Numerical Generation and Contact Analysis of Rough Surfaces in Concrete

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Abstract

In concrete structures, opened cracks contribute significantly to the transfer of shear and normal stresses through the contact forces occurring between fractured surfaces. Such contact forces are due to protruding asperities, engaged by interlocking and friction. In this paper, the role played by roughness on shear resistance is investigated numerically. First, micro computed tomography and digital microscope measures of concrete surfaces are used to validate a novel numerical generator of realistic cracked concrete surfaces. Secondly, a contact solver based on the boundary integral approach allows an extremely fine description of typical cracked surface topologies. Roughness changes drastically the predictions, so that the shear resistance computed numerically matches the prior experimental results reported in the literature. The proposed model does not need any fitting procedure, making it a reliable and physically based method for predicting shear transfer phenomena in concrete. An empirical power-law predicting the shear resistance in concrete is a direct outcome, which accounts for micro-scale roughness and aggregate distribution.

1. Introduction

The topography of solid surfaces and its characteristics are of great importance for interfacial phenomena such as contact, friction and wear. One such situation where contacting interfaces are of great importance is for the study of concrete structures presenting cracks, which appear way before the structural failure. Such cracks are assumed to initiate under pure Mode I loading and once initiated, they can undergo both normal opening as well as tangent slipping, i.e. mixed mode. The slip of a fully developed crack leads to contact between its surface asperities and to interfacial transfer of stress. This effect mitigates the stress concentrations at crack tips, and can therefore reduce evolution of cracks, resulting in an increase of the shear-carrying capacity of concrete structures. It has been shown that in concrete structures without shear reinforcements shear transfer action across cracks carry up to 80% of the total shear load (Campana et al. 2013). Therefore, understanding the contact occurring between cracks in concrete is crucial to design concrete structures prone to be subject to shear loads. Over the years, numerous studies have been conducted to either experimentally investigate the behavior of a single crack in concrete specimens (Jacobsen 2012; Østergaard et al. 2007; Carpinteri and Brighenti 2010; Tirassa et al. 2018) or to develop analytical approaches capable of predicting experimental observations (Walraven 1981; Li et al. 1989; Bazant and Gambarova 1980; Gambarova and Karakoç 1983; Dei Poli et al. 1987; Vecchio and Collins 1986; Bujadham and Maekawa 1992; Jacobsen 2012; Calvi et al. 2017; Sagaseta and Vollum 2011; Nagle and Kuchma 2007; Mattock and Hawkins 1972). These approaches allowed to calculate interfacial forces from the mechanical parameters of concrete and thus have been helpful in formulating guidelines to design safe structures fib (2013). In these analytical models, the topographies of cracks were simplified to a 1D profile in order to derive a simple analytical expression. Walraven (1981) and Calvi et al. (2017) simplified the crack profile as a flat profile with protruding circular aggregates whereas Li et al. (1989) simplified it by expressing the distribution of profile slopes ρ(θ) as a cosine function 12cosθ. Later, Bujadham and Maekawa (1992) provided a distribution for high strength concrete as the normal distribution 5/6 exp(−21 θ2/π2). The topography of a crack in concrete is undoubtedly affected by the presence of aggregates: cracks propagate mainly where the strength is lower, i.e. within the interfacial transition zone (ITZ) (Scrivener and Technik 2004) and through the matrix. However, the cracked surfaces are also inherently rough and possess self-affinity characteristics (Thomas 1999; Persson et al. 2005), usually characterized by a power law behavior of the auto-correlation function of surface profile. Cracks in concrete also possess such characteristics, as shown in the literature (Saouma et al. 1990; Hammad and Issa 1994; Issa et al. 2003; Balankin et al. 2005) as well as confirmed by digital microscope measurements (see Section 2). Therefore, both self-affinity of rough surfaces and distribution of aggregates need to be taken into consideration to obtain an accurate representation of crack profiles in concrete.

Thus, the simplification of crack profiles for estimating the resistance force makes the existing models [Walraven (1981); Li et al. (1989); Bujadham and

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Maekawa (1992)] less robust. Therefore, the aim of this paper is to study the role played by roughness, and to allow better predictions of the shear resistance by including representative surface profiles in numerical and semi-analytical models.

This paper starts in Section 2 by characterizing the topography of cracks in concrete. This is done by analyzing the so-called Hurst exponent (Persson et al. 2005; Yastrebsov et al. 2015) of cracked surfaces as well as the distribution of aggregates along a section of an actual concrete sample. Experimental results obtained by micro-CT and digital microscope are first compared with analytical predictions from the literature (Walraven 1981; Li et al. 1989; Bujadham and Maekawa 1992). In Section 3 a methodology is proposed to generate rough surfaces in concrete numerically while prescribing several important characteristics of real concrete surfaces, leading to representative concrete surfaces. In Section 4 the mathematical formulation necessary for determining the shear resistance is described, by starting from first principles. The numerical framework and the numerical setup considered for analyzing the contact between rough surfaces is explained in Section 5. In Section 6, the effect of roughness on shear resistance is investigated numerically by using an elasto-plastic contact solver based on the boundary integral approach. The artificial rough surfaces synthesized from the methodology proposed in Section 3 are sheared by imposing a relative displacement. The effect of roughness on the true contact area as well as on the contact forces is demonstrated thanks to a fine discretization of the surface. The statistical expectation of shear resistance for mixed-mode loading is computed and analyzed for various loading kinematics. A simple analytical formula is shown to reproduce the numerical results, opening the path to use a traction separation law in the experimental results of Jacobsen (2012) show that the experimental profile auto-correlation follows a power law:

$$\Delta h(\delta x) = \langle (h(x + \delta x) - h(x))^2 \rangle^{1/2} \sim \delta x^H$$  \hspace{1cm} (1)

where \(\Delta h\) is the root-mean-square of height difference between two points separated by distance \(\delta x\) along the crack surface and \(H\) is the Hurst exponent, with \(0 < H < 1\) for usual self-affine surfaces. The Wiener-Khinchin proves that the power spectral density (PSD) follows a power law. In real surfaces this decay only holds within a spectral range:

$$\Phi(q) \sim A|q|^{-2H-D} \quad \forall q \in [q_{min}, q_{max}]$$  \hspace{1cm} (2)

with \(D = 1\) for a profile (Milanese et al. 2019) and \(D = 2\) for a surface (Persson et al. 2005; Ponson 2016). The use of discrete Fourier transforms is therefore a notorious method to extract Hurst exponents from experimental and numerical surfaces (Jacobs et al. 2017). The Hurst exponent, the spectral range \([q_{min}, q_{max}]\) and the constant \(A\) describe together the magnitude of waves in a surface.

