3, and 4 are not clear.
- Sec. 3.3: the strain energy distribution results unclear to me. Moreover, how is "predefined radius" decided? This quantity seems to have a great influence on the value of the magnitude Me.
- Sec. 3.4: The experiment of reference should be described in more detail. I cannot agree on the assumption that differences between rock types can be assigned to the Weibull parameter gamma only.
- Some of the micro-parameters are not defined.

- What is the meaning of "Masked response" in experiments? This is not at all clear, neither from the figure nor from the text.
- Results in Fig. 10, with a concentration of (micro-)cracks in the lower-centre areas are not at all surprising in a three point bending test.
- Some of the observations in Sec. 5 are a consequence of the specific model adopted (e.g., the clusters and weak zones), that is can be hardly be considered outputs.

In conclusion, many assumptions and empirical solutions are proposed in the transfer from the IELD distribution to DEM simulations. Or, at least, not sufficient details are given to assess the accuracy of the present approach, and specifically of this particular implementation.

Reviewer 2 (Anonymous)

This study presents a methodology for modeling AE in heterogeneous rock fracturing. The manuscript is well organized and presented. I have some minor comments that the authors may consider to improve the manuscript.

- The authors use the length of interacting edge to represent the bond strength between particles. I understand this is an
 assumption used to simplify the stress intensity issue in DEM modeling. However, the authors need to provide more
 evidence to justify this assumption. Clearly, this assumption is not consistent with the physics behind the bonding
 strength. The bonding strength is independent of the contacting area (or edge length). The edge length is governing the failure at the bond through altering the local stress state. With smaller edge length, stress intensity is more
 significant that the bond breaks first (it is not because the bond strength is lower).
- 2. The EILD is implemented by altering the contact radius (area). It is true that this approach can change the bonding strength accordingly, but it also changes the bending stiffness at the contact. I am not sure if bending is involved in the model presented in this manuscript. So the authors may need to add some discussions about this effect. Whether changing the bending stiffness will change the behaviors or not at sample scale.
- 3. page 12 line 184. Could the authors explicitly provide the v_{p1} and v_{p2} as a function of density and time step?
- 4. page 14 line 211, two specimens
- 5. page 16 line 247, the two citations should be in parentheses.

Reviewer 3 (Giovanni Grasselli)

The use of a Weibull function to account for the heterogeneity of bond strength in a particle based DEM is an interesting approach that addresses several of the current constraints associated with that methodology, especially when trying to model AE. The edge interaction length distribution proposed by the author is really intriguing and I think could be extended to other discrete methodologies. I am also wondering if it could work on more shear based loading conditions. I think that point should be addressed in the text. The introduction is well written, but quite limited to relatively old papers, while there has been quite a bit of new developments and publications in the past 5 years. The other minor issue I have is related to the only experimental data used for validation (Labuz's group) does not really provide all the details necessary to fully calibrate the model, thus resulting in much more events recorded in the model with respect to the published lab results. My opinion is that the paper should be accepted. It is well written and easy to read, and certainly introduce an intriguing numerical approach that is worth to be disseminated.

Other suggestions:

- Add colour code/scale to bonds and dots in figures 12-13-14. As it is now, it is very unclear if colour refers to stress, magnitude, time, or something else.
- Loading velocity of 0.01m/s is very high with respect to what used in the lab. The authors should mention the reason for using it and also explain why that velocity could be still used to model quasi-static tests.
- Line 73. Remove "recently". A 2004 paper is not recent anymore.

Author Response

The author thank all reviewers for their excellent feedback. It is clear they each read the article from a critical perspective and there is no doubt that their feedback has improved the quality of the article. The author attempted to address each comment individually with details here and clarifications in the manuscript.

(ed) Regarding the existing paper on Zenodo:

With the goal of assisting other users who wished to use the acoustic emissions model in Yade, the authors released an earlier version of this work for free and without peer review on Yade's website and open science repository Zenodo.org in 2018. In comparison, the present paper's Appendix B, "Comparison of numerical and experimental elastic waves", was performed and added to improve model and result confidence. Additionally, the present document contains improved writing, clearer equation presentation, and available test scripts. As is usual with other pre-publication research materials stored on Zenodo, we retain all rights to share, adapt, and modify this text. Authors have added a note citing the document on Line 78

Response to Reviewer 3

The use of a Weibull function to account for the heterogeneity of bond strength in a particle based DEM is an interesting approach that addresses several of the current constraints associated with that methodology, especially when trying to model AE. The edge interaction length distribution proposed by the author is really intriguing and I think could be extended to other discrete methodologies.

I am also wondering if it could work on more shear based loading conditions. I think that point should be addressed in the text.

