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

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This paper is devoted to the construction of a new fast-to-evaluate model for the prediction of 2D crack paths in concrete-like microstructures. The model generates piecewise linear cracks paths with segmentation points selected using a Markov chain model. The Markov chain kernel involves local indicators of mechanical interest and its parameters are learnt from numerical full-field 2D simulations of cracking using a cohesive-volumetric finite element solver called XPER. The resulting model exhibits a drastic improvement of CPU time in comparison to simulations from XPER.

Keywords Markov chain, concrete, cracking prediction, machine learning

1 Introduction

Aging of materials is a major issue in industrial applications. It is particularly the case in nuclear framework where the aging of cementitious materials can cause safety issues. Among various degradations due to aging, a special attention is devoted to concrete cracking induced by Internal Sulfate Attack (Safuiddin et al. 2018). These degradations generally lead to the development of a network of cracks. They considerably influence the strength of structures, reduce their tightness. Knowing the characteristics of cracking is essential in the study of the life extension of nuclear power plants.

At mesoscopic scale, concrete, used in design of nuclear power plant containments, can be viewed as a two-phase composite material with mortar matrix and aggregates inclusions. The granular particles are randomly distributed in a matrix of mortar. The heterogeneities of this kind of material (Gangnant 2016) and the different associated scales (Huong 2011) increase the complexity of its study.

In the context of research on the safety of Pressurized Water Reactors, IRSN, in collaboration with the LMGC (Mechanics and Civil Engineering Laboratory) through the joint laboratory MIST (Micro-mechanics and Integrity of Structure Laboratory), has developed a micro-mechanical approach for the analysis of the behavior of materials during hypothetical accidental transients (Péralès 2005). This approach is based on the concepts of Cohesive Friction Zone Model (MZCF) (Monerie et al. 2001) associated with numerical modeling methods for multi-body systems based on the Non Smooth Contact Dynamics (NSCD) approach (Jean 1999). The developed parallelized numerical platform, XPER (eXtended cohesive zone models and PERiodic homogenization) (Perales, Dubois, et al. 2010; Perales, Bourgeois, et al. 2008), allows to simulate the initiation and two-dimensional propagation of multi-cracks in heterogeneous materials. However, each simulation is very expensive in terms of computing time, since it can involve several days of computation on a few dozen processors. This CPU time can therefore become prohibitive in the context of probabilistic safety studies.

In order to reduce this CPU time, this paper proposes the construction of a probabilistic model that allows to quickly predict a set of crack paths from the discretization of the microstructure associated with a local law of probability based on a Markov chain model. The transition core of the introduced model depends on two geometrical indicators. The parameters of the model are estimated from a set of training crack paths obtained numerically using full-field cohesive-volumetric finite element analysis with XPER.

Several recent works are dealing with the development of statistical and machine learning tools for cracking data analysis. They study for example crack classification or detection of type of cracks (Kumar Das et al. 2019; Kim et al. 2019). The crack path prediction has been also addressed in Willot 2015; Le Mire et al. 2021 or Bayar et al. 2019 but none of them leads to a surrogate model providing local information on the crack path which is the originality of our development.

This paper is organized as follows. The Section 2.1 is devoted to the reminder of some elements related to cracking of materials that are exploited in the construction of the model and allows to define working hypotheses. The Section 2.2 describes the test case considered in this document and the computer code

used for the simulations. The Sections 3 and 4 deal with the construction of the prediction model. After the introduction of the discretization of the problem, the two geometric indicators chosen to capture the local configuration of the aggregates are defined and an efficient procedure is proposed to evaluate them. On the basis of these indicators, a Markov chain model is then developed to perform the prediction of the crack path. Finally, the performance of the new model is studied in Section 5 for different shapes of aggregates.

2 Concrete crack

2.1 Phenomenology of cracking

The objective here is to describe the behaviour of cracks in concrete in order to retain general assumptions that characterize the crack path. The crack path is directly related to the heterogeneous composition of the concrete. In general, cracking studies are performed at the mesoscopic scale where concrete can be considered as a bi-material composed of a matrix (mortar) and inclusions (aggregates).

Concrete is often considered as **quasi-brittle material** (Gangnant 2016). It is clearly established that aggregates have a strong influence (Chen et al. 2012) on the fracture facies. This influence is due, on the one hand, to a **high fracture resistance of the aggregates** and, on the other hand, to **the relative weakness of the aggregate/matrix interfaces**. The interface properties depend on a zone around the aggregates called the Interfacial Transition Zone (ITZ) (Elices et al. 2008; Pope et al. 1992). This area is very porous, reducing significantly its strength. Thus, the cracks, during their propagation, preferentially follow the aggregate/matrix interfaces (see Figure 1) (Chen et al. 2012; Alexander et al. 1964; Akçaoglu et al. 2004).

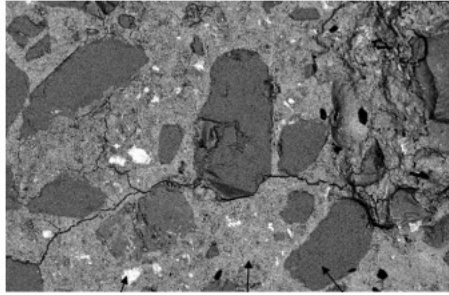


Figure 1: Example of a crack that propagates and follows the aggregate-matrix interface

It is established that aggregates and their boundaries have a significant influence on the mechanical behavior of concrete. Indeed, according to Husem 2003, the compressive strength of a concrete depends for 21% on cement paste, for 12% on aggregates and 67% on interphase. To summarize, the presence of aggregates leads both to (Walker et al. 1960):

- a heterogeneity of local mechanical fields,
- an increase in areas of weakness (aggregate/matrix interfaces) which locally constitute privileged cracking zones.

In addition, the local stress state implies a **direction of propagation of the crack**. The crack displacements are therefore restricted by a half-plane oriented ahead of the crack tip due to the impossibility to move backwards.

This analysis of the behavior of cracking in concrete allows to identify four working hypotheses:

- (H1) the matrix is elastic brittle,
- (H2) the aggregates are stiff and unbreakable,
- (H3) the matrix aggregate interface is the weakest zone in the composite material,
- (H4) the crack propagates mainly in mode I and thus in a half-plane oriented in the local direction of propagation, in front of the crack tip perpendicularly to the local tensile stress

2.2 Numerical simulation of cracking

In this section, the numerical representations of the concrete and the XPER software, that allows to numerically simulate the crack, will be presented. Numerical samples of concrete are constructed from morphological descriptors. These descriptors are statistical and geometric informations identified on real concrete, like n-point moments and spatial covariance (Jeulin 2015) allowing to characterize the spatial arrangements of different phases. The numerical microstructure are qualified as statistically similar to real concrete in the sense of these descriptors. An example of such microstructure is given in Figure 2.

The test case deals with a rectangular domain ($l \times L = 0.225m \times 0.600m$) submitted to a symmetrical traction on both sides (up and down) of the sample (Figure 2). The microstructure, composed of a matrix with 25% of polygonal aggregates (square shapes in the Figure 2), is considered as isotropic. Cracks can propagate through the matrix and not through aggregates (assumptions (H1) and (H2)).

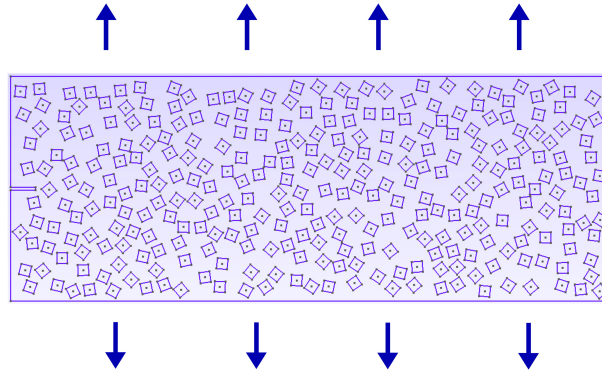


Figure 2: Test case submitted to traction (drawing process for the distribution of aggregates in the microstructure : HCPP (Hard Core Point Process))

All full-field crack simulations are performed with XPER code. The CPU time for a complete microstructure cracking simulation like Figure 2 is about 44 hours for a computer : Intel(R) Xeon(R) Gold 6126 CPU @ 2.60GHz connected in Infiniband - 256Go RAM - Nodes of 24 processors. The simulation parameters are given in Table 1 to Table 3.

	Matrix	Aggregates
ρ (kg/m^3)	2900	2900
E (Pa)	12e9	60e9
ν	0.2	0.2

Table 1: Volumic parameters of the simulations

	Matrix-Matrix	Aggregate-Aggregate	Matrix-Aggregate
$C_n=C_t$ (Pa/m)	1e17	1e17	1e17
σ_0 (Pa)	4.6e7	2.4e9	1.4e7
w (J/m^2)	20	∞	20

Table 2: Surface parameters of the simulations

Area of aggregates	$0.6 \times 0.225 \text{ m}^2$
Degrees of freedom	48666
Number of processors	24
Computation time	44h

Table 3: Numerical parameters of the simulations

Figure 3 shows an example of simulation with square-shape aggregates.