From \(A, H\) and \(q_{max}\), one can deduce the root-mean-square of slopes, defined as \(\left( \bar{V}h^2 \right)^{1/2}\), where \(\bar{\omega}\) is the surface average operator. It is widely used when considering flat-on-rough systems in linear elasticity conditions to predict that the applied pressure \(P\) and the contact area \(A\) are linked by:

$$\frac{A}{A_0} \sim \frac{P}{e(\bar{V}h^2)^{1/2}}$$  \hspace{1cm} (3)

where \(A_0\) is the nominal contact area and \(E\) is the effective Young’s modulus (Persson et al. 2005; Johnson 1985; Hyun et al. 2004; Campanà and Müsser 2007). The root-mean-square of slopes is therefore a characterizing scalar with a particular importance to contact mechanics.

In this work, \(H\) and \(\left( \bar{V}h^2 \right)^{1/2}\) are used as signatures for the roughness of surfaces.

In the following, several cracked surfaces will be analyzed. Surfaces extracted from real concrete samples as well the theoretical profiles proposed by Walraven (1981), Li et al. (1989) and Bujadham and Maekawa (1992) will be considered. Deviations of current analytical models
will be demonstrated. Then profiles generated with a novel algorithm will be shown to match the surface signatures of real specimens.

### 2.1 Experimental samples

The real concrete sample presented in Fig. 1 is one of the four post-mortem specimens that have been studied. All were cast with hard-medium gravel aggregates having diameters in the range \(d \in [0.063 - 8] \text{ mm}\) and with the cement mix type CEMII A-LL42.5n (white). Several sieves were used to select the aggregates so that the granulometric probability curve, \(P(d)\), follows as much as possible the theoretical Fuller’s distribution Fuller and Thompson (1907) (the desired distribution is shown in Fig. 2), which is a typical requirement for concrete casting. The concrete samples have been loaded under mixed-mode kinematics: initially in Mode-I and then with an imposed mixed displacement (normal and tangential) at a constant loading angle. Each specimen was loaded with a different loading angle. Under these conditions, a primary crack developed and propagated, leading to the creation of a rough surface [for further details refer to Tirassa et al. (2018)]. The surfaces thus created have been scanned using a digital microscope to measure the surface elevation, i.e. \(h(x, y)\). Figure 3 shows the scan of one of such surface.

Figure 6(b) (yellow color line in the plot) shows the PSD of \(h(x, y)\), which decays as a power-law matching a Hurst exponent of \(H = 0.8 \pm 0.05\). This is consistent with Balankin et al. (2005) where a measure performed on rough concrete profiles reported \(0.7 < H < 0.8\). This suggests that Hurst exponents are depending only on local fracturing processes, and are therefore rather independent of loading kinematics (i.e. loading angle). The root-mean-square of slopes for the rough surfaces presented in Fig. 3 are all within the range \((\sqrt{h^2})^{1/2} = 1.16 \pm 0.19\).

In order to characterize the placement of aggregates on surfaces, one of the samples presented earlier has been scanned using micro-computed tomography PIXE (EPFL-ENAC 2021), which was developed at the School of Architecture, Civil and Environmental Engineering (ENAC) of the Swiss Federal Institute of Technology Lausanne (EPFL). By assuming a straight crack cutting through the sample (and aggregates), one can use the images from micro-CT scans to extract \(C(d)\) and \(g(r)\). Figure 4(a) shows, for a given height, the sliced image extracted from the micro-CT scan. Several scans have been analyzed to compute the cumulative density of aggregate surface-diameters and the radial distribution function. To this end, each pixel belonging to an aggregate is segregated from the pixels in matrix or voids, with the Training Weka Segmentation plugin (Arganda-Carreras et al. 2017) of the Fiji software (Schindelin et al. 2019). Figure 4(b) shows the result of a segmentation. As a consequence of the segregation process, tiny aggregates with visible areas smaller than 0.02 mm\(^2\) have been excluded (the equivalent cutoff diameter is \(2\sqrt{0.02/\pi} = 0.16\)
mm). Since the aggregates have irregular shapes far from being circles [see Fig. 4(c)] the diameter of an aggregate is approximated as the largest side-length of its bounding box.

Figure 5(a) (line plot in orange) shows the obtained cumulative density of aggregate surface-diameters averaged over 100 micro-CT images (sliced at different heights) issued from the same concrete sample. Figure 5(b) (line plot in blue) shows the obtained radial distribution function averaged over 100 micro-CT images (sliced at different heights). The peak value in $g(r)$ corresponds to the most probable distance between aggregates, which is 0.83 mm for these micro-CT scanned surfaces. As expected it is comparable with the average surface-diameter (0.86 mm). A bias in the measure of both $C(d)$ and $g(r)$ is expected for small values of $d$ and $r$ since we do not account for the tiniest aggregates during image segregation.

2.2 Analytical models and surface profiles

In this section, several analytical models are studied for the surface and bulk signatures presented earlier. In Walraven (1981), derives the distribution of aggregate diameters from the Fuller’s grading curve and with the assumption that the aggregates are spherical in shape. As shown in Fig. 5(a) (line plot in blue), Walraven’s model parameterized with a maximal aggregate diameter $d_{\text{max}} = 8$ mm leads to a cumulative density function $C(d)$ which strongly differs from the one obtained in Section 2.1. It is possible that such a strong bias is introduced when the smallest aggregates are neglected during image analysis. However, it should not impact the distribution for diameters much larger than 0.16 mm.

The radial distribution function is not well defined for these models. Walraven’s model considers the placement of aggregates as a purely random process, without a constraint for an average distance between aggregates. To the best of our knowledge, this leads to a constant average density of aggregates, and therefore $g(r) = 1$ uniformly. On the other hand, the models based on a slope distribution function (Li et al. 1989; Bujadham and Maekawa 1992) consider a unique material phase, making it impossible to distinguish mortar from aggregate, and thus to derive a relation for $g(r)$.

Concerning the surface roughness, the assumptions of Walraven (1981) (flat surface with spherical bumps and holes), and that of Li et al. (1989) and Bujadham and Maekawa (1992) (a random walk constrained to a statistical slope distribution) lead to distinct profiles. Figure 6(a) shows such theoretical crack profiles, generated

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Fig. 4 (a) A micro-CT scan from a concrete sample at a particular height. (b) Post-processed scan after segregation of aggregates: 0 = aggregate, 1 = matrix, 2 = void. (c) The largest side of the bounding box is considered as the effective diameter of an irregular aggregate.
based on these models assumptions. The power spectral densities and the Hurst exponents for such analytical crack profiles are shown in Fig. 6(b). Walraven’s kind (line plot in blue) has $H > 1.0$ suggesting that it is not self-affine. The profiles of Li et al. (1989) (line plot in green) and Bujadham and Maekawa (1992) (line plot in green) have a too rough $H \approx 0.3$, irrespective of the considered slope distribution. This suggests that surfaces representative of a crack profile roughness cannot be obtained by adjusting the slope distribution.

In this perspective, none of the available analytical models consider crack profiles matching actual concrete surfaces. Next section presents a novel methodology to generate cracked concrete surfaces numerically, which respect aggregate placement as well as self-affinity roughness.