The authors did not explore shear based loading conditions. Considering other studies have seen success simulating acoustic emissions in compressive tests without the consideration of heterogeneity, the authors expect the introduction of this heterogeneity model to yield the same results presented within: increasing heterogeneity should increase the size of the spatial distribution of AE activity in shear based loading conditions. Authors comment on the method's applicability to shear based loading conditions on Line 251.

In case the reviewer is also concerned about the logistics of applying the methods to other geometries and loading conditions: the software implementation of the presented methodology is not confined to a single loading condition. Instead, future researchers need only to set up their desired geometry and loading conditions in Yade. The AE/heterogeneity models will operate automatically and generate the visualization of AE locations and magnitudes.

The introduction is well written, but quite limited to relatively old papers, while there has bees quite a bit of new developments and publications in the past 5 years.

The authors have included included additional works on AE monitoring in rocks, AE simulation in DEM or FEMDEM, heterogeneity modeling, and fracture modeling (Line 26, 40, 89, 124, 156, 157, 158):

- Meng, Q., Zhang, M., Han, L., Pu, H., & Nie, T. (2016). Effects of Acoustic Emission and Energy Evolution of Rock Specimens Under the Uniaxial Cyclic Loading and Unloading Compression. Rock Mechanics and Rock Engineering, 49(10), 3873–3886. https://doi.org/10.1007/s00603-016-1077-y
- Iturrioz, I., Birck, G., & Riera, J. D. (2019). Numerical DEM simulation of the evolution of damage and AE preceding failure of structural components. Engineering Fracture Mechanics, 210(2018), 247–256. https://doi.org/10.1016/j.engfracmech.2018.02.023
- Birck, G., Riera, J. D., & Iturrioz, I. (2018). Numerical DEM simulation of AE in plate fracture and analogy with the frequency of seismic events in SCRs. Engineering Failure Analysis, 93(December 2017), 214–223. https://doi.org/10.1016/j.engfailanal.2018.06.024
- Saksala, T. (2015). Rate-Dependent Embedded Discontinuity Approach Incorporating Heterogeneity for Numerical Modeling of Rock Fracture. Rock Mechanics and Rock Engineering, 48(4), 1605–1622. https://doi.org/10.1007/s00603-014-0652-3

- Nitka, M., & Tejchman, J. (2016). Mesoscopic Simulations of Concrete Fracture Based on X-ray CT Images of Interial Structure. 9th International Conference on Fracture Mechanics of Concrete and Concrete Structures. https://doi.org/10.21012/fc9.039
- Da Cruz, F., Emam, S., Prochnow, M., Roux, J. N., & Chevoir, F. (2005). Rheophysics of dense granular materials: Discrete simulation of plane shear flows. Physical Review E Statistical, Nonlinear, and Soft Matter Physics, 72(2). https://doi.org/10.1103/PhysRevE.72.021309
- Nitka, M., & Tejchman, J. (2015). Modelling of concrete fracture at aggregate level using DEM based on X-Ray CT images of internal structure. Proceedings of the 4th International Conference on Particle-Based Methods Fundamentals and Applications, PARTICLES 2015, 147, 343–354. https://doi.org/10.1016/j.engfracmech.2015.08.010
- Bai, Q. S., Tu, S. H., & Zhang, C. (2016). DEM investigation of the fracture mechanism of rock disc containing hole(s) and its influence on tensile strength. Theoretical and Applied Fracture Mechanics, 86(July), 197–216. https://doi.org/10.1016/j.tafmec.2016.07.005
- Tan, Y., Yang, D., & Sheng, Y. (2009). Discrete element method (DEM) modeling of fracture and damage in the machining process of polycrystalline SiC. Journal of the European Ceramic Society, 29(6), 1029–1037. https://doi.org/10.1016/j.jeurceramsoc.2008.07.060

The other minor issue I have is related to the only experimental data used for validation (Labuz's group) does not really provide all the details necessary to fully calibrate the model, thus resulting in much more events recorded in the model with respect to the published lab results.

The difference in acoustic event number is also a result of the Piezoelectric transducer's detectable amplitude, sampling rate, and the storage capacity of the experimental collection system. In Zietlow 1998, their system sampled at 20 MHz (50 ns between data points). Further, they only collected events that triggered the transducers beyond 10mV. Other storage and RAM limitations ultimately led the authors to estimate that their setup enabled the recording of a maximum of 64 events if they occurred simultaneously. In comparison, the DEM model does not use an event size threshold, records much smaller events, and does not have a limit on the number of events that can occur simultaneously. Of course, the reviewer is right to point out that the lack of full calibration contributes to the differences in AE activity. However, a full calibration is beyond the scope of this paper. Instead, the objective of the paper is to explore the effect of the EILD on the numerical IPZ and to use the experimental results to verify trends.

This point has been elaborated in the manuscript at Line 325.

My opinion is that the paper should be accepted. It is well written and easy to read, and certainly introduce an intriguing numerical approach that is worth to be disseminated.

