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**Damage Quantification via Digital Volume Correlation
with Heterogeneous Mechanical Regularization:
Application to an In Situ Meso-Flexural Test on Mortar**

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Abstract Background. The mechanical response and damage mechanisms of heterogeneous cementitious materials result from the mechanical properties of their

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3 constituents at the mesoscale. Objective. In this study, a finite element based Digital
4 tal Volume Correlation (FE-DVC) method with mechanical regularization tailored
5 for heterogeneous materials was applied to study crack propagation in mortar.
6 Method. A realistic 3D mesh was built consistently with the actual microstructure
7 based on high resolution X-ray tomography. A notched mesobeam was subjected
8 to *in situ* three-point flexure. Results. The introduction of mechanical contrast
9 in DVC analyses allowed the strain heterogeneities related to the underlying mi-
10 crostructure to be described and inelastic strain localization due to cracks to be
11 captured. Furthermore, the relaxation of mechanical regularization in damaged
12 elements improved the trustworthiness of displacement measurements. Conclu-
13 sion. Estimations of crack opening displacements and characterization of the crack
14 morphology were carried out, providing insights into the damage processes at the
15 mesoscale.

16 **Keywords** Digital Volume Correlation (DVC) · X-Ray tomography · Three-point
17 flexural test · Microscale · Mechanical regularization

18 1 Introduction

19 X-ray Computed Tomography (XCT) has become a powerful tool for the acqui-
20 sition of 3D images and is widely used in material science [1]. Static 3D images are
21 being utilized for morphological and quantitative microstructure characterization
22 that can be considered for image-based numerical modeling [2,3]. Tomographic
23 studies have found numerous applications for cementitious materials due to their
24 high heterogeneity and complex compositions. One example among various ap-
25 plications is the microstructure characterization based on X-ray imaging. Studies

26 were carried out on aggregate and cement particle shapes [4–9], pore and crack
27 networks [5,10–15], and cement paste morphology [16,12]. Such studies allowed
28 for example estimations of concrete permeability and hydration processes. More-
29 over, X-Ray based microstructures were used for mechanical and thermal property
30 estimations [17], as input to finite element (FE) models [18–20] and FFT-based
31 simulations [21].

32 Beyond static imaging, the continuation of these studies was the observation
33 of microstructural changes due to exposure to aggressive environments or thermo-
34 hydro-mechanical loadings. Taking sequences of 3D images under different environ-
35 mental conditions allowed the microstructure changes to be tracked. Tomographic
36 studies were reported on cementitious materials subjected to leaching [22,23], sul-
37 fate attacks [24], corrosion [25], and water migration [26]. One of the extensions
38 to this technique is *in situ* testing when experiments are carried out inside CT
39 scanners [27]. Registering 3D scans allows different deformation mechanisms such
40 as damage growth, crack opening, or shear banding to be quantified as a function
41 of time or mechanical loading. In particular, it allowed complex damage processes
42 to be visualized in concrete. The characterization of damage growth with X-CT
43 scanning was carried out under mechanical [20,28–31] and hydrostatic *in situ* load-
44 ings [32], subjected to freezing-thawing cycles [33] or autogeneous shrinkage [34].

45 Apart from image analyses and processing, Digital Volume Correlation (DVC)
46 became a popular technique to measure three-dimensional displacement and strain
47 fields with subvoxel resolution [35,36]. DVC appeared as an extension of Digital
48 Image Correlation (DIC) that was developed for 2D images [37]. The principle
49 of these methods first consisted in measuring displacements of small subvolumes
50 registered between reference and deformed volumes. Later on, finite element ap-

51 proaches were introduced [38]; the registrations are performed at the level of the
52 whole region of interest. DVC analyses were performed for concrete subjected to
53 *in situ* mechanical loadings [43,42,39–41], hydrothermal loadings [44], carbona-
54 tion [45] and reinforcement corrosion [46]. The study of damage development was
55 possible by analyzing displacement or strain fields as they normally indicate crack
56 locations [47] respectively as discontinuities or high values. Another way of dis-
57 playing crack networks was via residual fields, which are the difference images
58 between the reference volume and the deformed volume corrected with the mea-
59 sured displacement field [48,49,47,50].