### 3. Numerical generation of rough surfaces in concrete

In numerical works previously issued in the literature (Wriggers and Moftah 2006; Grassl and Jirásek 2010; Yilmaz and Molinari 2017), a concrete sample is generally modeled as a random packing of aggregates, which allows to simulate mechanical behaviors. Usually, gravel aggregates, which have rather smooth surfaces, are modeled as perfect spheres while crushed rock aggregates are modeled with arbitrary shaped polyhedrons. In a packing, the size distribution of aggregates $[d_{\text{min}}, d_{\text{max}}]$ is typically required to follow a granulometric curve such as Fuller’s (Fuller and Thompson 1907), so as to match an actual concrete casting. For the present study, the take-and-place algorithm as proposed by Wriggers and Moftah (2006) is employed to generate concrete packing numerically (Wittmann et al. 1985; Wang et al. 1999). The aggregates are progressively placed inside a box such that there is no overlap with already introduced aggregates. New aggregates are introduced until a targeted packing density, i.e. the aggregate volume ratio $\rho$, is reached. Figure 7(a) shows a numerically generated concrete sample with dimensions $50 \times 50 \times 50$ mm$^3$.

In real concrete, aggregates usually occupy 60% to
80% of the total volume. However it is computationally difficult to achieve a packing with such densities. To overcome this, other authors considered coarse aggregates only \((d_{\text{min}} > 4.75 \text{ mm})\) which led to packing densities around 40% (Wriggers and Moftah 2006; Grassl and Jirásek 2010; Ylmaz and Molinari 2017; Gatuingt et al. 2013). In this work, we want to model the concrete sample studied in Section 2.1 for which aggregates have been identified to be in the range \(d \in [0.063, 8] \text{ mm}\). Modeling only aggregates above \(d = 4.75 \text{ mm}\) greatly influences the granulometric curve, as shown in Fig. 2. Signatures issued from the distribution of visible aggregates, i.e. \(C(d)\) and \(g(r)\), will also be impacted [line plot in red in Fig. 5(b)] and line plot in green in Fig. 5(b)]. Selecting aggregates satisfying \(d > 0.3 \text{ mm}\) allowed to reach a packing density of 50% and a reduced mismatch of the granulometric curve, even if the real minimum aggregate size is \(d_{\text{min}} = 0.063 \text{ mm}\). Nevertheless, it will be shown, later in this section, that this approximation does not affect significantly the surface signatures \(C(d)\) and \(g(r)\).

Once a packing is generated, the procedure to generate a crack plane continues by cutting it at a given (random) height and by passing aggregates either beneath or underneath (depending on the height at which a spherical aggregate is cut). This assumes that ITZ is the weakest region in concrete. Figure 7(b) shows one such surface generated from the concrete packing of Fig. 7(a). The PSD for the generated surface is shown in Fig. 8(a) (line plot in blue). While it decays as a power-law, the corresponding Hurst exponent \(H > 1\) does not match the value of \(H\) observed for real concrete surfaces (see Section 2.1).

In order to generate a surface with the desired \(H\), a Fourier based filtering algorithm (Hu and Tonder 1992) can be employed to generate a self-affine surface numerically. With such an algorithm, it is possible to choose both the Hurst exponent \(H\) and the root-mean-square of slopes. Figure 7(c) shows such a numerically generated self-affine rough surface for \(H = 0.8\) and \((\Phi(h^2)^{1/2}) = 0.1\).

However, such surfaces do not have the holes and bumps typical of cracks breaking through the ITZ regions. Combining the surfaces extracted while cutting a concrete packing with purely fractal surfaces will allow to generate self-affine rough surfaces numerically, acknowledging the placement of aggregates. Hence, a surface \(S\) generated from the aggregate packing can be super-imposed to a self-affine surface \(S_{\text{affine}}\) generated for a given spectrum \((q_{\text{min}} = L/q_{\text{max}}, q_{\text{max}} = L/q_{\text{min}})\) as shown in Fig. 8(a).

While generating the self-affine rough surface, the Hurst exponent and the root-mean-square of slopes (keeping the spectrum fixed) is optimized to obtain a super-imposed surface with a targeted \(H_{\text{target}} = 0.8\):

\[
\text{argmin}_{\{q_{\text{min}}, q_{\text{max}}\}} \left[\Phi(h_{S_{\text{affine}}}(H_{\text{target}})^{1/2}) - H_{\text{target}}\right]\]  \(4\)

where \(H\) uses Fast Fourier Transform and log-log regression in \([q_{\text{min}}, q_{\text{max}}]\) to return Hurst.

Figure 8(a) shows an artificial concrete surface generated from the proposed algorithm. The input surface \(S\) is cut from an artificial concrete sample with \(\rho = 50\%\) and \(d = [0.3 - 8] \text{ mm}\) [see Fig. 7(a)] and has a Hurst exponent \(H \approx 1.1\). \(S\) is added to the optimal self-affine rough surface \(S_{\text{affine}}\) which is generated within the fixed spectral range \(q \in [2, 1024]\). The Nelder-Mead simplex algorithm (Nelder and Mead 1965) available as a Python package (Virtanen et al. 2020) was used to find the optimum \(H = 0.7\) and \((\Phi(h^2)^{1/2}) = 0.6\). The output surface verifies \(H = 0.8 \pm 0.01\). Figure 8(b) shows the power spectral density computed for a super-imposed surface (line plot in green). As can be seen, the PSD follows a power-law with an exponent leading to \(H \approx 0.8\).

As mentioned earlier, along with the Hurst exponent, the root-mean-square of slopes can be used as a signature for the surface roughness. The \((\Phi(h^2)^{1/2})\) averaged over 100 artificial surfaces is \(1.23 \pm 0.06\) which proves to be
in reasonable agreement with the values of actual concrete surfaces $1.16 \pm 0.19$.

To characterize the distribution of aggregates, the cumulative density function of aggregate surface-diameters, as well as the radial distribution function are computed for several numerically generated surfaces. By averaging over 100 surfaces $(C(d))$ and $(g(r))$ have been computed. Figure 5(a) shows that $(C(d))$ (line plot in green) is in fine agreement with the one obtained from the micro-CT scans (line plot in orange). Figure 5(b) shows the radial distribution of aggregates (line plot in orange), also matching the one obtained from the micro-CT scans (line plot in blue). In particular the expectation for the distance between aggregates is 0.85 mm which is close to 0.83 mm as obtained from micro-CT scans (see Section 2.1). It is again linked with the average surface-diameter here measured as 0.87 mm. These validations suggest that the surfaces generated with this novel approach have surface characteristics that are representative of real concrete surfaces.

Adding roughness over aggregate-based surfaces is not only an artificial method: the remnants of mortar sticking after crack development, as well as a crack evolution breaking through aggregates would both lead to roughness. Also, small wave-length roughness accounts for the smallest aggregates that could not be included in the numerical generation of packing samples due to computational limitation, which eventually compensates for the bias in the granulometric curve.

