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Review of “A probabilistic model for fast-to-evaluate 2D crack path prediction in heterogeneous materials”

Kathleen PELE^{1,4}, Jean BACCOU^{3,4}, Loïc DARIDON^{2,4}, Jacques LIANDRAT¹,  Thibaut LE GOUIC¹,  Yann MONERIE^{2,4},  Frédéric PERALES^{3,4},  J. M. CHANDRA KISHEN^{5,R}, and  Anna PANDOLFI^{6,E}

¹ Aix Marseille Univ., CNRS, Centrale Marseille, I2M, UMR7373, 13451 Marseille, France

² LMGC, Univ. Montpellier, CNRS, Montpellier, France

³ Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Cadarache, France

⁴ MIST, Univ. Montpellier, CNRS, IRSN, France

⁵ Department of Civil Engineering, Indian Institute of Science, Bangalore, India

⁶ Dipartimento di Ingegneria Civile ed Ambientale, Politecnico di Milano, Milan, Italy

^R Reviewer

^E Editor

Review of version 1

Permalink: hal-03295926v1

Author We would like to thank the two reviewers for their remarks and comments that have helped us to improve the clarity of the paper.

Reviewer 1 (J. M. CHANDRA KISHEN)

Reviewer In this work, the authors have developed a probabilistic model to predict a 2D crack path in heterogeneous materials such as concrete. The model is developed in two stages - the first involves geometrical parameters including the distance and angle to obtain the aggregate configuration while the second stage is the realization of the Markov chain model. The manuscript is well written and the work is of importance for prediction of cracking in concrete especially given the fact that it is faster and efficient. The paper may be accepted for its publication. However, the following comments may be addressed by the authors

Author We thank the referee for these comments. They were all taken into account.

Reviewer Line 4 of the abstract: Typo "craking".

Author Done, thank you

Reviewer Page 2, line 13: Change "facies" to "faces"

Author Done, thank you

Reviewer Page 2, last paragraph: 25% of polygonal aggregates is considered in the example. How do you justify this? Since in concrete, the volume of aggregates would be in the range of 40 to 70%

Author In this paper, our objective is to provide a generic prediction model that predicts the crack behavior which is controlled by the presence of aggregates in the field of view of the crack tip. To achieve that, our model should favor aggregates close to the crack tip (distance indicator), aggregates located in the local direction of propagation (angle indicator) but also aggregates further away from the crack tip and located in the local direction of propagation (interaction term). This last situation does not occur for high volume fraction. That is why a volume fraction

of 25% has been chosen in order to consider all the possible situations in the training set that could be encountered in mechanical applications. In this way, it is expected that our model remains valid for a wide range of volume fraction including [40%,70%]. This precision is added in the article in section 3.3.2 in Remark 1 : "The previous numerical tests show that the crack can reach an aggregate further way from the crack tip but located in the direction of propagation. This situation does not occur for high volume fraction of aggregates. That is why a volume fraction of 25% has been chosen for the analysis provided in this paper to consider all the possible situations that could be encountered in mechanical applications. In this way, it is expected that our analysis and the prediction model developed in the next section remain valid for a wide range of volume fraction including [40%,70%] that corresponds to concrete."

Reviewer What is the basis of choosing the parameters reported in Table 2?

Author To complete the lack, several references are proposed to understand the choice of these values. A precision is added in the section 2.2 : "For more information on the parameters, we refer the reader to the following article Blal et al. 2012 and the following theses: Bichet 2017, Socie 2019. These parameters are chosen in the case where there are no associated experimental measurements."

Reviewer According to the definition of tortuosity (Figure 5), the numerator in the ratio is generally smaller than the denominator and hence the ratio should be smaller than unity. Then, why are the values greater than 1.0 in Figure 23?

Author We are sorry, figure 5 for the tortuosity was not clear and could be confusing. It has been updated. The quantity l (numerator) corresponds to the length of the crack path (green lines on figure 5) that is influenced by the presence of aggregates. L_{mean} is simply the length of the straight line connecting the starting point and the last point of the crack path. l is therefore always larger than L_{mean} so the ratio will always be greater than 1.