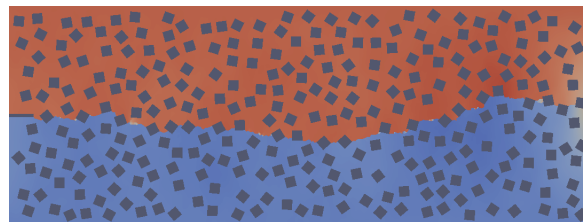


Figure 3: Crack path (colour discontinuity) obtained with XPER for the case described in the Figure 2. The colours stand for the vertical displacement.

The crack is represented by the colour discontinuity (colour stand for vertical displacement). The main direction of crack path is therefore almost perpendicular to the direction of the load. It turns out that two numerical concretes sharing the same morphological descriptors (covariogram, percentage of aggregate) can exhibit different crack paths (Figure 4).

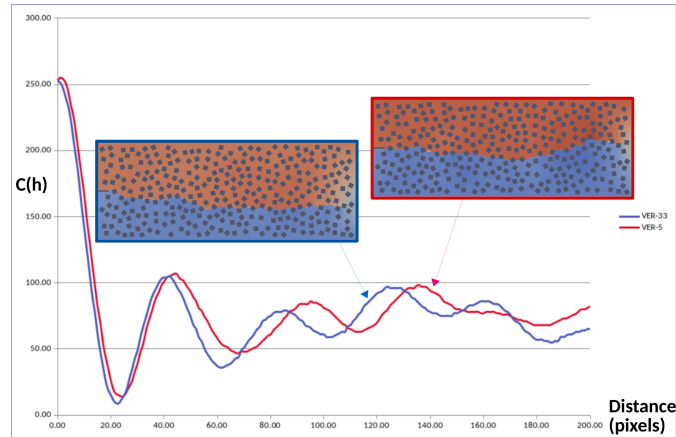


Figure 4: Comparison of two covariograms for two different microstructures

As a result, they lead to different values for mechanical quantities of interest such as the tortuosity (Figure 5), which definition is recalled below.

Definition 1 – Tortuosity : the tortuosity τ of a crack is the ratio between the length l of the crack path and L_{mean} the length of the line joining the first and last points of the crack: $\tau = \frac{l}{L_{mean}}$.

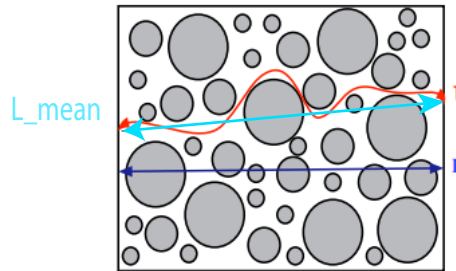


Figure 5: Schematic representation of the tortuosity : $\tau = \frac{l}{L_{mean}}$

In view of the cracked microstructure of Figure 3, it appears that the *local* configuration of the aggregates strongly influences the path of the crack. This information is central in our construction of the new crack indicators.

3 Definition and evaluation of local crack indicators

In this section, several key notions are presented in order to satisfy the hypotheses (H₁) to (H₄) (Section 2.1) describing the local behavior of a crack. The definition and the evaluation of the local crack indicators are described in subsections 3.2 and 3.3.

3.1 Discretization of the microstructure

Although the main crack propagates in the mode I direction, the local propagation of a crack depends strongly on the microstructure configuration (the aggregates) near the crack tip. Therefore, we propose a discretization of the microstructure, at this scale, allowing to estimate the step by step crack path. In this work, each aggregate is approximated by a polygon where each side is discretized by 5 points. This allows to simulate the propagation of the crack along the side (Figure 6). The crack path can leave or join an aggregate at several positions along the side of the aggregate and not only at the corners of the polygon.

The matrix is not discretized which implies that either the crack crosses the matrix following a straight line between two points of the discretization belonging to two distinct aggregates (assumption (H₁) of Section 2.1) or it follows the side of an aggregate (assumption (H₃) of Section 2.1).

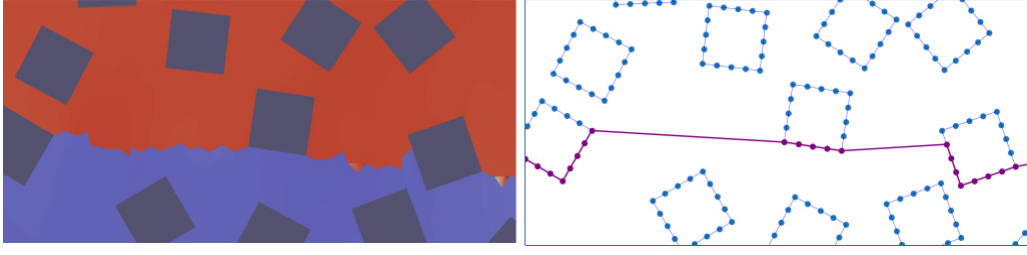


Figure 6: Discrete representation of a microstructure and crack path: on the right, the blue dots stand for the discretization points (y_i^E) and the purple path represents the XPER crack crossing the points (x_i^E).

For a microstructure E , the set of discretization points denoted by $\mathcal{Y}_E = \{y_i^E\}_{i=1,\dots,N_E}$ constitutes the discrete granular microstructure (Figure 6). The crack path is then approximated from a subset of \mathcal{Y}_E denoted by $\mathcal{X}_E = \{x_i^E\}_{i=1,\dots,m_E}$. We can define the discretized crack as follows.

Definition 2 – Discretized crack : if one considers the Cartesian coordinate system whose origin is at the bottom left corner of the microstructure, the crack path can be parametrized by $(x^1, h_E(x^1))$ where $h_E : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a piecewise linear function such that: if $(x_i^{E,1}, x_i^{E,2})$ denotes the coordinate of x_i^E in the Cartesian system,

$$\forall x^1 \in [x_i^{E,1}, x_{i+1}^{E,1}], h_E(x^1) = \frac{x_{i+1}^{E,2} - x_i^{E,2}}{x_{i+1}^{E,1} - x_i^{E,1}} (x^1 - x_i^{E,1}) + x_i^{E,2}.$$

Assumption (H4) implies that, starting from a point of the discretized crack path, only a subset of discretization points can be reached. They are located in a *field of view* defined as follows (an example is exhibited in Figure 7).

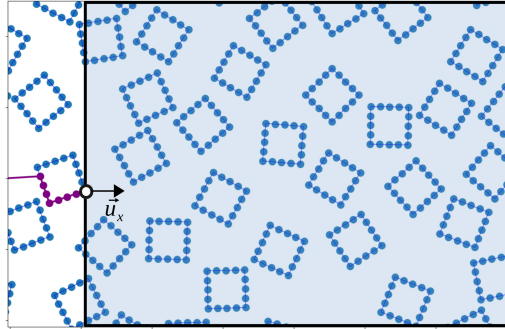


Figure 7: Example of a *field of view* (blue area) at the crack tip (white circle), following the local direction of propagation u_x . The purple line stands for the path of the crack

Definition 3 – Field of view : if E is a microstructure, $x \in \mathcal{X}_E$ the crack tip and \vec{u}_x is the local direction of crack propagation at x , the *field of view* of the crack path at x is defined by the area containing the set of I discretization points $\{y_i^E\}_{i \in I} \subset \mathcal{Y}_E$ such that:

$$\langle xy_i^E, \vec{u}_x \rangle \geq 0, \forall i \in [1, \dots, N_E] \quad (1)$$

where $\langle \cdot, \cdot \rangle$ denotes the euclidean scalar product in \mathbb{R}^2 .

Remark 3.1 Note that it is possible to take into account a non constant local direction and locally orientate the field of view. In the numerical studies of this paper, \vec{u}_x is a constant vector orthogonal to the loading direction. We refer to chapter 4 of Pele 2021 for an example where \vec{u}_x is evaluated through a mechanical simulation.

Depending on the configuration associated of the tip of the crack, the field of view may not contain point in the same aggregate. This strongly influences the crack path and should be taken into account in the prediction model developed in this paper. Consequently, it is important to distinguish the two following configurations of the *field of view*:

- **Configuration F1:** *field of view* including possibilities to follow the aggregates sides or to cross the matrix (Figure 8),

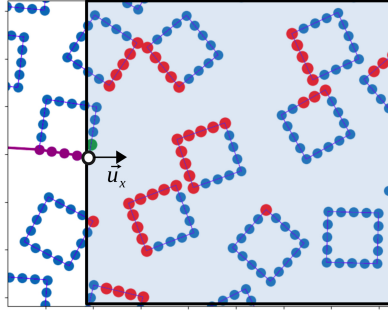


Figure 8: Field of view (F1): the green point stands for the candidate point belonging to the original aggregate, the red points stands for the candidate points on the other aggregates (implying to cross the matrix). The purple line stands for the path of the crack

- **Configuration F2:** *field of view* only including possibilities to cross the matrix (Figure 9).