Other suggestions:

Add colour code/scale to bonds and dots in figures 12-13-14. As it is now, it is very unclear if colour refers to stress, magnitude, time, or something else.

In fact, these colors are used to distinguish between events, the actual color themselves have no quantity besides an arbitrary Event ID number. The goal of these figures is to demonstrate the number of broken bonds (colored lines) that ultimately cluster together to yield a single event (colored circle). This was not clear enough in the manuscript and has now been added to Figure 12-13-14 captions.

Loading velocity of 0.01m/s is very high with respect to what used in the lab. The authors should mention the reason for using it and also explain why that velocity could be still used to model quasi–static tests.

The reviewer makes an excellent point. We consider the simulation quasi-static and therefore we aim to keep the inertia number of the system below a conservative 10^{-3} , even though it is recommended that quasi-static experiments keep the inertial number beflow 10^{-2} by the highly cited paper:

• Da Cruz, F., Emam, S., Prochnow, M., Roux, J. N., Chevoir, F. (2005). Rheophysics of dense granular materials: Discrete simulation of plane shear flows. Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 72(2). https://doi.org/10.1103/PhysRevE.72.021309

Further, the same inertia management methodology was implemented for a three point DEM bending test of concrete in:

• Nitka, M., & Tejchman, J. (2015). Modelling of concrete fracture at aggregate level using DEM based on X-Ray CT images of internal structure. Proceedings of the 4th International Conference on Particle-Based Methods - Fundamentals and Applications, PARTICLES 2015, 147, 343–354. https://doi.org/10.1016/j.engfracmech.2015.08.010

In our particular case we follow the same logic:

 $I = \dot{\varepsilon} \sqrt{\frac{m}{Pd}} = 0.0009 < 10^{-3}$ $\dot{\varepsilon} = \frac{0.01m/s}{0.08m}$ m = 2.98x10kg $d_{min} = 0.0022m$ P = 1kPa

Where P is the pressure used to create the random dense packing before adding the cohesive bonds to the particles. Since $0.0009 < 10^{-3}$, the selected loading rate keeps the simulation from entering the "dense flow" inertial regime. By increasing strain rate in this way, we reduce the computational cost for reaching solution, while maintaining the accuracy of the results. The authors have added this note to the text at Line 257.

Line 73. Remove "recently". A 2004 paper is not recent anymore.

Done.

Response to Reviewer 2

This study presents a methodology for modeling AE in heterogeneous rock fracturing. The manuscript is well organized and presented. I have some minor comments that the authors may consider to improve the manuscript.

1. The authors use the length of interacting edge to represent the bond strength between particles. I understand this is an assumption used to simplify the stress intensity issue in DEM modeling. However, the author need to provide more evidence to justify this assumption. Clearly, this assumption is not consistent with the physics behind the bonding strength. The bonding strength is independent of the contacting area (or edge length). The edge length is governing the failure at the bond through altering the local stress state. With smaller edge length, stress intensity is more significant that the bond breaks first (it is not because the bond strength is lower).

As the reviewer points out, failure in DEM is commonly modelled using strength criteria. From a micromechanical perspective, if we consider two particles bonded by a beam (cement), the criteria is physically accurate considering the maximum allowable tensile force of the beam depends on its cross-sectional area and tensile strength. Same in shear. Thus, variation of material "toughness" emerges naturally in the system, as noted by the reviewer. This use of DEM to model realistic rock/concrete fractures is extensive in literature, and we have added this discussion to the text at Line 155.

2. The EILD is implemented by altering the contact radius (area). It is true that this approach can change the bonding strength accordingly, but it also changes the bending stiffness at the contact. I am not sure if bending is involved in the model presented in this manuscript. So the authors may need to add some discussions about this effect. Whether changing the bending stiffness will change the behaviors or not at sample scale.

Bending stiffness is not considered in the model presented. Only normal and shear stiffnesses/strengths are considered. Authors have clarified in Line 153 that the current DEM model does not include bending stiffness.

3. pg 12 line 184. Could the authors explicitly provide the v_{p1} and v_{p2} as a function of density and time step?

The p-wave velocities of the particles are a function of density and young's modulus

$$v_p = \sqrt{E/\rho}$$

We added this to the text at Line 222 and we encourage the reviewer to refer to the definition and usage of the pwave velocity made in the source code for further details [1].

https://gitlab.com/yade-dev/trunk/blob/master/pkg/dem/JointedCohesiveFrictionalPM.cppL448

4. pg 14 line 211, two specimens

The second word "specimen" is now removed from the text.

5. pg 16 line 247, the two citations should be in parentheses.

The sentence was edited to refer directly to the two studies.