60 In the present study, an FE-DVC method with mechanical regularization tai-
61 lored for heterogeneous materials was used to quantify damage in mortar. Me-
62 chanical regularization was initially introduced in a homogeneous setting for DVC
63 analyses [51,52]. Then, it was adapted to heterogeneous materials in a DIC frame-
64 work [53] by taking into account the contrast in elastic properties of different
65 phases. Damage was also added to allow localized solutions to be retrieved [47]. In
66 the present case, a mesh was built consistently with the underlying microstructure,
67 based on an X-ray microtomography scan acquired prior to the *in situ* test. Then, a
68 notched microbeam was subjected to *in situ* three-point flexure. In order to image
69 a larger part of the beam, a lower resolution was selected. The realistic volume
70 mesh was backtracked via DVC from the high resolution scan to the *in situ* scan.
71 The influence of mechanical contrast on the trustworthiness of 3D displacement
72 and strain fields was studied. Furthermore, the damaged elements were detected
73 in order to take into account their reduced stiffness in mechanical regularization.
74 This technique allowed the displacement measurements to be consistent in the

75 damaged areas. The final DVC results were used for crack opening estimations
 76 and a study of the crack morphology at the mesoscale.

77 The study workflow (Figure 1) summarizes the different steps of the present
 78 study, whose aim is to demonstrate the potential of mechanically regularized DVC
 79 based on the underlying microstructure for the study of damage at low scales.

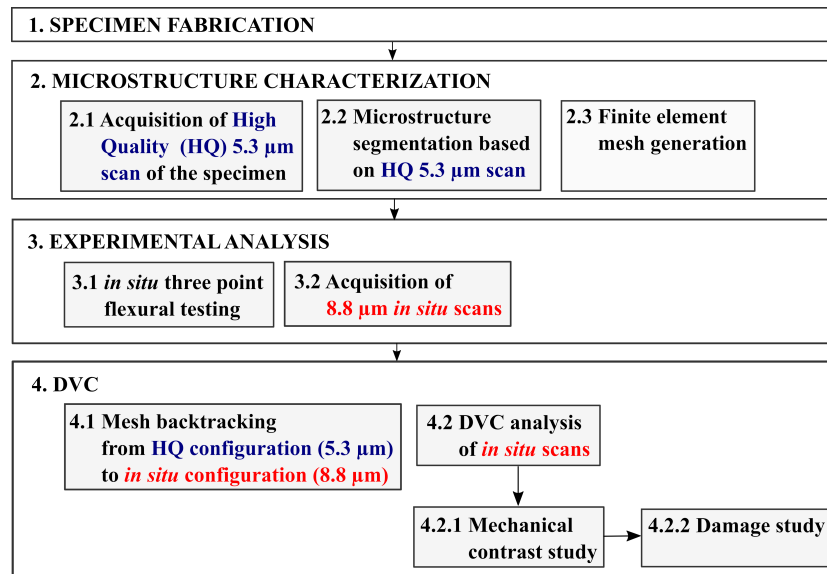


Fig. 1 Experimental and numerical workflow

80 2 Material and Methods

81 This section describes the specimen fabrication process and provides a description
 82 of the microstructure characterization procedure that was used to reconstruct a
 83 realistic 3D mesh. The experimental setup and protocol are then detailed. The
 84 section ends with a description of heterogeneous regularization within an FE-DVC
 85 framework.

86 2.1 Material and Specimen

87 A mortar batch was mixed using a CEM I Portland cement with a water-to-cement
88 ratio of 0.525. A low sand-to-binder ratio was used (0.5). Sand was sieved to obtain
89 a granulometric distribution within the range 200 μm to 2 mm in diameter. The
90 reduction of the sand volume fraction to 18%, and elimination of fine particles,
91 made the resulting microstructure more suitable for efficient image processing as
92 less geometric details were distorted or lost. A thin mortar plate with dimensions
93 $65 \times 35 \times 8$ mm was cast in a silicon mold and unmolded after 1 day. By means of
94 X-ray radiography, the mortar plate was checked for the absence of mesocracking
95 and defects. After control, the plate was selected for further fabrication.

96 First, the top surface was ground and polished until a 5 mm thickness was
97 reached with simultaneous control of parallelism of the top and bottom faces.
98 The thickness deviation was of the order 0.1 mm, which corresponds to a $\angle 1.5\%$
99 inclination between the top and bottom surfaces. Second, the plate width was
100 adjusted to 20 mm with a wire saw. Third, $5 \times 5 \times 20$ mm microbeams (Figure 2)
101 were cut from the plate with a diamond disk saw to ensure planar parallel sides.
102 Fourth, the notch was cut with a saw equipped with a fine (0.1 mm) wire and low
103 tension to avoid sample degradation. The notch width was approximately 0.15 mm
104 and its height was 1.5 mm. The specimen were stored at 100% air humidity. During
105 preparation, the specimen surfaces were re-wetted to prevent them from drying
106 cracking.