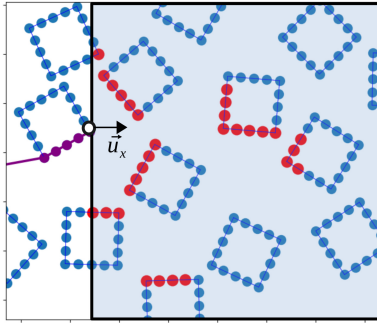


Figure 9: Field of view (F2) : the red points represent the candidate points on the other aggregates (implying to cross the matrix). The purple line stands for the path of the crack.

3.2 Definition of the two indicators

This section is devoted to the definition of two geometrical indicators to capture the local behavior of a crack. These indicators will characterize all the couples (x, y_i^E) where x is the tip of the crack and y_i^E a point of the field of view E . The first indicator is the angle that each vector $\overrightarrow{xy_i^E}$ makes with the local direction of propagation, \vec{u}_x (assumption (H4)). The second indicator is the Euclidean norm of $\overrightarrow{xy_i^E}$. These indicators are evaluated at each increment of the crack propagation.

Definition 4 – Crack indicators : let E be a microstructure, $x \in X_E$ be the tip of the crack and \vec{u}_x be the local direction of propagation at x . If $\langle \cdot, \cdot \rangle$, resp. $\|\cdot\|$, is the euclidean scalar product, resp. norm, in \mathbb{R}^2 , for any y in the *field of view* of x , the two local indicators are defined by:

$$d_x(y) = \|\overrightarrow{xy}\|,$$

$$\theta_x(y) = \arccos\left(\frac{\|\langle \overrightarrow{xy}, \vec{u}_x \rangle\|}{\|\overrightarrow{xy}\| \cdot \|\vec{u}_x\|}\right),$$

For any x , normalized distance and angle are also introduced as:

$$\tilde{d}_x(y) = \frac{d_x(y) - d_{min}}{d_{max} - d_{min}},$$

$$\tilde{\theta}_x(y) = \frac{\theta_x(y) - \theta_{min}}{\theta_{max} - \theta_{min}},$$

where d_{max} , d_{min} and θ_{max} , θ_{min} are the maximum and minimum values of the indicators associated to the candidate points in the field of view for a given location of the crack tip.

The Figure 10 illustrates the defined indicators.

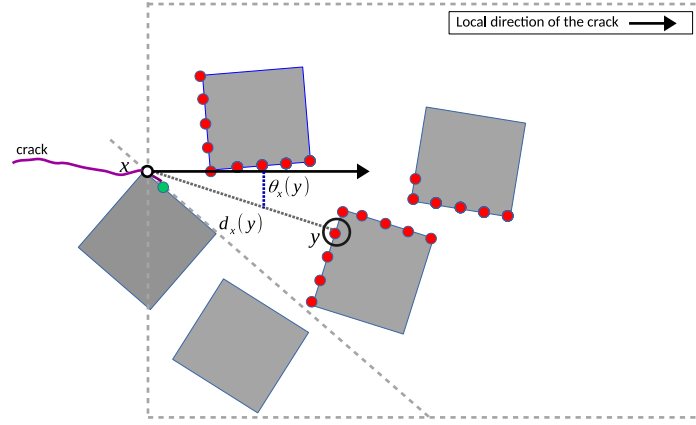


Figure 10: Illustration of the indicators of the candidate point y for the crack tip x in the configuration F1. The red points correspond to candidate points on neighbouring aggregates and the green point to the possibility of going along the same aggregate.

3.3 Evaluation of the indicators

This section is devoted to the evaluation of the two previous indicators. In the first section 3.3.1, an efficient procedure to select the points actually reachable by the tip of the crack in the field of view is developed. In the second section 3.3.2, a numerical study of these indicators is performed by analyzing a training set of microstructures cracked with XPER code.

3.3.1 Procedure to select the candidate points

For each point x of the crack, a straightforward strategy for indicator evaluation would require the computation of the distance and the angle, $d_x(y_i^E)$ and $\theta_x(y_i^E)$, for all the discretization points located in the *field of view* of x . However, following Assumption (H2), some points cannot be reached by the crack due to the presence of aggregates and should be deleted from the candidate points. For a given aggregate, the deletion procedure is based on the detection of an area not visible from x because it is hidden by the aggregate. This area is called in the sequel the shadow area.

The method to identify this shadow area and to delete the corresponding discretization points is given by Procedure 3.1. To prevent a dependence to the local crack propagation orientation, the position and the shape of the aggregate, it relies on computational geometry (Boissonnat 2017).

Procedure 3.1 – Deletion of the discretization points in the shadow area of an aggregate : let E be a discrete granular microstructure, $x \in \mathcal{X}_E$ be a crack tip and $\{y_j^E\}_{j=1,\dots,n_E}$ be the n_E points discretizing the sides of an aggregate A in the field of view of x . For any $(i, k) \in \{1, \dots, n_E\}^2$, we denote by $\angle(\overrightarrow{xy_i^E}, \overrightarrow{xy_k^E})$ the angle between two vectors $\overrightarrow{xy_i^E}$ and $\overrightarrow{xy_k^E}$ in $[0, \pi]$. The deletion is based on the identification of the points lying in the shadow area of the aggregate. We first find the two points y_1^* and y_2^* such that $\angle(\overrightarrow{xy_1^*}, \overrightarrow{xy_2^*}) = \max_{(i,k) \in \{1,\dots,n_E\}^2} \angle(\overrightarrow{xy_i^E}, \overrightarrow{xy_k^E})$. This angle defines a search cone (Figure 11). A point z in the field of view belongs to the cone if :

$$\det(\overrightarrow{xy_2^*}, \overrightarrow{xz}) \det(\overrightarrow{xy_1^*}, \overrightarrow{xz}) < 0,$$

A point z in the cone belongs to the shadow area and is deleted if (Figure 12):

$$\det(\overrightarrow{xy_1}, \overrightarrow{y_1^*z}) \det(\overrightarrow{y_1^*z}, \overrightarrow{y_1^*y_2^*}) < 0.$$

This procedure is repeated for all aggregates, allowing the capture of the candidate points of the field of view respecting the assumption (H2).

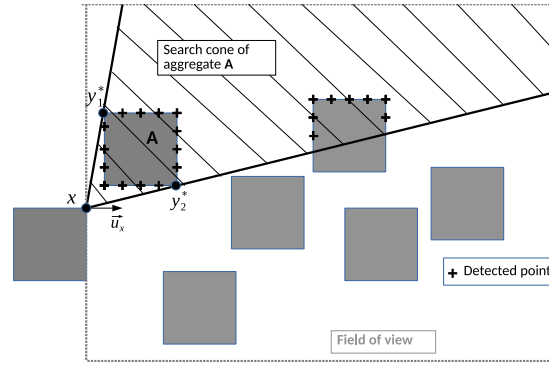


Figure 11: Illustration of Procedure 3.1 : construction of the search cone (hatched area) associated to aggregate A.

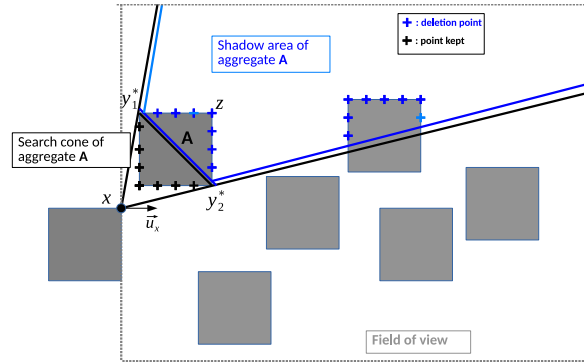


Figure 12: Illustration of Procedure 3.1 : construction of the shadow area (blue area) associated to aggregate A

3.3.2 Analysis of the relevance of the indicators

In this section, we analyze the relevance of the two indicators angle and distance to capture the local characteristics of the crack path. This analysis is also exploited to define the different terms of the prediction model developed in section 4.

The two indicators are evaluated for each discretization point located on the crack path using Procedure 3.1 for a set of 35 microstructures whose cracking is simulated by the XPER code following Section 2.2. In this study the local direction of the field of view is always orthogonal to the loading (mode I). The indicator evaluation is performed for the two configurations of the field of view : F1 (see Figure 8) and F2 (see Figure 9). Figure 13 displays the results of the set of indicator pairs selected by the cracks of the 35 microstructures.