Response to Reviewer 1

The paper addresses the ability of a new experimental/numericla approach to predict acoustic emission related to fracture in rocks. The methodology involves a combination of digital image analysis to infer cracks heterogeneity in rock samples and Discrete Element simulations. Despite the relevance of the topic and the high potentiality of the approach, I find the quality of the work insufficient for publication in this journal. General and detailed comments are reported below.

General comments:

- There are too many acronymous and over-technical words that make the article impervious to read.

The reviewer's concern is valid, the article contains too many unnecessary acronyms, the full list follows: CL, BPM, IPZ, FPZ, AE, DEM, EILD, REV

Authors removed the following acronyms in an attempt to improve the readability of the article: CL, BPM, FPZ, REV

Due to the frequency of usage in both the literature and the present paper, authors opted to keep the remaining acronyms: AE, DEM, IPZ

And finally, authors elected to keep the acronym EILD, which was created for this paper to improve readability.

The authors also attempted to simplify/remove any words/discussion they believed to be "over-technical" and unnecessary throughout the paper.

- It is not clear if the approach that combines image analysis to infer EILD and implementation of this distribution in DEM samples has been proposed in this paper for the first time, it has been proposed by the authors (or other authors) in a previous paper.

With the goal of assisting other users who wished to use the acoustic emissions model in Yade, the authors released an earlier version of this work for free and without peer review on Yade's website and open science repository Zenodo.org in 2018. In comparison, the present paper's Appendix B, "Comparison of numerical and experimental elastic waves", was performed and added to improve model and result confidence. Additionally, the present document contains improved writing, clearer equation presentation, and available test scripts. As is usual with other pre-publication research materials stored on Zenodo, we retain all rights to share, adapt, and modify this text. Authors have added a note citing the document on Line 78

- It is unclear how the experimental procedure described in Sec.3 is applied to the specific case in Sec.4. Is the EILD distribution inferred from the experiments in (Zietlow and Labuz, 1998) and then applied to the DEM sample?

The reviewer's confusion regarding Sec 3.1 is valid and the authors have clarified this in the document at Line 191. Since we do not have access to thin sections associated with the rocks used in Zietlow 1998, we instead present Sec. 4 as a parametric sweep of Weibull shape factors, with the goal of demonstrating the effect of increasing numerical heterogeneity on the intrinsic process zone. Thus, the example rock thin section used in Sec 3.1 is only used to demonstrate the image analysis method and confirm the validity of the Weibull type statistical distribution for the edge-interaction-length-distribution. On

the other hand, Sec 3.2 (implementation of EILD), 3.3 (numerical AE model), and 3.4 (3pt bending test procedure) are all used in Sec 4 for the simulation of AE activity with respect to various Weibull shape factors during numerical 3pt bending tests (Line 244).

How are the other parameters in Table1 defined? How is the size distribution of the DEM particles decided?

The DEM microproperties highlighted in Table 1 represent a generic rock with similar strength and deformation characteristics to the quartzite, sandstone, and granite specimens tested by Zietlow 1998. A perfect calibration of each rock type was not performed since a) Zietlow 1998 did not release full deformation curves for each rock type and b) this study aims to isolate the effect of the Weibull shape parameter, Weibull shape parameter, on acoustic emission spatial distributions during failure. Therefore, the DEM rock specimens used throughout the study maintains the same micro parameters (Tab.1) while varying Weibull shape parameter. The point is clarified and rewritten in Sec. 3.4. The size distribution of the particles is bounded by AE resolution (i.e. obtaining realistic AE activity as shown in Fig. 8) and computational efficiency (the basis of the paper, see Line 17).

- I do not see a real match in the macroscopic response between experiments and DEM. In order to discuss about AE in "that specific" experimental sample, a proper calibration should be performed on the same rock either on the stress-strain response of the test or (better) via an independent experiment. This is missing in the present paper. Moreover, the validation phase is somehow confused with a parametric study on the influence of γ on the materials response. The two aspects should be treated independently. After proper calibration, the response should be validated against experimental data and later the parametric study can be performed.

It is worth noting here that the original manuscript discussed the lack of full calibration twice in an attempt to make the interpretation of results as transparent as possible (original manuscript Lines 212 and 260). However, the authors accept that the point is not made well enough, and the reviewer is correct to point out the confusion. In brief: the paper does not aim to simulate directly the AE in any specific experimental sample. Instead, the paper aims to demonstrate the effect of the Weibull shape parameter (numerical heterogeneity) on the numerically generated acoustic emissions. Ultimately, the goal is to demonstrate that the presented numerical heterogeneity model is capable of adding heterogeneity (depending on the magnitude of the Weibull shape parameter) to the specimen in a way that increases the size of the numerical intrinsic process zone, similar to experimental observations of the intrinsic process zone for rocks containing various magnitudes of heterogeneity.