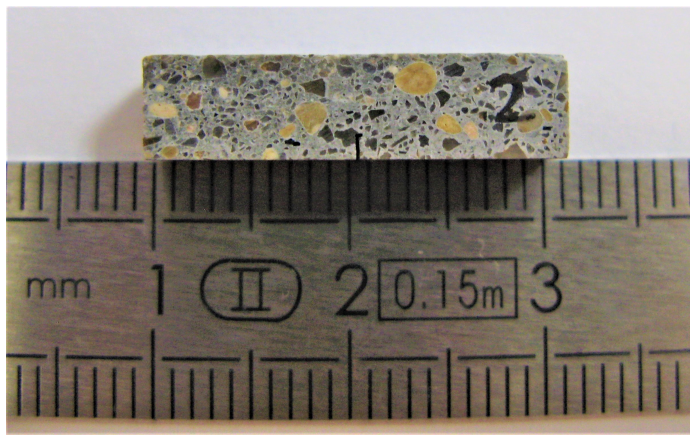


Fig. 2 Notched mortar microbeam

107 2.2 Microstructure Segmentation and Microstructure-Based Mesh

108 Before the *in situ* test, a High Quality (HQ) scan of the central part of the mi-
109 crobeam was acquired with a 5.3 μm resolution using a GE Phoenix v|tome|x m
110 CT system. The acquisition parameters are detailed in Table 1.

Table 1 DVC hardware parameters

Parameters	High Quality Scan	<i>In situ</i> Scan
CT device	GE Phoenix v tome x M	
Target	high-flux target	
Filter	0.1 mm Cu	
Voltage	180 kV	200 kV
Current	57 μ A	90 μ A
Tube to detector	807.3 mm	
Tube to object	21.5 mm	35.5 mm
Detector	GE Dynamic 41 100	
Definition	1992 \times 2000 (2 \times 2 binning)	
Number of projections	2500	1600
Angular amplitude	360°	
Frame average	5 per projection	3 per projection
Frame rate	2 fps	3 fps
Acquisition duration	2.5 h	45 min
Gray Level amplitude	14 bit (16 bit format)	
Pixel size	5.3 μ m	8.8 μ m

111 Avizo[®] data visualization and analysis software was used for further image
112 processing. After mechanical testing (Section 2.3), a Region Of Interest (ROI)
113 containing the notch with dimensions 2.6 \times 5 \times 5 mm was selected for further
114 segmentation (Figure 6). First, a median filter (3 \times 3 \times 3 voxels) was applied to
115 mitigate noise (Figure 3(a)).

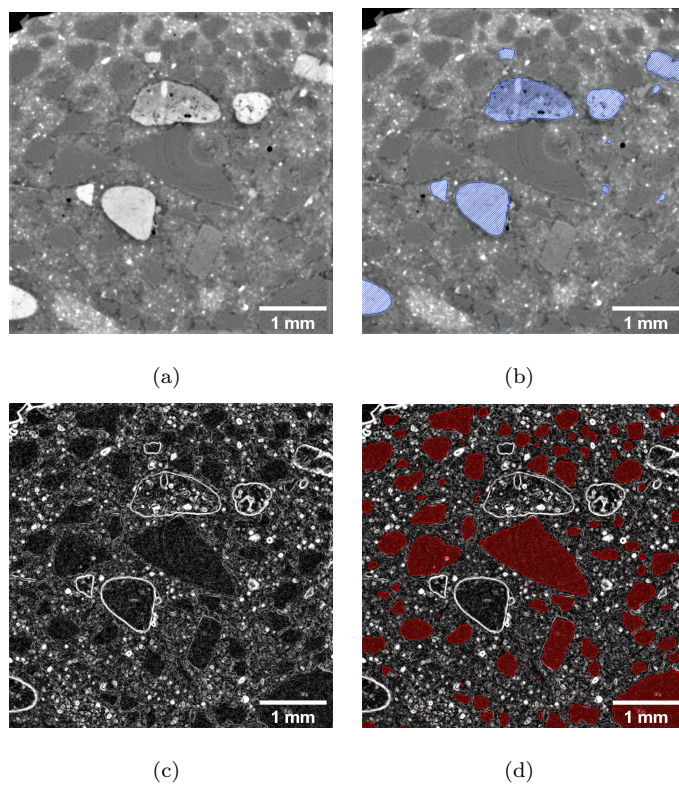


Fig. 3 Inclusion segmentation. (a) Filtered image (light inclusions - limestone aggregates, gray inclusions - siliceous aggregates). (b) Segmentation of limestone aggregates. (c) Contrast (norm of image gradient). (d) Segmentation of siliceous particles

116 Second, the segmentation of aggregates was carried out as follows. Two types
117 of inclusions (limestone – CaCO_3 , silica – SiO_2) were present in mortar with
118 different morphology and levels of attenuation that define their representation on
119 images. Limestone inclusions were brighter (higher X-ray absorption) than the
120 cementitious matrix, and were separated by simple thresholding (Figure 3(b)).
121 Silica inclusions had similar gray levels as the cement paste matrix, but showed less
122 internal contrast and appeared as very homogeneous regions. The calculation of the
123 image gradient norm gave a field with low values in homogeneous zones, and high

124 levels in heterogeneous regions (Figure 3(c)). This tool allowed the homogeneous
 125 inclusions to be distinguished from the heterogeneous matrix (Figure 3(d)). These
 126 two families of inclusions were considered as a unique "aggregate" phase with
 127 identical elastic properties. Mesoporosity was present in the specimen in a small
 128 amount, and did not seem to have a major effect on the crack path during the
 129 flexural test. For these reasons, mesopores were not segmented as a separate phase
 130 and were incorporated in the matrix. Last, the notch surfaces were segmented from
 131 the volume (Figure 4(a)).