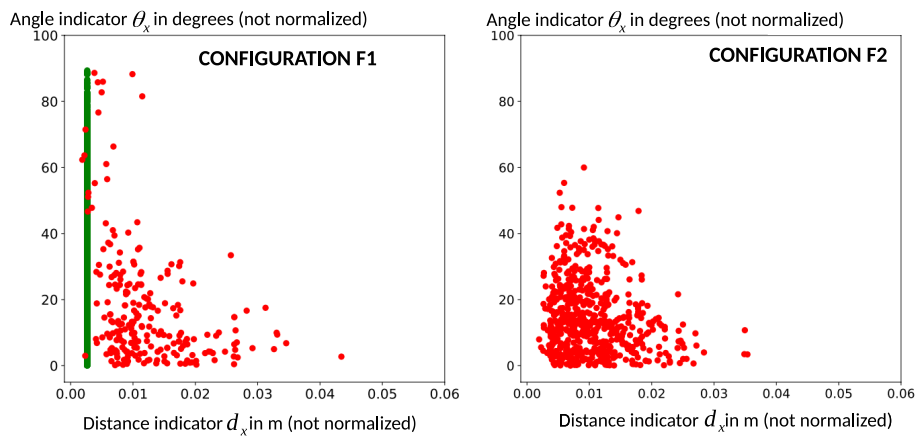


Figure 13: Indicator values in configurations F1 and F2 associated to points on the crack for 35 microstructures with square aggregates. Each point represents a couple of not normalized values (d_x, θ_x) . The red dots stand for candidate points present on neighbouring aggregates (cross the matrix) and the green dots stand for the candidate points belonging to the same aggregate

- Configuration F₁ (Figure 8)

Figure 13 (left-hand side graph) confirms that the crack is likely to follow the aggregate side. This situation corresponds to the large number of green points with the shortest distance and a variation range between 0 and $\frac{\pi}{2}$ for the angle. For this points on the same aggregate, the distance indicator is not influential. It is important to note that the attraction of the point on the same aggregate may be reduced in some cases. Indeed, the observation of our training base highlights that the crack sometimes chooses to leave the aggregate side and to cross the matrix even if it has the possibility to follow the aggregate (red points on Figure 13). This change of behaviour in the crack propagation is due to two situations that simultaneously occur: following the same aggregate involves a large angle while crossing the matrix is associated to the combination of small angle and short distance.

- Configuration F₂ (Figure 9)

In this configuration (right-hand side graph of Figure 13), since there is no candidate point on the aggregates sides, the crack can only propagate into the matrix. The indicators values of the candidates points reached by the crack are in the bottom left hand corner of the graph (i.e short distance and small angle). This reflects the fact that the crack is at the same time constrained by the direction of the stress and attracted by the closest aggregates.

The two local indicators are therefore relevant to characterize and discriminate the local behavior of a crack. They are integrated into a probabilistic prediction model that is described in the next section.

4 Markov chain model for crack prediction

This section is devoted to the construction of the fast-to-evaluate surrogate model for crack path prediction. The crack is modelled by a Markov chain with a set of parameters. In this section, we describe the development of the model with a specific transition kernel involving the two indicators presented in the section 3.2. The parameters are estimated in section 5.1. Finally, section 4.2 fully describes the crack path prediction using the proposed model.

4.1 Construction of the model

The prediction model is based on a Markov chain model. This type of model relies on the property that the prediction of future states of a system only depends on its present state. It is therefore particularly well suited to the modeling of the crack whose propagation only depends on local information at the crack tip and not on the whole path before the tip. Let us recall the definition 5 of a Markov chain. For more details on Markov chains, the reader is invited to refer to the first chapter of Norris 1998 or any text book on Markov Chains.

Definition 5 – A Markov chain : a sequence of random variables $(X_n)_{n \in \mathbb{N}}$ with values in a set \mathcal{E} is a Markov chain of state space \mathcal{E} if for all $k \in \mathbb{N}$, $\forall (x_0, \dots, x_{k+1}) \in \mathcal{E}^{k+2}$ such that $P(X_0 = x_0, \dots, X_k = x_k) > 0$,

$$P(X_{k+1} = x_{k+1} | X_0 = x_0, \dots, X_k = x_k) = P(X_{k+1} = x_{k+1} | X_k = x_k).$$

Here, $P(X_{k+1} = y | X_k = x)$ denotes the conditional probability of $X_{k+1} = y$ given $X_k = x$. We set $\nu_0(x_0) = P(X_0 = x_0)$, so that for all $(x_0, \dots, x_n) \in \mathcal{E}^{n+1}$,

$$P(X_0 = x_0, \dots, X_n = x_n) = \nu_0(x_0) \prod_{k=0}^{n-1} P(X_{k+1} = x_{k+1} | X_k = x_k).$$

Moreover, the chain is said to be homogeneous if for all $k \in \mathbb{N}$ and for all $(x, y) \in \mathcal{E}^2$, $P(X_{k+1} = y | X_k = x) = P(X_1 = y | X_0 = x)$.

The discretization points of the crack are assumed to be a realization of homogeneous Markov chain. The discussion of Section 3 leads to propose that the probability of transition is evaluated from a transition kernel depending on the two local geometrical indicators introduced in Definition 4. The following modelling defines the general structure of transition probability between two points in the crack.

Modeling 4.1 – Transition probability of crack : for any microstructure E , we suppose that $(X_i^E)_{i=1, \dots, m_E}$ is a sequence of random variables that constitutes a homogeneous Markov chain. $(x_i^E)_{i=1, \dots, m_E}$ defines a sequence of realizations of the Markov chain and the transition kernel of the chain defining the probability of transition from x to y is given by:

$$P_E(X_{i+1}^E = y | X_i^E = x) = c_{x, \Lambda} f_{\Lambda}(\tilde{d}_x(y), \tilde{\theta}_x(y)), \quad (2)$$

where P_E denotes the conditional probability given E , $c_{x,\Lambda}$ is a normalization constant in order to define a probability and f_Λ is a function parametrized by a set Λ of parameters to be determined. We set the first realization $X_0 = x_0$: it is the starting point of the crack and is chosen in the microstructure. In particular we have,

$$P_E \left(X_0^E = x_0, \dots, X_{m_E}^E = x_{m_E}^E \right) = \prod_{i=0}^{m_E-1} P_E \left(X_{i+1}^E = x_{i+1}^E | X_i^E = x_i^E \right). \quad (3)$$

The aim of this model is to reproduce the crack behaviour by weighting the probability of propagation of the crack with the importance of the indicators according to the local configuration at the tip of the crack in the microstructure. Since the presence of candidate points on the aggregate sides influences the local direction of propagation, the expression of f_Λ depends on the configuration (F1 or F2). We use a decreasing exponential function in order to penalize high values of the indicators.

Based on the modelling 2 and our assumptions, the following model presents the final transition probability by specifying $c_{x,\Lambda}$ and f_Λ .

Modeling 4.2 – Probabilistic cracking model : let x be a discretization point reached by the crack and belonging to an aggregate A . If $\{y_k^E\}_{k=1,\dots,K_E}$ is the set of candidate points in the field of view of x , then the transition kernel is given by:

- Configuration F1 (Figure 8): let $\Lambda_{F1} = (\mu_1, \mu_2, \mu_3, \mu_4, \mu_5, \mu_6)$ be the parameters associated to this configuration. If $\{y_k^E\}_{k=1,\dots,r_E}$ defines the set of candidate points on A and $\{y_k^E\}_{k=r_E+1,\dots,K_E}$ the candidate points on the other aggregates, $c_{x,\Lambda} = c_{x,\Lambda_{F1}}$ and $f_\Lambda = f_{\Lambda_{F1}}(\tilde{d}_x(y), \tilde{\theta}_x(y))$ with :

$$f_{\Lambda_{F1}}(\tilde{d}_x(y), \tilde{\theta}_x(y)) = \begin{cases} e^{-\mu_1(\tilde{\theta}_x(y))^{\mu_2}} & \text{if } y \in A \\ e^{-\mu_3(\tilde{d}_x(y)\tilde{\theta}_x(y))^{\mu_6} - \mu_4(\tilde{d}_x(y))^{\mu_5}} & \text{else} \end{cases} \quad (4)$$

and the normalizing constant $c_{x,\Lambda_{F1}}$ is thus,

$$c_{x,\Lambda_{F1}} = \frac{1}{\sum_{k=1}^{K_E} f_{\Lambda_{F1}}(\tilde{d}_x(y), \tilde{\theta}_x(y))} \quad (5)$$

- Configuration F2 (Figure 9): let $\Lambda_{F2} = (\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6)$ be the parameters associated to this configuration, then $c_{x,\Lambda} = c_{x,\Lambda_{F2}}$ and $f_\Lambda = f_{\Lambda_{F2}}(\tilde{d}_x(y), \tilde{\theta}_x(y))$ with :

$$f_{\Lambda_{F2}}(\tilde{d}_x(y), \tilde{\theta}_x(y)) = e^{-\lambda_1(\tilde{d}_x(y)\tilde{\theta}_x(y))^{\lambda_5} - \lambda_2(\tilde{d}_x(y))^{\lambda_6} - \lambda_3(\tilde{\theta}_x(y))^{\lambda_4}} \quad (6)$$

and the normalizing constant $c_{x,\Lambda_{F2}}$ is thus,

$$c_{x,\Lambda_{F2}} = \frac{1}{\sum_{k=1}^{K_E} f_{\Lambda_{F2}}(\tilde{d}_x(y), \tilde{\theta}_x(y))} \quad (7)$$

The different variables integrated in this modeling come from the analysis performed in Section 3.3.2. The mixed term allows to take values of distance and angle of the same order of magnitude. The distance term allows to take into account the neighboring attraction of the aggregates. The angle term allows to take into account the direction of propagation. In the configuration F_1 , the distinction between the possibility of following the aggregate and crossing the matrix is taken into account in the expression of $f_{\Lambda_{F1}}$ that depends on the two previous situations. Moreover, as observed in section 3.3.2 for candidate points on the same aggregate, the distance has no influence and therefore, only the angle indicator is included in the model. For candidate points that require crossing the matrix in the configuration F_1 , experimentally, it is the presence of an aggregate close to the crack tip that has the most important influence on the change of crack behavior. That is why the angle indicator is only taken into account in the interaction term contrarily to the transition kernel in configuration F_2 . It allows reducing the number of parameters in the model and the variability of their estimate.