The authors agree with the reviewer that this does not constitute a true "validation". Instead it is a verification that the release of energy in the numerical system during failure is more widely distributed with the introduction of heterogeneity, similar to experimental trends. Further, the elastic waves are traveling through the system in a similar manner to what we would expect experimentally (Appendix B). Therefore, the authors have rewritten the article to make this point clearer (e.g. Line 71, Sec 3.4, Line 387).

- There are often cross references to analysis in other papers (e.g. line 291-292). A paper cannot rely on informations in different paper. Rather, it should be self-explaining.

Line 291-292 (of the original submission) refers to the present numerical analysis only. Authors have attempted to clarify this in the paper at Line 367.

- Many figures are not properly introduced or commented, e.g. Figs. 3,9,11, 12, 13.

Fig. 3 caption improved Fig. 9 ordering corrected (now Fig. 8) Fig. 11 reordered so that Fig. 11a is referenced before Fig. 11b Fig. 12 no longer referenced early in the text Figs. 12-14 caption improved and introduced more clearly in the text. Line 346

Minor comments: - Eq.2: there is a mismatch in the definition of kn.

The definition of kn is corrected.

- I would hesitate to relate kt/kn to the Poisson's ratio.

The comment is removed

- Eq7: how are the friction and cohesion at contact calibrated?

Generic DEM calibration is performed using the deformation parameters first to obtain proper macroscopic young's modulus (of the experimental sandstone Zietlow 1998). Next, the strength parameters (friction, cohesion, θ_{int}) are calibrated to obtain the correct failure strength (of the experimental sandstone Zietlow 1998). A brief description of the calibration is added to the paper at Line 266.

- Eq8: how does θ_{int} enter in the equations? How is θ_{int} calibrated/validated?

 θ_{int} factors the allowable interaction range for two particles. See Eq.8, if two particle centers are within D_{eq} , they are considered interacting and possibly cohesive depending on if they are within the range when cohesion is set. The point has been clarified at Line 164.

- Is it plausible to assume that the grain strength follows EILD? Is this anyhow validated in this or previous works?

There is no evidence presented in this paper to suggest that the strength distribution of individual grains follows the same distribution as the EILD.

- I don't understand why the assumption of a Weibull distribution is needed if the actual edges size and distribution is obtained via image analysis.

The assumption of the Weibull distribution is needed so that we can fit a statistical model to the obtained imagery data. The statistical model is necessary so we can generate random deviates ($alpha_w$) which can be used to factor the bond properties in DEM.

- Line 170: γ is not defined.

γ is now defined.

- The steps between Figs. 2-3-4 are not clear.

Sec. 3.1 is now clarified. In brief, 1) the image analysis is used to gather the edge length data (histogram, Fig 2), 2) Maximum likelihood is used to estimate the Weibull model parameters to fit the image analysis data (model, Fig 2), 3) The estimated Weibull shape factor is used to generate random deviates (Fig 3) which are used to factor the bond strengths (Eq. 12+Eq. 6). Fig 4 shows the final distribution of tensile bond strengths in the specimen. As expected, it follows closely to a squared Weibull distribution.

- Sec.3.3: the strain energy distribution results unclear to me. Moreover, how is "predefined radius" decided? This quantity seems to have a great influence on the value of the magnitude Me.

The radius defines the neighborhood surrounding the broken bond that experiences the greatest contribution of the total strain energy change of the system. Hazzard and Damjanac (2013) showed that a volume constrained by 2 to 5 particle diameters captures the strain energy change of the entire system due to one broken bond (Line 215). Beyond this neighborhood, the strain energy change contribution is so small that it is not worth the computational effort required to obtain it. Thus, the value does not have an influence on the value of the magnitude. The authors have clarified this point at Page 13 footnote 1.

- Sec.3.4: The experiment of reference should be described in more detail. I cannot agree on the assumption that differences between rock types can be assigned to the Weibull parameter γ only.

The paper does not try to model the experimental rocks directly. Instead, the paper uses the experimental results to demonstrate the trend of IPZ dimensions and load based AE activity with respect to specimen heterogeneity. Authors have improved the description of this in Sec 3.4.

- Some of the micro-parameters are not defined.

Authors added λ (AE neighborhood radius) to the microparameter table (Table 1).

- What is the meaning of "Masked response" in experiments? This is not at all clear neither from the figure nor from the text.

The stiffness associated with the experimental apparatus needs to be considered when interpreting experimental results. If experimental loads are high enough, the true load displacement curve is "masked" by the effect of apparatus stiffness during loading and failure. In other words, the experimental data contains the deformation of the apparatus in addition to the rock deformation. Figure 7b shows how the stiffness of the experimental specimen should be higher if the experimental apparatus did deform during the experiment. In DEM, the "experimental apparatus" has an infinite stiffness and therefore the results should be unmasked. Authors clarify on Line 294, 295.

- Results in Fig.10, with a concentration of (micro-)cracks in the lower-centre areas are not at all surprising in a 3-points bending test.