Reviewer The notations used in Table 2 need to be defined

Author Please see answer to the previous comment about the parameters of Table 2.

Reviewer 2 (Anonymous)

Reviewer The paper presents a new fast-to-evaluate model for 2D crack propagation in concrete-like composites. The model provides stochastic criteria for crack orientation and propagation in a composite domain constituted by unbreakable inclusions immersed in a brittle matrix. The approach is totally geometric. The proposed procedure is interesting, and it deserves to be diffused. Accordingly, the paper deserves to be published, provided the following points be addressed.

Author Thank you very much for your reading and your helpful comments.

Reviewer Authors should clarify how the proposed procedure can be integrated within a mechanical model to perform simulations of mechanical relevance. In mechanical fracture models, stress concentration (or energy distributions in variational approaches) drives the crack propagation. How the proposed crack path criteria interact with mechanical fracture evolution laws and integrate with them? This aspect should be clarified.

Author We develop in this article a fast-to-evaluate prediction model that is able to approximate a crack path instead of performing the cracking simulation with the mechanical code. The objective is not to accurately reproduce the mechanical simulation but to propose a complementary tool to identify situations of interest that would require new simulations for example (this refers to the so-called design of experiment approach). Therefore, there is no interaction with the mechanical laws implemented in the code in the prediction step. Our model does not explicitly include mechanical elements but is built up from geometric information : the indicators. This indicators were selected after an analysis of the crack behaviour calculated by XPER (section 1). They were thus retained for their capacity to well transcribe the behaviour of the crack in the studied cases. Mechanical information is only contained in the XPER training database that is used to estimate model parameters.

A precision is added in the abstract: "This model does not include directly any mechanical elements. It is the database, derived from the XPER crack, that contains the mechanical information and optimises the probabilistic model."

A precision is also added to the introduction: "All the mechanics are contained exclusively in the training step of the model."

Reviewer This point is related to the previous one. The crack path procedure does not distinguish different shapes of aggregates. Indeed, irregular aggregates with prominent corners should produce stress concentration, reducing the effective fracture toughness, and, on the other hand, they should increase tortuosity. All this aspect should influence the crack path, but they are not considered in the proposed model. Is it correct? Are they demanded to the superposed mechanical model? Contrary, if there is dependence on the aggregate shape, this should be commented, providing numerical results

Author In this paper, the influence of the shape of the aggregates has been numerically investigated through the choice of different training sets with different convex polygonal aggregate shapes (Figure 22). It was observed that:

- the model whose parameters are learnt on the square training base shows good performances on a test base with multiform aggregates
- the training sets with pentagon and octagon aggregates leads to the same magnitude for the Frechet distance as in the case of square aggregates. Since our model seeks to reproduce a general behaviour of the cracking, one can conclude that there is not a significant impact of the convex polygonal shape on the prediction results even if the set with the square aggregates leads to the smallest error for the largest number of microstructures.

We have added these precisions in section 5.2 : "However on the 30 microstructures studied, the 3 training bases show good performances on the test set with the same error magnitude. We can therefore conclude that there is no significant influence of the shape of the training set."

Reviewer Authors should give a brief description of XPER code, which the model is based on, pointing out the main algorithmic ingredients.

Author Some basics on XPER is now presented in section 2.2 : "XPER implementation involves a multi-contact modeling strategy based on the Non-Smooth Contact Dynamics (NSCD) (Jean, 1999) method where cohesive models are introduced as mixed boundary conditions between each volumetric finite element. Each element or group of elements of the mesh can be considered as an independent body and the interface between bodies follows a frictional CZM (Nordmann et al. 2020) with no regularization nor penalization (Perales, Dubois, et al. 2010)."

Reviewer Graph of figure 4 should be explained. What do $C(h)$ and $Distance(pixel)$ stand for?