4. Formulation for contact between rough surfaces

In this section is presented the mathematical formulation determining the total resistance force $F^R$ acting against the relative slipping of two surfaces in contact. Such surfaces are crack lips entering in contact because of the mixed mode loading. By definition, the total resisting force is the sum of all the forces acting along the area $A$ where the two surfaces are in contact. Describing such
forces with a contact pressure field $p$ leads to the following integral equation:

$$F^R = \int p(x)ndA$$

(5)

where $n$ refers to the unit vector field normal to the surface. The contact area $A$ can be decomposed into $N$ smaller contacting patches $(a_i)_1 \ldots N$ such that $a \cup a_i = A$ (as shown in the figure below). With $\bar{f}$, the force acting on the $i$th contact patch, the average contact force per patch $\bar{f}$ can be linked to the total force $F^R$:

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f(x)nda = \frac{1}{N} F^R$$

(6)

where $\cdot$ denotes the surface average operator. The number of independent contact patch $N$ is linked to the total contact area $A$ and the average area per contact patch:

$$\bar{a} = \frac{1}{N} \sum_{i=1}^{N} a_i = A \Rightarrow N = \frac{A}{\bar{a}}$$

(7)

This allows to write the normalized total resistance force:

$$\frac{p^R}{A_0} = \frac{\bar{f}}{\bar{a} A_0}$$

(8)

The previous equation is valid for a single contact situation, and so far, does not contain any approximation. Assuming a kinematic loading, most of the quantities presented above will depend on a global displacement vector, named $\delta$ hereafter. However, the problem of shear resistance in cracked concrete has to be stochastic because of random roughness created during the crack propagation. This was motivated by the analysis of post-mortem cracked surfaces in concrete Section 2. Such a randomness invites to employ the ensemble average operator ($\cdot \cdot$), which averages any quantity over an ensemble of surfaces generated with the algorithm presented in Section 3. This way, the expectation of the shear resistance will be independent from fluctuations due to the random roughness.

$$\frac{\langle p^R \rangle \delta}{A_0} = \frac{\langle \bar{f} \delta \rangle}{\langle \bar{a} \delta \rangle A_0}$$

(9)

The above expression can be further simplified by expressing the total contact area $A^\delta$ as $\bar{a}^\delta N^\delta$, $N^\delta$ being the number of contact patches.

$$\frac{\langle p^R \rangle \delta}{A_0} = \frac{1}{A_0} \left( \frac{\langle \bar{f} \delta \rangle}{\langle N^\delta \rangle} \right)$$

(10)

In the following sections, we will compute and characterize the quantities $\bar{f} \delta$ and $N^\delta$ thanks to an elasto-plastic contact solver.

5. Numerical framework

In this section, we briefly describe the elastic-plastic contact solver and the numerical setup employed in this study to simulate the contact between the concrete surfaces generated from the algorithm described in Section 3.

5.1 Elastic-plastic contact solver

Modeling self-contact between crack surfaces needs a pair of surfaces, initially perfectly conforming. Obtaining a relative displacement is achieved by considering the lower one as fixed and rigid, while the upper one will be the boundary of a semi-infinite elasto-plastic half space. The required mixed-mode displacement is applied onto the top surface as a weak (average) constraint. The global displacement vector $\delta = \delta_\nu + \delta_\sigma$, $\delta_\sigma$ is defined with a normal component $\delta_\nu$ and a tangent component $\delta_\sigma$. Similarly to the experiment of Jacobsen (2012), a Mode-I initial displacement $\delta_\nu$ is imposed, then followed by a progressive mixed-mode loading, which is characterized by the ratio $\gamma = \delta_\nu/\delta_\sigma$. Similar to the experiments, 2 different loading ratios ($\gamma = 1.2, 1.73$) and 3 different initial openings ($\delta_\nu = 0.025, 0.04, 0.1$ mm) are considered for this study. A detailed schematic for the loading and boundary conditions considered in this study is presented in Fig. A21.

At each loading step, an interpenetration between the two surfaces will occur, as shown in Fig. 9(a). Indeed, prior to solving contact mechanics, the configuration for the upper surface at a given displacement vector $\delta$ will be $h_{up}(x) = h(x - \delta_\nu, \delta_\sigma)$, and a tangent component forces will be resolved with a boundary-element approach (Polonsky and Keer 1999; Rey and Anciaux 2017) available in the open-source contact software Tamas (Frérot et al. 2019), which is computationally much faster than a traditional finite-element resolution. This allows to perform many large scale simulations, each with a finely discretized surface.

Nevertheless, there are several necessary approximations for using a Boundary-integral formulation to this problem. In order to benefit from accelerated Fast Fourier Transform approaches, in-variance/symmetry hypotheses are required so that only systems with a flat-deformable surface in contact with another rough-rigid surface can be used. In principle, this does not apply to the rough on rough case of this study. Assuming that the bottom surface is rigid, the trial gap $g^*$, before any contact mechanics resolution, is given as:

$$g^*(x) = h_{up}(x) - h(x) = h(x - \delta_\nu, \delta_\sigma) - h(x) + \gamma^* \delta_\nu + \delta_\sigma$$

(11)

where $\gamma^* \neq \gamma$ is considered as a trial loading angle. As illustrated in Fig. 9(b) a negative gap is considered as an interpenetration. The final gap will be modified with the vertical displacement field $u$ produced while resolving contact elasto-plastic constraints. The final gap becomes:

$$\tilde{g}^*(x) = h_{up}(x) + u(x) - h(x) = g^*(x) + u(x)$$

$$\tilde{g}^* = \tilde{u} + \gamma^* + \delta_\sigma$$

(12)

It is important to note that the final vertical opening $\delta_\sigma$, and therefore the effective loading angle, are unknown since they depend on the contact resolution. This is somewhat similar to how the loading kinematics are enforced in experiments (Jacobsen 2012), where a control loop measures constantly the average relative displacements
\( \Delta u_n \) and \( \Delta u_x \) with four strain gauges placed along the crack, in order to adjust the vertical opening (in real-time) and to achieve the sought loading ratio \( \gamma = \Delta u_n / \Delta u_x \). For the numerical method presented, the loading remains displacement-controlled and the trial loading angle \( \gamma^* \) will lead to an effective loading angle \( \gamma \) which will be computed a posteriori.

The overall procedure to find displacements, tractions and \( \gamma \) is achieved in two stages. First, the rough on rough configuration is mapped onto a rough on flat normal configuration: the rough profile is taken as the trial gap field \( g^* \), and is assumed rigid. A trial displacement \( u^* \) is produced by canceling interpenetrated regions (where \( g < 0 \)). The displacement field \( u \) which complies with a mean gap \( \bar{g} \delta = g^* \delta + u^* \), as well as contact constraints can be found with the boundary element solver under linear elasticity hypotheses. This displacement leads to the deformation of the flat half-space, with the accompanying surface pressures [see Fig. 9(c)].