More generally, in both configurations F_1 and F_2 , the interaction term between distance and angle allows integrating the effect of the combination of small values of the two indicators that was observed in section 3.3.2. It constrains the crack to follow a propagation direction while keeping the attraction of the closest aggregates.

The model parameters are estimated from a training set of microstructures whose cracking has been simulated with XPER code. Under the independence assumption of the microstructures, the estimate is performed by maximization of the likelihood. More precisely, if $\{E_i\}_{i=1,\dots,Q}$ denotes the training set of microstructures and $(x_j^{E_i})_{j \in I_{E_i}^{F1}}$ et $(x_j^{E_i})_{j \in I_{E_i}^{F2}}$ are the sequences of I points selected by the crack on the microstructure E_i in both configurations, the parameters Λ_{F1}^* and Λ_{F2}^* are solutions of:

- Configuration F1:

$$\Lambda_{F1}^* = \arg \max_{(\mu_1, \dots, \mu_6)} \left\{ \prod_{i=1}^Q \prod_{j \in I_{E_i}^{F1}} P_{E_i} \left(X_{j+1}^{E_i} = x_{j+1}^{E_i} | X_j^{E_i} = x_j^{E_i} \right) \right\} \quad (8)$$

- Configuration F2:

$$\Lambda_{F2}^* = \arg \max_{(\lambda_1, \dots, \lambda_6)} \left\{ \prod_{i=1}^Q \prod_{j \in I_{E_i}^{F2}} P_{E_i} \left(X_{j+1}^{E_i} = x_{j+1}^{E_i} | X_j^{E_i} = x_j^{E_i} \right) \right\} \quad (9)$$

where P_{E_i} is given by Modeling (4.2).

4.2 Cracking prediction with the probabilistic model

This section describes the crack path prediction for a given microstructure using the Markov chain model introduced in Modeling 4.2. The parameters of the transition kernel are assumed to be known, their estimate is studied in Section 5. This prediction relies on a procedure that starting from the crack tip, provides the next point of the field of view that is reached by the crack.

More precisely, the local indicators introduced in Definition 4 are first evaluated integrating Procedure 3.1 to reduce the set of candidate points in the field of view. Then, the Markov chain model can evaluate the probability of each point of the set to be the next point reached by the crack. Finally, a realization is retained according to the evaluated probability to select the next point of the crack. This procedure is described below:

Procedure 4.1 – Process of a local prediction to determine the next point of the crack : given x_i^E the crack tip in a microstructure E and $\vec{u}_{x_i^E}$ the local propagation direction, the prediction includes three steps:

- Step 1: construct the field of view of x_i^E , identify the candidate points following Procedure 3.1 ($\{y_k^E\}_{k=1,\dots,K_E}$ is the set of remaining points) and evaluate the normalized indicators $\tilde{d}_{x_i^E}(y_k^E)$ and $\tilde{\theta}_{x_i^E}(y_k^E) \forall k$.
- Step 2: according to the configuration, compute $\{P_E(X_{i+1}^E = y_k^E | X_i^E = x_i^E)\}_{k=1,\dots,K_E}$ using Modeling 4.2.
- Step 3: select a realization from the discrete law $\sum_{k=1}^{K_E} P_E(X_{i+1}^E = y_k^E | X_i^E = x_i^E) \delta_{y_k^E}$.

In this procedure, the objective is to randomly drawn the next point of the crack among the points with the highest probabilities and not to select the candidate point with the highest probability. It is considered that several points can be good candidates for to be the next point of crack. Starting from the crack tip (initial position), this procedure is successively applied to any new point on the crack until the boundary of the domain is reached.

Thus the prediction model is stochastic. Starting from the same initial position, it can be applied to obtain several realizations of the crack path. Therefore, it allows to quantify the uncertainty associated to the prediction and to the mechanical quantities of interest. In the next section 5, tools to use this set of realizations to determine the most optimal crack path will be presented.

Figure 14 provides an illustration of the prediction procedure in the F2 configuration. The algorithm 1 summarizes the three steps of the procedure.

Algorithm 1 Local prediction

```

1: E is the discrete granular microstructure
2:  $x^E$  is the point of crack tip
3: DirectionProp is the local direction in mode I
4: MarkovChainModel is the model in 4.2 (gives the probabilities for the candidate points)
5: RandWeighted performs a weighted draw for select the next point of the crack
6: ParamModel are the estimated parameters of the prediction model
7: function CRACKING( $E, x_0^E, ParamModel, DirectionProp$ )
8:   FieldviewAgg = set of aggregates in the field of view of the point  $x^E$  associated to DirectionProp
9:   FieldviewPoint = set of points located on the aggregates of FieldviewGran
10:  for G in FieldviewAgg do
11:    ShadowG= shadow zone of aggregate G
12:    for point in FieldviewPoint do
13:      if point in ShadowG then
14:        Deletes the point in FieldviewPoint
15:      end if
16:    end for
17:  end for
18:  ProbaPoint=MarkovChainModel(FieldviewPoint,ParamModel)
19:  PositionPointChosen=RandWeighted(ProbaPoint)
20:  return PositionPointChosen
21: end function

```

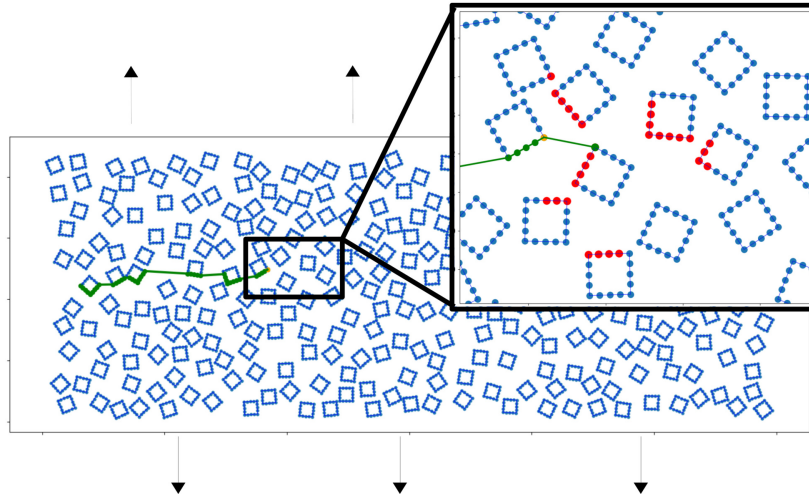


Figure 14: Illustration of the prediction (procedure 3.1) in the F2 configuration with a zoom on the region of interest. The field of view is orientated with respect to a propagation direction orthogonal to the stress effort. The orange point is the crack tip, the red points are candidate points in the field of view where the probability to be reached is evaluated, the green points are the candidate points selected by the model

5 Numerical application

Several types of numerical applications are considered in this section. They first concern the estimate of the parameters (Section 5.1) of the transition kernel. Then, we focus on the ability of the model to correctly predict the crack path (Section 5.2) and the associated mechanical quantities of interest.

5.1 Parameter estimate

The parameter estimate exploits a training set of 35 microstructures numerically cracked with the XPER code from the test case described in Section 2.2 with square shape aggregates. The estimation of the parameters of the Markov chain are obtained by maximising the likelihood (Equations (8) and (9)). The maximisation is performed with an optimized version of the BFGS algorithm (Yunhai et al. 2008).

Table 4 provides the estimated values for Λ_{F1} and Λ_{F2} .

Let us recall that in Modeling 4.2, the parameters $\mu_1, \mu_3, \mu_4, \lambda_1, \lambda_2, \lambda_3$ correspond to multiplicative factors, the others are exponents.