The authors agree with the reviewer. Fig.10 attempts to demonstrate how the large AE events track through the center of the macro failure (broken bonds in red). Authors have clarified this on Line 325.

- Some of the observations in Sec.5 are a consequences of the specific model adopted (e.g. the clusters and weak zones), that is can be hardly be considered outputs.

The authors agree that tough regions and microdefects are infact model inputs. Authors intended to use this comment to explain the development of the numerical IPZ. Authors have clarified this on Line 391.

In conclusion, many assumptions and empirical solutions are proposed in the transfer from the IELD distribution to DEM simulations. Or, at least, not sufficient details are given to asses the accuracy of the present approach, and specifically of this particular implementation.

The transfer of the EILD to the DEM simulations follows these steps: 1) measure grain edge lengths, generate a histogram of these data 2) fit a statistical model to the data 3) use the statistical model to generate random deviates which are used to factor DEM bond strengths. Authors hope the changes highlighted throughout this review help to clarify this point.

Review Round 2

Reviewer 1 (Vanessa Magnanimo)

The authors have made a strong effort to improve clarity and readability of the paper, working out several details.

However, I still find that the work doesn't have the sufficient focus and structure to be published in this journal. Rather the paper strongly resembles the open access material previously made available by the same authors in Zenodo.org in 2018.

The novelty of the paper with respect to the previously published material seems to be limited to the content of Appendix B and improved writing, equations etc. In my view, this is not sufficient to justify the publication of an "original" paper. Related to this, the actual papers experiences defects typical of an open documentation, which is lack of focus and structure.

I suggest that the authors select a clear goal and rewrite the paper accordingly for a new submission. For example, the application of their methodology (already available in Zenodo.org) to an experiment where data on the distribution along with the acoustic emission are available would be extremely interesting, including a careful calibration and validation.

Similarly an extensive parametric study could be of great use for the scientific community. In that case the (incomplete) comparison with experiments in (Zietlow and Labuz, 1998) is not needed and is source of confusion.

Reviewer 2 (Anonymous)

The authors addressed all my previous concerns and questions. I have no further comments to the revised manuscript. I recommend to accept the revised manuscript for publication.

Reviewer 3 (Giovanni Grasselli)

As mentioned in the introduction, the paper aims to "introduce a methodology designed for the investigation of rock matrix heterogeneities and their effect on pre- and post- fracture Acoustic Emission (AE) distributions" using DEM.

However, it focuses only on spherical discrete elements (see reductive definition of DEM at line 136) and not on general e.g., tetrahedral, or cubical shapes. This is not clearly stated in the paper, making the message a bit misleading.

From my experience, spherical DEM are good approximation to simulate particulates, however, have great limitations in capturing the real mechanical response of cohesive, or where the angularity of the rock constituent grains has to be considered. Another major issue of spherical DEM relates to the model generation: the cohesive rock matrix has to be simplified into packed spheres, with all macroscopic material properties to emerge from the interaction of spheres connected through bonding with assigned microscopic properties. However, no clear and unbiased methodology has proposed, so far, for the packing procedure (size distribution of the particles, etc...) or the assignment of the contact properties.

This work is an interesting attempt to develop a methodology to assign contact properties based on rock microstructure imaging; however, I do not see enough experimental data to support the proposed methodology, as the EILD analysis in section 3.1 is not directly used together with the laboratory tests as stated at lines 191-194. Furthermore, it appears that the alpha parameter is function of the sphere sizes, and thus, on the user modeling strategy.

With respect to section 3.3, it appears to me that the work presented is a simple re-implementation in Yade of the approach proposed by Hazzard in 2002, which is highly sensitive to the chosen spatial window. Furthermore, this approach can just model the location and magnitude of the AE, however, it disregards the mechanism and the temporal trajectory of the propagating crack, which might be much more interesting from both scientific and engineering perspective.

Looking at Figure 10, for example, modelling results and the experimental data are also quite different.

Personally, I also disagree with several statements present in the paper. For example: at line 127 and following, it is stated that "tensile tests generally produce clean fractures with very few (if any) broken bonds in regions surrounding the fracture (Cai and Kaiser, 2004; Ma and Huang, 2017; Mahabadi et al., 2009). These "clean" fractures are likely due to the typical

uniform distribution of particle sizes and the corresponding skewed distribution of bond strengths of traditional DEM." However, no mention is made to the fact that the rock is loaded in a very different manner, with compressive failure more prone to a mixed mode I and mode II cracking, versus only mode I for the tensile failures. This difference, in my opinion, can also explain the difference in AE types and modes.

Despite all my above criticisms, I want to really commend the authors for making all their work available as open source, greatly supporting the scientific community working on Particle element methods. As such I think the specific implementation will be certainly useful to others and as such it is worth to be disseminated. However, specifically to the current paper, as mentioned above, I have several reservations with respect to the value of its scientific contributions.