By considering only elastic interactions, non-physical values of contact pressures (beyond the yield limit) will be encountered. In reality plastic flow should have occurred, with the effect of saturating pressure, roughly leading to a plateau at a maximal value \( p_{\text{max}} \approx k \sigma_y \) (Johnson 1985; Tabor 1951; Hill 1950). Therefore plasticity needs to be resolved in a second stage, similarly to (Johnson 1985; Tabor 1951; Hill 1950). Therefore plasticity needs to be resolved in a second stage, similarly to the classical return mapping algorithm. For this purpose, the pressure saturation model (Almqvist et al. 2007) will be employed. However, this algorithm is formulated in its dual form (unknowns are gaps or displacements), so that the input is the applied average pressure. The previous elasticity resolution was performed as a primal problem (average gap was prescribed, pressures were unknown). Switching to a dual pressure formulation, is performed by evaluating a compatible average pressure. In order to do so, the contact patches (where pressure is strictly positive) are located with a flood-fill algorithm considering 8 neighbors. For each contact cluster, its average pressure \( p_{\text{cluster}} \) is computed. Wherever \( p_{\text{cluster}} > p_{\text{max}} \), the cluster pressure is predicted as completely saturated, as shown in Fig. 9(d).

This projection of the contact pressure per cluster leads to a trial pressure field \( p \) compatible with plasticity constraints. Then the final pressure field is obtained with the saturation model (Almqvist et al. 2007) by requiring that the average pressure must be \( p^* \) which provides the final displacements and tractions in the rough-rigid on flat-deformable space [Fig. 10(b)]. The displacement and pressure fields thus obtained provide the deformed rough-on-rough configuration by mapping them back to the original configuration. In order to account for the curvature, the outward vector normal to the original rough surface \( n \) is giving the direction of the contact force that prevents interlocking of the contacting asperities [see Fig. 10(c)].

After solving the elasto-plastic contact problem, the final loading angle can be computed with,

\[
\gamma = \frac{\delta_x (x) - \delta^*}{s_x} = \frac{\delta_x (x) + \delta^* - \delta_u}{s_x} = \gamma^* + \frac{\delta^*}{s_x} \quad (13)
\]

It is observed that the \( \gamma \) computed for a given input

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**Fig. 9 Elastic resolution procedure.** (a→b): Mapping a rough-on-rough configuration onto a rough-on-flat configuration.
(b→c): Solving for interpenetration by enforcing a mean gap \( \bar{g} \). The outputs are pressure field \( p \) and displacement field \( u \).
(c→d): Projection of the average pressure at each cluster by saturating it to \( p_{\text{max}} \), producing a predictor state. This trial pressure \( p^* \) allows to compute a compatible mean pressure \( p^* \).

**Fig. 10 Elasto-plastic resolution procedure.** (a→b): Starting from the configuration Fig. 9(c), the initial condition \( u, p^* \), solve for a prescribed average pressure \( p^* \) using the pressure saturation model (Almqvist et al. 2007). The resolution leads to a new displacement \( u \) and a new pressure field \( p \). (b→c): The new displacement field \( u \) is used to obtain the deformation in rough-on-rough configuration. The new pressure field \( p(x) \) is mapped back to the rough-on-rough configuration along the outward normal field \( n \) at each contact point.
(\gamma^*, \delta^*) remains constant independently of the sliding displacement \delta_s with only a small standard deviation. The deviation of \gamma from the loading angle considered in Jacobsen (2012) (\theta = \tan^{-1}(\gamma)) is well within \pm 1° for the entire loading history as shown in Fig. A21

5.2 Numerical setup
In this section, the numerical setup considered for analyzing contact between rough surfaces is described. For our study, surfaces with a superposed self-affine roughness (class \( S_A \)) and surfaces with only protruding aggregates (class \( S_p \)) will be considered. Thus, the values of \( f_p \), \( N \) and \( \tau \) will be compared. The surfaces used throughout this work are generated with the algorithm presented in Section 3 for a packing density of \( \rho = 40\% \) and a distribution of aggregate diameters within the range \( d = [4 \text{ - } 8] \text{ mm} \). The aggregates are placed in a concrete sample of characteristic compressive strength \( \sigma_{c, \text{fib}} = 20 \text{ MPa} \) according to the empirical relation \( \bar{\sigma} = 36 \text{ MPa} \) and \( \begin{bmatrix} \rho \approx 0.49 \text{ mm} \end{bmatrix} \end{bmatrix} \) (Van Mier and Van Vliet 2003; Ylmaz and Molinari 2017). The packing density and the aggregate distribution are chosen similar to the concrete samples that Jacobsen (2012) used for evaluating the entire loading history as shown in Fig. 11

6. Results
In this section, the results obtained from simulating the contact between surfaces show the effect of roughness on the evolution of contact area, contact forces \( f^\delta \) and number of contact patches \( N \). Furthermore, these findings will be used to formulate analytical expressions for \( f^\delta \), \( N \) and \( \tau \) acknowledging the surface roughness as well as the aggregate distribution.

6.1 Evolution of contact area
The effect of roughness on the real contact area is now presented. One surface with roughness (of class \( S_A \)) and one surface without (of class \( S_p \)) will be loaded with the kinematic constraint following a loading ratio \( \gamma = 1.73 \) and an initial opening \( \delta_s^i = 0.025 \text{ mm} \). Figure 11 shows the contact pressure field obtained for a shear displacement \( \delta_s = 0.073 \text{ mm} \). As expected, the contact patches for a surface without roughness have crescent shapes following the protruding aggregates contours. While including roughness produces the same global shapes, it adds small patches distributed randomly throughout the surface. Figure 12 shows the contact pressure field at a larger shear displacement \( \delta_s = 0.49 \text{ mm} \). This time both \( S_A \) and \( S_p \) share comparable features, revealing that the additional contact spots initially induced by the roughness tend to vanish for large displacements.

In order to obtain meaningful statistics, 50 realizations are studied for each surface class (\( S_A \) and \( S_p \)). Every such surface is a cut, at a specific height, through the same numerical concrete packing. The real contact area is calculated from the contact pressure field since a positive value of pressure \( p(x) > 0 \) corresponds to a contact point where the gap vanishes (\( g = 0 \)). The real contact area is shown in a normalized form \( A/A_0 \), where \( A_0 \) is the nominal area. Figure 13(a) shows the expected real contact areas (\( A_{S_A} \)) and (\( A_{S_p} \)) as function of the shear displacement \( \delta_s \). It can be observed that for small shear displacements, the real contact area (\( A_{S_A} \)) is greater than the real
contact area \((A)_{SB}\). This confirms that roughness initially introduces many new contact spots. However, after reaching a maximum area for a specific shear displacement, \((A)_{SB}\) decreases. On the other hand, the real contact area expected for \(S_B\) follows a monotonic increase with the shear displacement. As a consequence of roughness, \((A)_{SB}\) becomes smaller than \((A)_{SA}\) for large displacements. In order to clarify the origin of this behavior, the contact area evolution close to the aggregate shown in the insets of Figs. 11 and 12 is shown on a series of snapshot at different shear displacements, in Fig. 13(b). The contact area around the \(S_B\)-type aggregate increases with the shear displacement whereas it decreases for a \(S_A\)-type, which is due to the added roughness. Thus, at large shear displacement, when contact occurs only through protruding aggregates, \(S_B\) has a large real contact area if compared to \(S_A\).