Author The principle of the covariogram is recalled, in the section 2.2 : "To illustrate this point, we propose an example on the Figure 4 with the covariogram (Jeulin, 2015) under stationary and isotropic assumptions. The covariogram allows to study the spatial distribution and the relative organisation of the phases of a random medium. Mathematically, it represents the probability that for a point x located in a given phase A , here an aggregate, $x + h$, where h is a translation vector, is in the same phase:

$$C(x, x + h) = P(x \in A, x + h \in A)$$

In the case of a stationary and isotropic process, the covariogram only depends on norm of the translation vector h and is noted for simplicity $C(\|h\|)$." And the legends are specified in the Figure 4 : " $C(\|h\|)$ represents the value of the covariogram and $\|h\|$ is the norm of the translation vector "

Reviewer Tortuosity should be measured by the red line in Figure 5, and not by the light blue line. Comment on this.

Author We are sorry, the Figure 5 for the tortuosity was not clear and could be confusing. It has been updated. On the new Figure 5, tortuosity is the ratio between the length of the crack path (green line) and the length of the "straight" path (red line) connecting the starting point and the last point of the crack

Reviewer In Figure 13, points belonging to the same aggregate (green points) belong to a vertical line, that is, they have the same distance from the crack tip point. Why? It is not clear.

Author The discretization of each aggregate is uniform. Therefore, when the crack is propagating along the aggregate side, the points reached by the cracks are equally spaced leading to the same value for the distance indicator. This explains why the green points are located on a vertical line. This precision is added in the paragraph of the Configuration F1 in the section 3.3.2 : "It is interesting to observe that the green points are all located on a vertical line since the discretization of each aggregate is uniform. Therefore, when the crack is propagating along the aggregate side, the points reached by the cracks are equally spaced leading to the same value for the distance indicator"

Reviewer Section on Markov chain model is very hard to be read by a not expert reader. Authors should do the effort of simplifying and making it clearer.

Author We clarify the section on the Markov chain model for non-expert reader by adding several sentences at the beginning of Section 4 to introduce the key ideas of Markov chain model: "For given crack tip and direction of propagation, several points can be reached and one of them will be selected by the model as the next crack tip. The Markov chain model proposed in this section allows to associate a probability to each of these points. The future crack tip is then chosen by a random draw based on these probabilities. The key point of this type of model is the construction of a transition kernel that precisely defines the probability for the crack tip at position x to reach a new point y ."

Concerning the technical details of Section 4.1, we describe the content of the technical details before providing them for a better understanding.

Reviewer Parameters μ_i and λ_i are calibrated from a training set of microstructures. This means that several XPER simulations are needed a-priori. Since the model is closely related to the composite topology, different sets of microstructures are needed for different topologies, such as composites with aggregates of different sizes, shapes, or density distributions. If this is correct, this constitutes a large limitation of the proposed model, whose aim is to reduce the computational cost, since, for any topology, a computational expensive procedure is needed to calibrate parameters. Authors should comment on this issue.

Author The framework of our study is specified in section 2.1 : In this paper, rectangular microstructures with 25% uniformly distributed aggregates of different shapes are studied. The model shows a good robustness with respect to the aggregate shapes (section 5.2). However, further investigations are required in particular for different density distributions (non-uniform) and different sizes of aggregates. Without further studies, there is no certainty that the same good performances are kept for all composite topologies. This is part of the perspectives. A precision is added in the conclusion : "In this paper, it was decided to study microstructures of similar uniform density with different shapes of aggregates. Further investigations should consider different microstructures, in particular non-uniform densities (presence of clusters) and aggregates of different sizes. The first step will be to test the robustness of the current model on these new types of microstructures. According to the results, adaptation of the model should be considered, taking in mind that our goal is not to calculate a new training set for each new case."

Review of version 2

Permalink: [hal-03295926v3](https://hal.archives-ouvertes.fr/hal-03295926v3)

Reviewer 1 (J. M. CHANDRA KISHEN)

Reviewer The authors have revised the manuscript satisfactorily based on the comments made by the reviewers. The manuscript may now be accepted for its publication.

Editor’s assessment (Anna PANDOLFI)

This paper presents a nice approach to model fracture propagation in concrete. The paper received two rather positive reviews, suggesting a minor revision. Authors provided an exhaustive answer to all the points raised by the reviewers, and provided a second version of the paper that has been approved by the reviewers and the editor.

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