Author Response

Response to Reviewer 3

The authors are sorry to hear that Reviewer 3 reversed his opinion on this matter between Revision 1 and Revision 2.

However, it focuses only on spherical discrete elements (see reductive definition of DEM at line 136) and not on general e.g., tetrahedral, or cubical shapes. This is not clearly stated in the paper, making the message a bit misleading.

We have edited the line referenced by the reviewer to specify that the current study uses spherical particles (Line 129):

"The present study uses a spherical Discrete Element Method (DEM) to treat particulate material as an assembly of various sized spheres, each characterized by density and stiffness."

In addition, we reference spherical nature of the method directly and indirectly throughout the remainder of the paper: Line 129, 130, 132, 141, 152, 159, 197, Eq 3, Eq 8, Eq 9, Table 1, Figure 6, Pg 12 Footnote 1, Eq 16

From my experience, spherical DEM are good approximation to simulate particulates, however, have great limitations in capturing the real mechanical response of cohesive, or where the angularity of the rock constituent grains has to be considered. Another major issue of spherical DEM relates to the model generation: the cohesive rock matrix has to be simplified into packed spheres, with all macroscopic material properties to emerge from the interaction of spheres connected through bonding with assigned microscopic properties.

There is plenty of literature evidence to support the use of spherical DEM for modeling mechanical behavior and failure of cohesive materials (e.g. Potyondy 2004, Scholtes 2012, Duriez 2016). Angular polyhedral are very expensive to model. Further, heterogeneity modeling is very expensive (Line 16). We highlight in the present paper that the objective of this paper is to make heterogeneity modeling computationally tractable (Line 69). Hence the use of spheres and statistical modeling.

- Potyondy, D. O., & Cundall, P. A. (2004). A bonded-particle model for rock. International Journal of Rock Mechanics and Mining Sciences, 41(8), 1329–1364. https://doi.org/10.1016/j.ijrmms.2004.09.011
- Scholtès, L., & Donzé, F.-V. (2012). Modelling progressive failure in fractured rock masses using a 3D discrete element method. International Journal of Rock Mechanics and Mining Sciences, 52, 18–30. https://doi.org/10.1016/j.ijrmms.2012.02.009
- Duriez, J., Scholtès, L., & Donzé, F. V. (2016). Micromechanics of wing crack propagation for different flaw properties. Engineering Fracture Mechanics, 153, 378–398. https://doi.org/10.1016/j.engfracmech.2015.12.034

However, no clear and unbiased methodology has proposed, so far, for the packing procedure (size distribution of the particles etc...) or the assignment of the contact properties. Furthermore, it appears that the alpha parameter is function of the sphere sizes, and thus, on the user modeling strategy.

We agree with the reviewer that our method poses some very interesting questions about how this acoustic emission model is affected by various discrete element method calibration methods and particle size distributions. The size distribution

here reproduces the expected acoustic emission magnitude distribution (Line 242), which is enough to continue presenting and demonstrating the method in this paper. The current manuscript is focused on the fundamental combination of the heterogeneity model with the discrete element and the acoustic emission models. It is our hope that the fundamental presentation here, along with full source code availability and a highly modifiable user interface, will bolster other scientists whose unique applications will undoubtedly call for various particle size distributions and calibration methods.

This work is an interesting attempt to develop a methodology to assign contact properties based on rock microstructure imaging; however, I do not see enough experimental data to support the proposed methodology, as the EILD analysis in section 3.1 is not directly used together with the laboratory tests as stated at lines 191-194.

The imagery in this paper is used to a) demonstrate the methodology for collecting grain contact quantities from imagery and b) demonstrate the validity of using a Weibull model to describe the distribution of grain contact quantities. We then generalize and implement the model to demonstrate the effect of the Weibull shape factor. We agree that a fully coupled acoustic emission experimental investigation would be favorable – but it is not possible for us to execute and therefore all we have to offer is the open sourced methodology in case other researchers believe a full experimental acoustic emission investigation is beneficial. We have updated the paper to further clarify the intent of the EILD analysis from Sec 3.1 (Line 163 and 175). We make it clear throughout the paper that the method presented is not a full experimental validation (Line 248, 306)

With respect to section 3.3, it appears to me that the work presented is a simple re-implementation in Yade of the approach proposed by Hazzard in 2002, which is highly sensitive to the chosen spatial window.

The strain energy based AE simulation method presented here follows Hazzard 2000 and 2013. In Hazzard 2013, the spatial window was investigated to show that 2 particle diameters was sufficient to match the total strain energy released by the specimen. Thus, we disagree with the reviewer that the method is "highly sensitive to the spatial window". The clustering scheme does depend on a small spatial window, but as mentioned, Hazzard 2013 verified that a spatial window within a few particle diameters resolves the change of strain energy in the entire specimen. We have improved this discussion at Line 217. We also discussed the sensitivity of the spatial window in our original manuscript, in the response to this particular reviewer, and in edits for the the revised manuscript. Pg 12.