	Estimated values
μ_1	7.06
μ_2	4.1
μ_3	30.2
μ_4	8.9
μ_5	0.2
μ_6	0.85
λ_1	34.2
λ_2	9.2
λ_3	13.16
λ_4	1.79
λ_5	1.08
λ_6	0.42

Table 4: Estimated parameters for Λ_{F1} and Λ_{F2} , $\Lambda_{F1} = (\mu_1, \dots, \mu_6)$ and $\Lambda_{F2} = (\lambda_1, \dots, \lambda_6)$

In the configuration F1, the two highest values of the multiplicative factors (μ_3 and μ_4) and the two lowest values of the exponents (μ_6 and μ_5) correspond respectively to the parameters of the distance and the interaction terms. These two quantities are associated to candidate point located on another aggregate. As a result, the crack will tend to favour a path on the same aggregate unless the angle to stay on the aggregate is high and the crossing of the matrix is associated to low distances and angles. This is consistent with the analysis of Section 3.3.2.

It is also interesting to study the variability of the estimate with respect to the size of the training set. More precisely, the parameter estimate is performed from a training set including an increasing number of microstructures. Figure 15 and Figure 16 display the estimate of each parameter. It is possible to observe a first stabilization for the majority of the parameters from about ten microstructures. In all cases, beyond 25 microstructures, the estimate can be considered to be stabilized for all parameters.

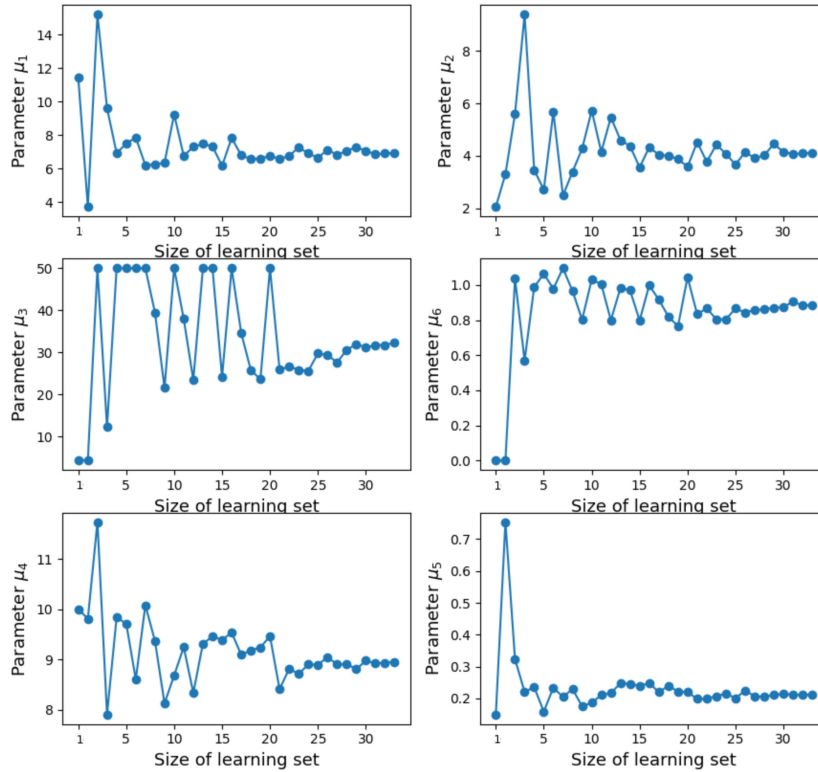


Figure 15: Parameter estimate with respect to the size of the training set in the F1 configuration. From top to bottom, parameters associated to θ_x (points on the same aggregate), to the interaction term (points requiring crossing the matrix) and to \tilde{d}_x (points requiring crossing the matrix)

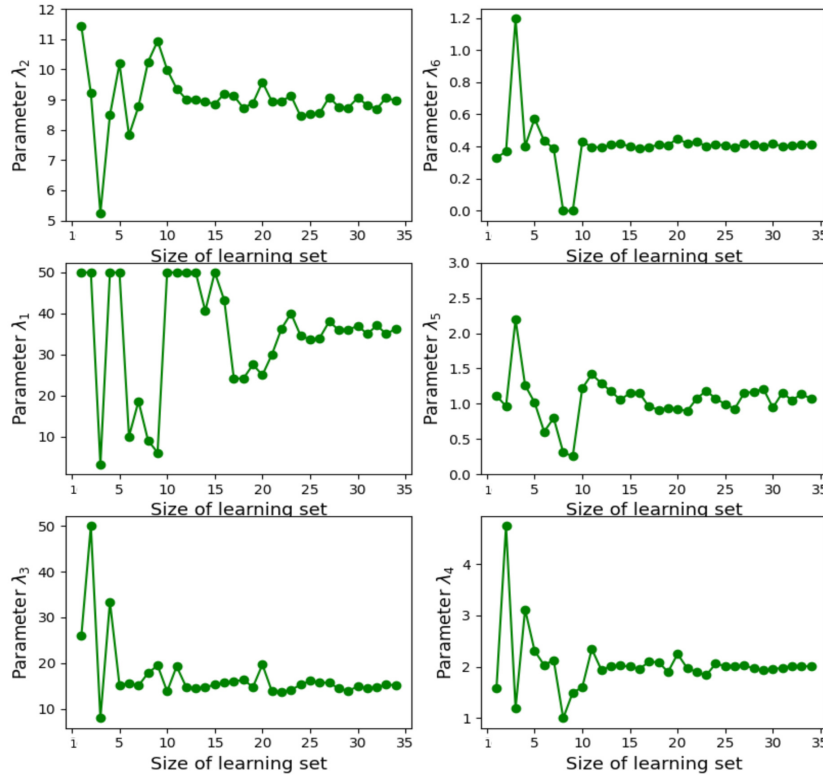


Figure 16: Parameter estimate with respect to the size of the training set in the F2 configuration. From top to bottom, parameters associated to \vec{d}_x , to the interaction term and to $\vec{\theta}_x$

5.2 Cracking prediction

We evaluate the performances of the prediction model with the estimated parameters provided by Table 4. Since the model is stochastic, for a given microstructure, its output is a random crack path. When run M times, we obtain a set of M cracks.

In this section, the model is applied to the training set for verification and to a test set (i.e. not used for the parameter estimate) of 30 microstructures with multiform aggregates (aggregates represented by regular polygons with a number of sides varying from 3 to 8) for validation. It is important to keep in mind that the change of aggregate shapes between the training and the test sets does not require new XPER simulations to construct the prediction model, and therefore there is no extra significant computational time for the crack prediction.

We first focus on the analysis of the crack paths then consider the prediction of the tortuosity.

5.2.1 Crack path

For a given microstructure E , we denote by $\mathcal{X}_E^k = (x_{i,k}^E)_{i=1,\dots,m_E^k}$ the sequence associated to the k^{th} ($k = 1, \dots, M$) crack realization.

Median path When the objective is to derive a unique crack path that approximates the deterministic computer code simulation at a low cost, we use a median path from the set of points \mathcal{X}_E^* satisfying:

$$\mathcal{X}_E^* = \arg \min_{\{\mathcal{X}_E^k\}_{k=1,\dots,M}} \left(\sum_{j=1, j \neq k}^M D(\mathcal{X}_E^k, \mathcal{X}_E^j) \right) \quad (10)$$

where D is the Fréchet distance (Driemel et al. 2012; Jekel et al. 2019) which is defined as follows :

Definition 6 – Fréchet distance : let X_1 and X_2 be two crack paths. The Fréchet distance between two crack is defined as follows :

$$D(X_1, X_2) = \inf_{\alpha, \beta} \max_{t \in [0,1]} \|X_1(\alpha(t)) - X_2(\beta(t))\|$$

where $X_1, X_2 : [0, 1] \rightarrow \mathbb{R}^2$ are parametrizations of the two crack and $\alpha, \beta : [0, 1] \rightarrow [0, 1]$

The median crack is considered the most optimal crack for a given microstructure.

Confidence region To quantify the uncertainty of the median, we define a confidence region. The region is constructed from point-value evaluations of percentiles. This type of construction requires a parametrization of each predicted path (see definition 2). In this test case, the crack is initialized on the left hand side boundary of the microstructure and propagates until the failure of the microstructure.

For any $x^1 \in [0, L]$, the uncertainty is quantified by estimating the 5% and 95% percentiles from the sample $(h_E^1(x^1), \dots, h_E^M(x^1))$. Denoting $(\tilde{h}_E^1(x^1), \dots, \tilde{h}_E^M(x^1))$ the ordered sample (increasing order), the uncertainty interval at x^1 is defined by $[\tilde{h}_E^{\lfloor 0.05M \rfloor}(x^1), \tilde{h}_E^{\lceil 0.95M \rceil}(x^1)]$ (where $\lceil \cdot \rceil$ is the ceiling and $\lfloor \cdot \rfloor$ the floor) which constitutes the upper curve and the lower curve. The region of confidence is finally taken as the convex hull and the uncertainty of the model prediction can be quantified by the diameter of this region computed as the Fréchet distance between the lower and upper curves defining this hull. The confidence region gives the area where the crack has the highest probability of passing.