It is clear, and was expected, that the addition of roughness modified the true contact area, which will consequently impact shear resistance. This is now studied by computing and comparing ensemble averages of the shear resistance stress, defined as:

\[
\langle t^\delta \rangle = \left\langle \frac{e^{RS}}{A_0} \right\rangle = \frac{1}{A_0} \left\langle (\beta \cdot e_y) S^\delta \right\rangle = \frac{1}{A_0} \left( \beta \cdot (\beta \cdot N)^\delta \right) \tag{14}
\]

After identifying every contact patch with a flood-fill, their number \(N\) and the average force per contact patch \(f^\beta\) are both extracted. The study of the covariance of \(f^\beta\) and \(N^\delta\) reveals that these two terms are independent of each other irrespective of loading kinematics for both surface classes (please refer to Appendix C for further details). Eventually the separation formula is obtained as Eq. (15), which allows to study contact forces and contact clusters separately, which is done in the following sections.

![Fig. 12 Snapshots of pressure field at loading kinematics, \(\delta = 0.49\) mm, \(\delta = 0.025\) mm and \(\gamma = 1.73\). (a) Surface class \(S_A\) and (b) Surface class \(S_B\). For both surface classes, contact patches are formed only due to protruding aggregates.](image)

![Fig. 13 (a) Ensemble average of real contact areas for a loading defined by \(\gamma = 1.73\) and an initial opening \(\delta = 0.025\) mm. Inset shows the ratio of ensemble average of real contact areas. The added roughness initially leads to an increase of the real contact area, and ultimately a decrease. (b) Zoom of the pressure map around an aggregate identified in the insets of Fig. 11 at four different shear displacements [highlighted in red on the curve Fig. 13(a)].](image)
of two regions, with and without a protruding aggregate, for shear displacements where the behavior is sensitive to the initial opening angle following the power-law decay. Such a switch of behavior has to be sought in the relative contribution of roughness and protruding aggregates to the total number of contact clusters.

Figure 14 shows the ensemble average of number of contact clusters \( N \) for classes \( S_A \) and \( S_B \), for the loading kinematics: \( \gamma \approx 1.73 \) and \( \delta_s^{\text{in}} = 0.025 \text{ mm} \) (line plot in orange for \( S_A \) and in red for \( S_B \)). The average number of contact clusters is always larger with roughness (for \( S_A \)). For shear displacements where \( (A)_{S_A}/(A)_{S_B} > 1 \) such a behavior was expected since many contact patches are created due to the additional roughness. However, at larger shear displacements such a difference is not trivial. Surfaces from class \( S_A \) have a large number of contact clusters with small areas, explaining how the number of contact remains large while the contact area drops. In order to demonstrate this, the probability density function of area of contact clusters \( \rho(a) \) is computed and shown in Fig. 15 for a shear displacement \( \delta_s = 0.49 \text{ mm} \) (where \( (A)_{S_A}/(A)_{S_B} < 1 \)). This probability density was computed from the 50 realizations for both surface classes. As expected the probability density of small contact areas is indeed larger with roughness.

Besides the large difference in the number of contact clusters for \( S_A \) and \( S_B \), their evolutions are decaying as a power-law of the shear displacement \( \delta_s \) (see Fig. 14). For surfaces with including roughness \( (S_A) \), the power-law decay initiates after a certain amount of slipping. At the onset, the expected number of contacts first increases before following the power-law decay. Such a switch of behavior is sensitive to the initial opening \( \delta_s^{\text{in}} \), a smaller \( \delta_s^{\text{in}} \) leads to a larger peak (shown by line plots in blue, orange, green in Fig. 14). The origin of this non-monotonic behavior has to be sought in the relative contribution of roughness and protruding aggregates to the total number of contact clusters. Figure 16 shows series of snapshots of two regions, with and without a protruding aggregate, taken from a loaded \( S_A \)-type surface. As can be observed the number of contact patches created due to the protruding aggregates decreases monotonically while \( \delta_s \) increases, whereas the number of contact patches created in the isolated region initially increases before decreasing. The combined effect of contact with aggregates and roughness leads to a non-monotonic evolution of \( N \) for surfaces having roughness.

The power-law behavior observed for the ensemble average of the number of contact clusters allows to analytically predict it as a function of the shear displacement \( \delta_s \):

\[
\langle N \rangle = B\delta_s^{-\kappa} 
\]

(16)

where \( B \) is a constant of proportionality and \( \kappa \) is a power-law exponent. Both these coefficients can be extracted by fitting the numerical results (please refer to Appendix D for a detailed description of the fitting procedure). For the surfaces with roughness and aggregates \( (S_A) \), the following analytical model is obtained:

\[
\langle N \rangle = B(\gamma)\delta_s^{-\kappa(\delta_s^{\text{in}})} \quad \text{with} \quad B(\gamma) = c + d, \kappa(\delta_s^{\text{in}}) = a\delta_s^{\text{in}} + b \quad (17)
\]

with \( c, d, a, b \) constants which are independent of the loading kinematics (The numerical values of such constants are shown in Appendix D). This power-law model is shown in Fig. 14, which matches quite well the numerical predictions, except at the onset of the shear displacement. At the beginning, the surfaces are indeed close to conformity with important true contact areas, dominated by aggregate shapes, and therefore leading to a monotonic behavior deviating from the power-law. On the other end, the power-law is a signature of rough contact, which happens only after a sufficient opening occurred, therefore depending on the initial opening and the loading angle.

![Fig. 14](image_url) Evolution of average number of contacts for surface class \( S_A \) and \( S_B \) in log-log scale for same loading ratio but different initial openings. The figure also shows the analytical fits over the power-law behavior.

![Fig. 15](image_url) Probability density function of area of contact clusters for surface class \( S_A \) and \( S_B \) at \( \delta_s = 0.49 \text{ mm} \). The loading ratio is \( \gamma \approx 1.73 \) and the initial opening is \( \delta_s^{\text{in}} = 0.025 \text{ mm} \).
6.3 Average contact force per contact cluster: Numerical and analytical predictions

Figure 17(a) shows the ensemble average of \( f_y \) for surface classes \( S_A \) and \( S_B \) under the loading kinematics: \( \gamma \approx 1.73 \) and \( \delta_o^1 = 0.025 \) mm (line plot in green for \( S_A \) and in red for \( S_B \)). The average force per cluster is always larger for surface without roughness (i.e. \( S_B \)). As observed earlier, the inclusion of roughness results in the formation of a large number of contact clusters with smaller areas (please refer to Fig. E29 for more details). Since the maximum contact pressure saturates to \( p_{max} \), it is expected that the force per contact cluster will be close to proportional with the contact area per cluster \( A \). As a consequence, the added roughness and plasticity diminishes substantially the average force per cluster.