Furthermore, this approach can just model the location and magnitude of the AE, however, it disregards the mechanism and the temporal trajectory of the propagating crack, which might be much more interesting from both scientific and engineering perspective.

The approach does not disregard the temporal trajectory of the propagating crack, as outlined in the methods section on Pg. 13 (as well as Hazzard 2013) where it discusses the clustering mechanism. A neighborhood can grow in the direction of failing bonds (crack trajectory) if it is occurring in the same spatial and time window as an existing AE event.

Looking at Figure 10, for example, modelling results and the experimental data are also quite different.

They should not look identical, we are using a stochastic method. But yes, the numerical method does show many more acoustic emissions than the experimental data. There are various reasons for this including 1) we are collecting at a higher sampling rate and 2) we have a higher sensitivity.

at line 127 and following, it is stated that "tensile tests generally produce clean fractures with very few (if any) broken bonds in regions surrounding the fracture (Cai and Kaiser, 2004; Ma and Huang, 2017; Mahabadi et al., 2009). These "clean" fractures are likely due to the typical uniform distribution of particle sizes and the corresponding skewed distribution of bond strengths of traditional DEM." However, no mention is made to the fact that the rock is loaded in a very different manner, with compressive failure more prone to a mixed mode I and mode II cracking, versus only mode I for the tensile failures. This difference, in my opinion, can also explain the difference in AE types and modes

We have corrected the statement. The clean fractures modeled in numerial Brazilian tests observed by Cai and Kaiser, 2004; Ma and Huang, 2017; Mahabadi et al., 2009 match macroscopic fractures but are not able to resolve the release of energy associated with experimentally observed acoustic emissions (Rodriguez 2016). Line 119.

Despite all my above criticisms, I want to really commend the author for making all their work available as open source, greatly supporting the scientific community working on Particle element methods. As such I think the specific implementation will be certainly useful to others and as such it is worth to be disseminated. However, specifically to the current paper, as mentioned above, I have several reservations with respect to the value of its scientific contributions.

The authors appreciate the comment made by the reviewer and agree that the work is worth disseminating.

Response to Reviewer 1

The novelty of the paper with respect to the previously published material seems to be limited to the content of AppendixB and improved writing, equations etc. In my view, this is not sufficient to justify the publication of an "original" paper. Related to this, the actual papers experiences defects typical of an open documentation, that is lack of focus and structure.

The main goal of submitting this paper to a journal was to receive a peer review. The zenodo document was not peer reviewed and therefore has no expert opinion associated with it. Besides the lack of peer review, the two documents referenced by the reviewer are similar. However it is worth pointing out all changes in comparison between the current paper and the paper hosted on zenodo:

- Sec 2.2 Discrete Element Method: rewritten and notation improved
- Sec 3.1 Image analysis: rewritten, presentation of methods changed
- Figure 5 added
- Sec 3.3, editorial changes recommended by reviewers
- Figure 6 recreated to include more detail
- Sec 3.4 Three Point Bending test: rewritten and inertial considerations added by request of reviewers
- Sec 3.5 Practical reproduction of results: added
 - Scripts added for reproducing results added
 - Directions for how to find and modify source code added
- Sec 4 Results: heavily edited and new analyses run to generate:
 - New Figure 7a
 - New Figure 9
 - New Figure 10
- Appendix B analysis added to improve confidence in the acoustic emission scheme and algorithm.
- Various editorial improvements throughout introduction and background.
- Various editorial changes by request of reviewers highlighted in detail in "Revision 1: response to reviewers" document attached.
- Rewritten abstract

Related to this, the actual papers experiences defects typical of an open documentation, that is lack of focus and structure.

We believe the paper is well organized, well written, and most importantly: reproducible.

For example, the application of their methodology (already available in Zenodo.org) to an experiment where data on the distribution along with the acoustic emission are available, would be extremely interesting, including a careful calibration and validation

We agree with the reviewer that the proposed methodology poses interesting questions and can be strengthened by a strict experimental validation. We look forward to making methodology and open source code available in OpenGeomechanics. There is no doubt that making this method available will enable other researchers to focus their time on developing proper acoustic emissions experiments (as suggested by the reviewer) instead of redeveloping the methods presented here.

Review Round 3

Reviewer 1 (Vanessa Magnanimo)

Recommendation: Accept Submission

Reviewer 3 (Giovanni Grasselli)

I am fine with the responses. No additional comments or suggestions.

Editorial Decision

At the end of Review Round Number 3, the managing Editor has decided to accept the revised version of the manuscript for publication without any further changes.