Figure 17 and Figure 18 provide two examples of median crack path and confidence region as well as a comparison with the XPER simulation for a microstructure of the training set (only square inclusions) and a microstructure of the test set (various shape inclusions).

The number of paths calculated by the prediction model is $M = 100$. To complement the previous comparison, Figure 19 and Figure 20 display the Fréchet-distance-based error between the XPER simulation and the median path as well as the uncertainty for all the microstructures of the training and test sets. For a better understanding of their values, the results of Figure 17 and Figure 18 correspond to the microstructures 31 and 28 on these figures.

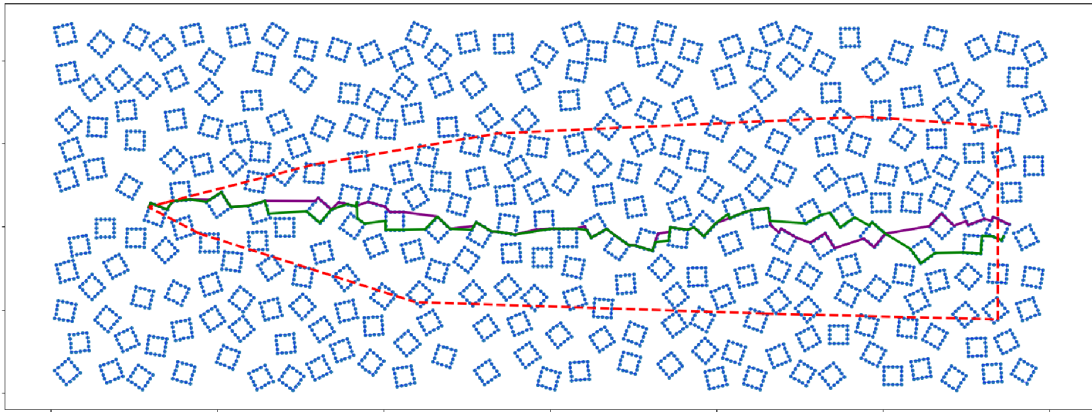


Figure 17: Example of path prediction for square aggregates: XPER simulation (purple), median path (green), region of confidence (dotted red curve)

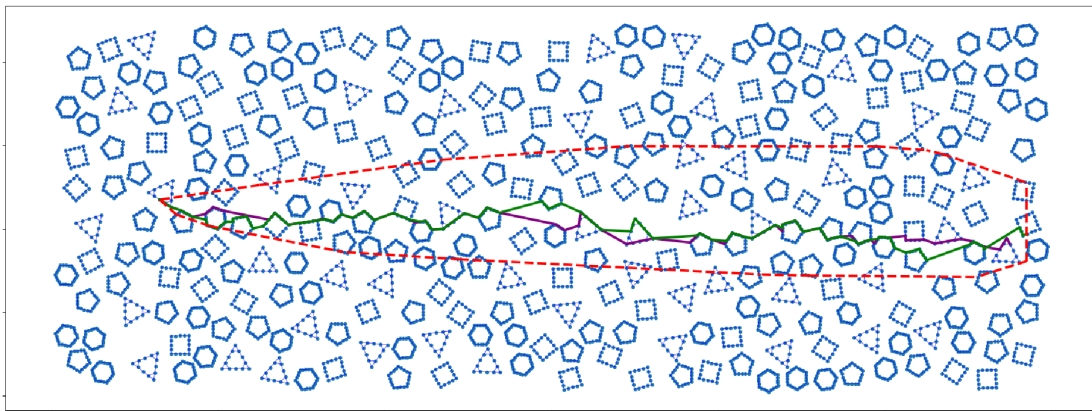


Figure 18: Example of path prediction for multiform aggregates: XPER simulation (purple), median path (green), region of confidence (dotted red curve)

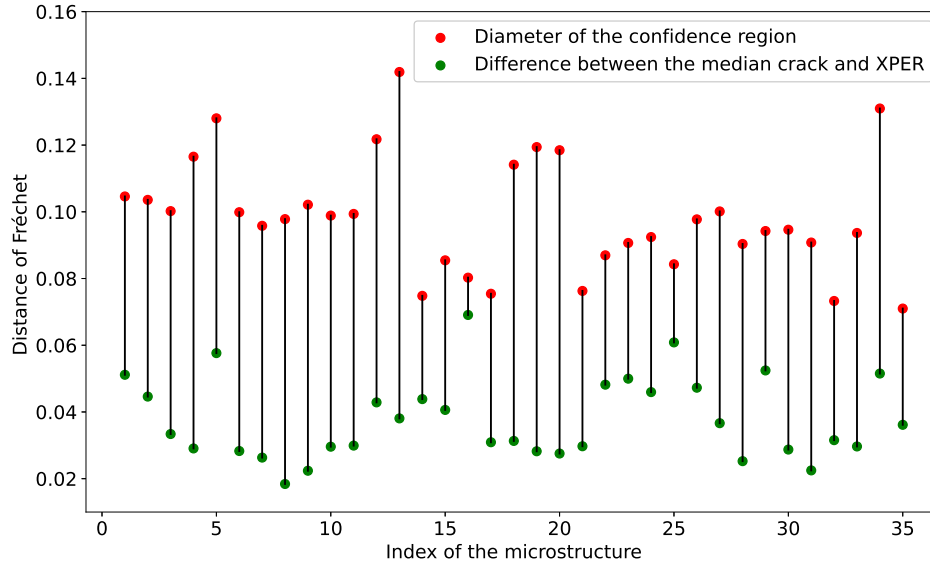


Figure 19: Prediction on the training set (square aggregates): Fréchet-distance-based error (green) between the median crack path and XPER simulation, radius of the confidence region (red)

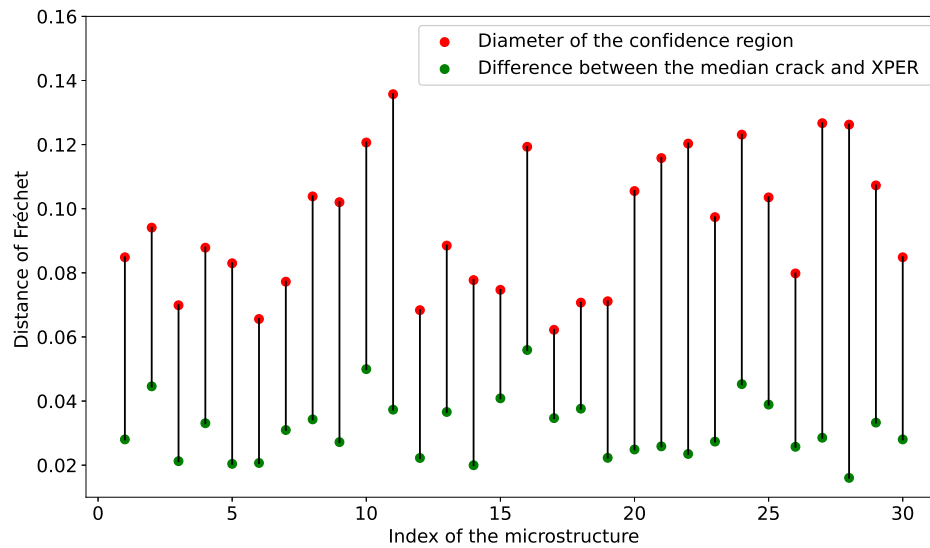


Figure 20: Prediction on the test set (multiform aggregates): Fréchet-distance-based error (green) between the median crack and XPER simulations, radius of the confidence region (red)

It can be observed that the error between the median crack path and the XPER simulation is always smaller than the uncertainty. The accuracy of the median prediction can be reduced for some microstructures of the training and test sets. As an example, Figure 21 shows the case associated to the largest error on the test set.

This lack of accuracy can be explained by a situation encountered by the crack where two candidate points of the field of view have similar values of their indicators. As a result, they exhibit the same probability to be the next point on the crack path. Since our model is stochastic, these two points are therefore reached by several crack realizations and it is not surprising that, for some microstructures, the median crack path does not correspond to the same local choice than the XPER simulation. However, despite this local bifurcation, the rest of the crack path is in good agreement with the mode I propagation direction. Moreover, the XPER simulation lies in the region of confidence. Note that this result holds for both microstructures of the training and test sets.