The details of the statistics of the force per contact cluster are presented in Appendix F, which includes the probability density of \( f_y \). The ensemble average of force per cluster \( \bar{f}_y \) follows an increasing power-law, as revealed in Fig. 17(b) for various loading kinematics. The following analytical expression can be deduced:

\[
\bar{f}_y \sim \delta^\alpha
\]

with an exponent \( \alpha = 1.34 \) for rough surfaces, and \( \alpha = 0.7 \) for the aggregate only surface. It is remarkable that \( \alpha \) only moderately depends on the loading kinematic parameters \( (\gamma, \delta_o^1) \), whereas it strongly depends on the roughness \( (S_A \text{ surfaces have } H \approx 0.8, \text{ and } S_B \text{ surfaces have } H \approx 1.1) \). Furthermore, the analytical expression defined in Eq. (18) with \( \alpha = 1.34 \) provides a good approximation of \( \bar{f}_y \) for large shear displacements as seen in Fig. 17(b).
6.4 Shear stress: Numerical and analytical predictions

Figure 18 presents the shear stress response for surface classes $\mathcal{U}$ and $\mathcal{S}$ for identical loading kinematics: $\gamma \approx 1.73$ and $\delta_o^\perp = 0.025$ mm (line plot in green for $\mathcal{U}$ and in red for $\mathcal{S}$). The shear stress for $\mathcal{U}$ increases initially before decreasing, whereas for $\mathcal{S}$ the shear stress monotonically increases. At small shear displacements $(\tau)_{\mathcal{U}}$ is greater than $(\tau)_{\mathcal{S}}$ and at large shear displacements it is reversed. This behavior is similar to the evolution of the total contact area $(\mathcal{A})_{\mathcal{U}}$ and $(\mathcal{A})_{\mathcal{S}}$ respectively [see Fig. 13(a)]. Furthermore, the peak stress observed for $\mathcal{U}$-type surfaces is likely due to the behavior of the total number of contact clusters (see Fig. 14) which is absent for $\mathcal{S}$-type surfaces.

Using Eq. (15) along with the expressions Eqs. (16) and 18) leads to a power-law approximation of the shear resistance:

$$\tau \approx \beta \delta_s^{-\kappa + \alpha}$$

(19)

where $\beta$ is a multiplicative factor that will condition the elevation of the resistance. With the approximations that were made, this expression is expected to fit the behavior of $\tau$ only for large shear displacements. Eq. (19) illustrates the predicted behavior of this simple power-law model for various loading kinematics and roughness (see Table 1 for the numerical values of the constants). While the tail of the curves fit particularly well, the peak stress cannot be reproduced correctly. In order to capture the bell shape, the expression of the shear resistance can be empirically modified as follows:

$$\tau = \beta (1 - e^{\delta_s \xi}) \delta_s^{-\kappa + \alpha}$$

(20)

where the exponential term $e^{\delta_s \xi}$ brings a saturation allowing to capture the entire numerical prediction. Figure 19 shows the analytic expression computed using Eq. (20) (see Table 2 for the numerical values of $\beta$ and $\xi$). An excellent agreement is demonstrated. Furthermore, the exponential term compensates for the uncertainty observed at the onset of shear displacement (for $N$ and $f_N$). The parameter $\xi$ is only a fitting parameter, which controls how quickly the saturation is reached and shows, as expected, a dependence on loading kinematics.

An important outcome of the presented work is considered to be Eq. (20), as it can be employed in large scale finite element simulations, where describing roughness of fractured surfaces would lead to extremely fine meshes and computationally expensive simulations. This simplified expression of the shear resistance stress can be used to formulate a traction separation law (TSL) which would account for interlocking phenomena occurring in fractured concrete, similarly to the traction-separation laws.
Table 2 Values of $\beta$ and $\zeta$ obtained after fitting $\tau$ to the entire regime using Eq. (20). The values of $\alpha$ and $\kappa$ used for fitting are taken from Table 1.

| $S_A$ | $\delta_s = 0.025$ | $\delta_s = 0.04$ | $\delta_s = 0.025$ |
|-------|----------------|----------------|----------------|
| $\gamma = 1.2$ | $\gamma = 1.2$ | $\gamma = 1.73$ |
| $\beta$ | 1.42 | 1.45 | 0.53 |
| $\zeta$ | 17.45 | 15.54 | 25.26 |

used for cohesive zone modeling (Camacho and Ortiz 1996). Such a TSL would incorporate the effects of roughness and the aggregate distribution present at micro and meso-scales. Therefore, macro-cracks can be modeled with their global shape, while the microscopic details due to surface roughness will be handled with cohesive elements placed along the crack surface. Figures G32 and G33 show the normalized contact pressure maps along the surface $p_x = f(\delta_x, \delta_s)$ and normal to the surface $p_z = f(\delta_z, \delta_s)$ computed from the presented numerical simulations.

7. Discussion and comparison to experiments

In this section, we compare our numerical predictions with the experimental results (Jacobsen 2012). All reported numerical results are based on the material properties of real concrete (Jacobsen 2012), without using any fitting parameter. Figure 20 puts in perspective the experiments and the presented numerical model: qualitative predictions are obtained for surfaces with roughness ($S_A$ type surfaces). Both pre-peak regime and the order of magnitude of the peak stress are within an acceptable range. While the positions of the peak stress (for $S_A$ type surfaces) are predicted with acceptable precision, the power-law issued from the measures of Jacobsen decays much faster than our numerical prediction. The roughness characteristics (i.e. $H$ exponent and root-mean-square of slopes) control the power law exponents of $(N)_{S_A}$ and $(f_y)_{S_A}$. The steep decay observed in the measurements could mean a much different roughness produced by fracturing the concrete employed by Jacobsen.

The absence of Coulomb friction cannot be at the origin of such a bias, since adding a tangential contribution would only increase $\tau$. On the other end, the proposed model does not consider crack nucleation or damage in the bulk or nearby the contacting surfaces. Nevertheless, a significant amount of damage is observed for highly confined concrete, which results in the degradation of the material stiffness (Di Prisco and Mazars 1996). This is why lower values of $(\tau)$ are observed experimentally, especially during the post peak regime. The damage can be modeled as a constitutive law using various damage mechanics approaches (Grassl and Jirásek 2006; Wu et al. 2017) However, this will require a full-scale finite element simulation with a fine discretization of rough surfaces. Indeed, it cannot be done with boundary integral methods as it requires translation in-variance, which precludes a varying constitutive behavior.

8. Conclusions

In this work, we have investigated the role played by cracks topography on the shear resistance of concrete loaded by mixed-mode displacements. This was motivated by the necessity to describe the interlocking nature of shear transfer across cracked surfaces, in order to use more reliable and physically based equations in design criteria.

An accurate representation of surfaces was shown to require a multi-scale description, built upon meso-scale aggregates and micro-scale roughness. A signature of the small-scale roughness was constructed with self-affine concepts, such as the Hurst exponent and the root-mean-square of surface slopes. micro-CT and digital microscope measurements have been made on actual surfaces, which were previously sheared until failure. A novel algorithm was presented to synthesis rough surfaces. The principle consists in adding a fractal-like roughness on protruding aggregates, which proves to reproduce the signature of the experimental samples.

To investigate the effect of roughness on shear resistance, a stochastic study was made using an elasto-plastic solver based on a boundary integral formulation. It is demonstrated that both meso-scale (aggregates) and
micro-scale roughness (small scale asperities) are crucial to obtain a non-monotonic evolution of shear stress, observed typically in standard shear-loaded experiments (Jacobsen 2012). The presented results showed that during the onset of displacement, the aggregates (meso-scale) dominate the behavior by introducing a peak shear stress whereas the post-peak decay, which follows a power-law behavior and makes it non-monotonic, is influenced by the roughness characteristics of the surface. While the presented study only considers a standard experimental setup (Jacobsen 2012) for validation, it is the first study of its kind that demonstrates the importance of surface roughness to the aggregate interlock action.

An empirical relation, acknowledging both aggregate distribution as well as surface roughness was shown to predict the resisting shear stress in accordance with the considered experimental observations. It is believed that the presented numerical methodology opens the path to develop empirical equations capturing the role of aggregate sizes/shapes and varying material properties on the aggregate interlock, for instance with modified power-law tails in Eq. (20). This will lead to reliable design guidelines/codes for estimating shear capacity of cracked concrete structures.

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Appendix A Schematic for the numerical setup

Fig. A21 (a) Concrete sample considered in the experiments of Jacobsen. The top part of concrete was load under mixed-mode loading ($\delta_0$ = opening displacement along $z$ direction and $\delta_s$ = shear displacement along the $y$ direction). (b) One of 50 concrete surfaces considered for the numerical simulations in this study. (c) Shows a cross-section of the two conforming concrete surfaces from (b) interlocked under mixed-mode loading.
Appendix B Values of loading angle computed for numerical simulation

Fig. B22 The expected value of $\gamma$ for different inputs ($\gamma^*, \delta_0^*$). The values of loading angle are within $\pm 1^\circ$ range (shown as dotted line) of the targeted angle $\theta = \tan^{-1}(\gamma)$.

Appendix C Covariance of $\langle N \rangle$ and $\langle \tilde{f}_y \rangle$

Fig. C23 Covariance of $\tilde{f}_y^\delta$ and $N^\delta$ for various displacement $\delta$ for surface class $S_\xi$.

Fig. C24 Covariance of $\tilde{f}_y^\delta$ and $N^\delta$ for various displacement $\delta$ for surface class $S_\eta$. 
Table D3 Obtained values of κ and B after fitting procedure shown in Fig. D25. The values of initial opening δ₀ are in mm.

| δ₀ | B   | κ    |
|----|-----|------|
| 0.025 | 218.8 | 1.79 |
| 0.025 | 115.1 | 1.92 |
| 0.025 | 45.7  | 1.90 |
| 0.04   | 188.2 | 1.72 |
| 0.04   | 71.0  | 1.78 |
| 0.04   | 59.2  | 1.58 |
| 0.1    | 217.2 | 1.00 |
| 0.1    | 124.8 | 0.87 |
| 0.1    | 100.9 | 0.78 |

Fitting parameter κ:
Figure D26 shows the values of κ obtained as a function of the initial opening δ₀ for different loading ratios. As can be observed, there is a linear dependency of κ on δ₀. Furthermore, the variation of κ due to different loading ratios γ remains small, suggesting that κ depends only on the initial opening and can be approximated as linear function of δ₀, i.e. κ = aδ₀ + b (as shown by the best fit in Fig. D26).

Appendix D Number of contact clusters (N) and fitting procedure
The expression \( \langle N \rangle = B \delta_s^{-\kappa} \) is fitted to the numerically obtained values of \( \langle N \rangle \). The fitting is done only for the values of \( \delta_s \) over which ensemble average of contact clusters decay as a power-law. Figure D25 shows the best fits obtained for various loading kinematics.

Fig. D25 Fitting of analytical expression \( \langle N \rangle = B \delta_s^{-\kappa} \) to the numerically obtained values of \( \langle N \rangle \). The loading ratios considered are 1.2, 1.5 and 1.73. The initial openings considered are: 0.025 mm, 0.04 mm and 0.1 mm.

Fig. D26 Variation of κ as a function of initial opening δ₀ for different loading ratios γ for surface class δₐ.
Fitting parameter $B$:  

The values of $B$ obtained from fitting are plotted as a function of the loading ratio $\gamma$ for different initial openings. Assuming that $B$ depends only on $\gamma$ allows to express $B$ as a linear function of $\gamma$, i.e. $B = c\gamma + d$ (as shown by the best fit in Fig. D27). Finally, the values of the constants $a$, $b$, $c$, $d$ used in the above fitting is given in Table D4.

| $a$  | $b$  | $c$  | $d$  |
|------|------|------|------|
| -13.3| 2.2  | -267.9| 526.9|

Table D4 Values of constants $a$, $b$, $c$, $d$ obtained for predicting $\kappa$ and $B$.

Appendix E Average contact area per cluster $\bar{a}$

The average contact area per cluster is computed for surface classes $S_A$ and $S_B$. The average is computed by considering data from all 50 realizations.

Fig. D27 Variation of $B$ as a function of initial opening $\gamma$ for different initial openings $\delta^i$ for surface class $S_A$.

Fig. D28 Prediction of ensemble average of number of contact clusters using proposed analytical expression. The analytical expression are in fine agreement with numerical results.

Fig. E29 Average contact area per cluster computed for surface classes $S_A$, $S_B$ for loading kinematics: $\gamma = \delta_o/\delta_s \approx 1.73$, $\delta^i = 0.025$ mm.
Appendix F Probability density of $S_A$ and $S_B$

Fig. F30 Probability density of contact force per cluster $f_y$ for surface class $S_A$ for various shear displacement values. The loading ratio is $\gamma \approx 1.73$ and the initial opening is $\delta_s = 0.025$ mm. The distribution follows power-law behavior irrespective of shear displacement.

Fig. F31 Probability density of contact force per cluster $f_y$ for surface class $S_A$ for various shear displacement values. The loading ratio is $\gamma \approx 1.73$ and the initial opening is $\delta_s = 0.025$ mm.

Appendix G Normalized map of contact pressure normal and tangential to the surface

Fig. G32 Normalized contact pressure along the surface $p_y$ as a function of opening and shear displacement. The values are linearly interpolated based on our simulations for different loading kinematics.

Fig. G33 Normalized contact pressure normal to the surface $p_z$ as a function of opening and shear displacement. The values are linearly interpolated based on our simulations for different loading kinematics.