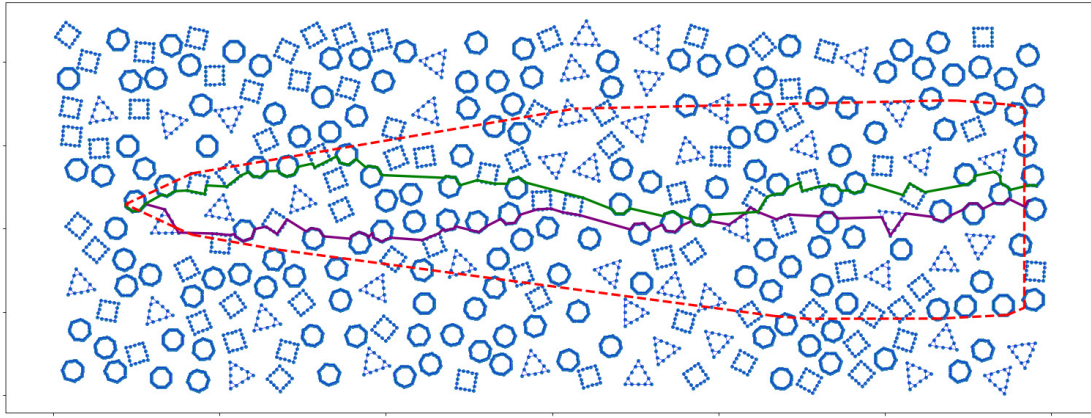


Figure 21: Example of path prediction for multiform aggregates: XPER simulation (purple), median path (green), region of confidence (dotted red curve)

Influence of the training set We also study the influence of training set on the predictions for microstructures of the test set. Besides the training set with square aggregates, we consider two new training sets of 35 microstructures with pentagonal, resp. octagonal, aggregates numerically cracked with XPER code under the same conditions as those of Section 2.2. The parameters of the prediction model are estimated with the BFGS algorithm. Figure 22 gives the results associated to the construction of the median crack path for the 3 training sets. The set with square aggregates leads to the smallest error for the largest number of microstructures.

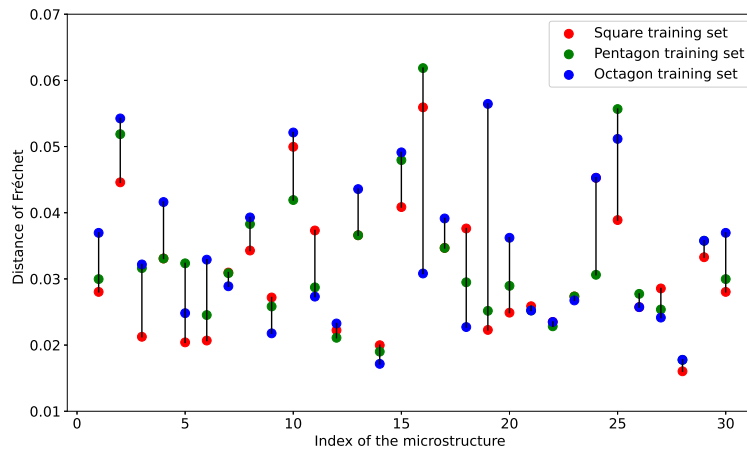


Figure 22: Comparison of Fréchet distances between the median crack path and the XPER simulations for different training sets

Evaluation of the computational time We conclude this section by focussing in Table 5 on the CPU time associated to the crack prediction by our model for both training and test sets.

One iteration of Algorithm 1	0.13
One crack realization ($M=1$)	13
Median crack ($M=100$)	1375

Table 5: Average computational time in seconds associated to the prediction using the probabilistic model in the case of a single processor

By comparing to the XPER simulation (Table 3), our model allows a drastic reduction of the computational cost (reduction by a factor 2575 for the median crack path when considering the same number of processors).

5.2.2 Analysis of a mechanical quantity: the tortuosity

For each microstructure, the tortuosities of the M predicted paths are computed and we focus on their median and uncertainty interval. This interval is obtained from percentile estimate similarly to the previous section. Figure 23 displays the results when $M = 100$ for each microstructure of the test set and a comparison with the tortuosity coming from the XPER simulation is performed as well.

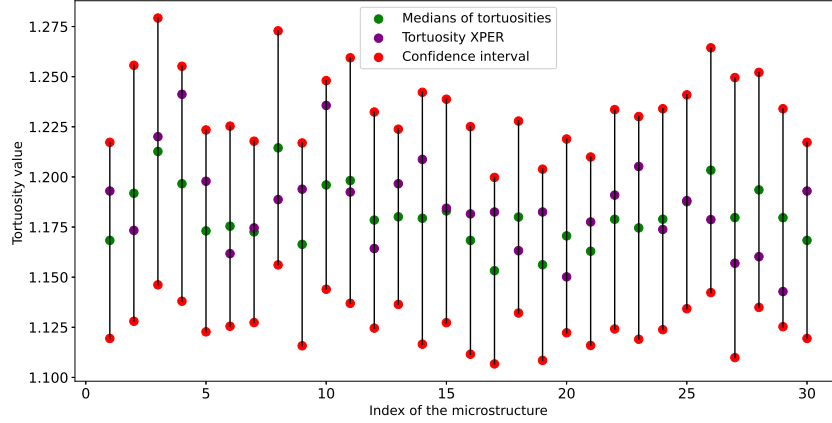


Figure 23: Tortuosity prediction on the test set (multiform aggregates): XPER simulations (purple), median predictions (green), uncertainty intervals (red)

It is also important to keep in mind that the model provides more information than a median and a confidence interval. It allows to derive the tortuosity histogram (see for example Figure 24) of each microstructure.

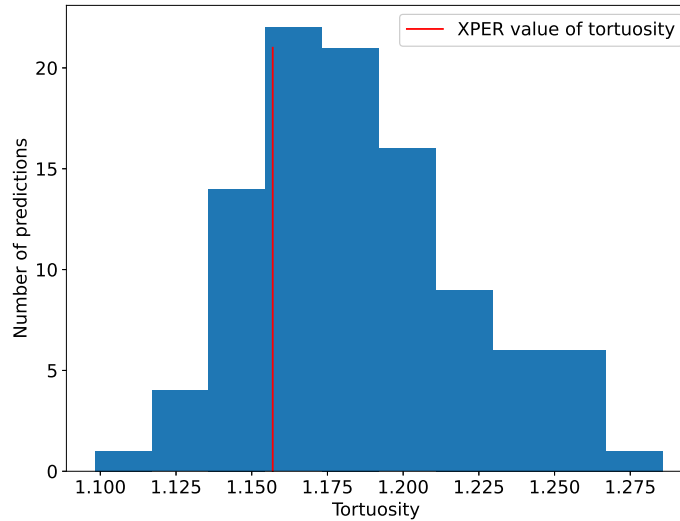


Figure 24: Tortuosity histogram for a microstructure of the test set

This statistical quantity can be exploited to evaluate the probability for the tortuosity to belong to a given variation range. This type of information is relevant for computational cost reduction since it allows performing targeted XPER simulations i.e. simulations leading to a tortuosity in a variation range of interest.

Finally, the performance of the model is studied in term of tortuosity density estimate taking into account the variability due to all microstructures. Figure 25 shows that the XPER tortuosity density can be accurately approximated.

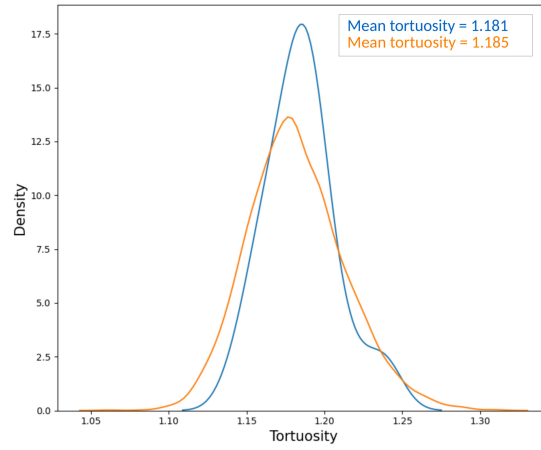


Figure 25: Comparison of the tortuosity densities constructed from the XPER simulations (blue) and the model predictions (orange) for microstructures with multiform aggregates (density obtained by kernel density estimate method)

6 Conclusion

We developed a probabilistic model for 2D fast crack prediction. This model leads to an algorithm that approximate at a low computational cost the local path of a crack.

The algorithm has been fully described and includes two steps. The first step is the computation of two local geometrical indicators (distance and angle) to capture the aggregate configurations in the vicinity of the crack tip. An efficient procedure exploiting a shadow cone has been proposed to evaluate them. The second step is the realization of a Markov chain model on the basis of the two indicators. The model parameters are estimated from a training set of numerically cracked microstructures. From any point of a crack in a microstructure, the model is able to evaluate the capability of any new point to be reached by the crack.

The numerical results show that, for a given microstructure with different aggregate shapes, the new model provides a set of predicted cracks that are in agreement with the computer code simulation. Moreover, it allows recovering the variability of mechanical quantities of interest such as the tortuosity.

The main advantage for practical issues is that the model is sufficiently flexible to be automatically adapted to any change in the local direction of the crack. A more complex application (a three-point bending beam test) is currently conducted on a mechanical test case where the crack direction is obtained through a mechanical simulation.

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