132 Based on the segmentation results, the Avizo[®] tools allowed surface triangular
 133 meshes to be generated and exported in .stl format. The size of surface triangles
 134 was controlled to be at least several voxels for consistency with DVC, and with si-
 135 multaneous check of excessive distortion of triangles. The surface meshes were then
 136 processed with the tools available in the Salome[®] platform ([https://www.salome-
 137 platform.org/](https://www.salome-platform.org/)) to obtain 4-noded tetrahedral elements (Figure 4(b,c)). The mesh
 138 consisted of 346,472 tetrahedra and 63,465 nodes. The distribution of mesh ele-
 139 ments and volume between the different phases is given in Table 2.

Table 2 Characteristics of the phases in the mesh. The physical size of one voxel is 8.8 μm

	Aggregates	Matrix	Interphase	Bulk matrix
Elements	74,120	272,352	134,474	137,878
Nodes	7,863	-	16,232	39,279
Volume, vx^3	$1.57 \cdot 10^7$	$5.50 \cdot 10^7$	$2.61 \cdot 10^7$	$2.89 \cdot 10^7$
Volume fraction	22%	78%	37%	41%
Element size, vx	6	6	6	6
Young's modulus, GPa	70.0	13.3	13.3	13.3
Poisson's ratio	0.26	0.26	0.26	0.26

140 In the matrix, elements adjacent to aggregates are denoted as interphase ele-
 141 ments, and the remainder of the matrix are bulk elements. The equivalent element
 142 size, which is defined as the cubic root of the volume of each element, was equal
 143 on average to $10 v_x$ (or $53 \mu\text{m}$) in the HQ configuration and $6 v_x$ in the LQ setting
 144 (Table 2). The mesh fineness was identical in the matrix and the aggregates.

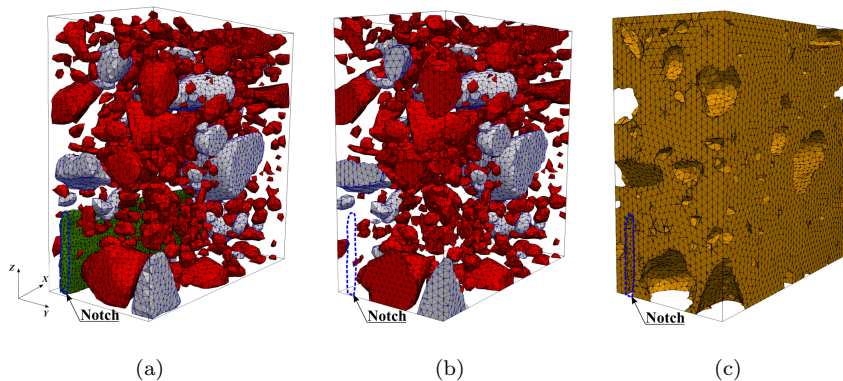


Fig. 4 Surface and volume meshes (red: siliceous aggregates, gray: limestone aggregates, yellow: matrix, green: notch). (a) Surface meshes. (b) Aggregate and (c) matrix meshes

145 2.3 Experimental Analysis

146 The *in situ* flexural test was performed with the LMT *in situ* Tension-Compression
 147 (TC) testing machine designed at the MATEIS laboratory [27]. The load capacity
 148 is ± 1 kN. Tensile or compressive loads can be applied by axial displacement of
 149 the bottom actuator. The adapted setup for three-point flexural tests is shown
 150 in Figure 5. The vertical motion of the bottom actuator with part A1 causes a
 151 horizontal motion of support parts B and C thanks to 45° contact surfaces. The
 152 shortening of the distance between B and C results in point load application to
 153 the sample that is equivalent to three-point flexure. The parts of the flexural setup

154 were manufactured in an aluminium alloy as it has a high stiffness and reasonable
 155 X-ray attenuation compared to mortar, which allowed additional artifacts to be
 156 avoided. Thin adhesive tape was attached to the top and bottom faces of the
 157 beam for maintaining the sample and improving its stability during testing. The
 158 adhesive tape was also used for fastening the parts of the setup to ensure better
 159 control over sample positioning inside it, and for safe insertion of the setup into
 160 the tube of the TC machine.

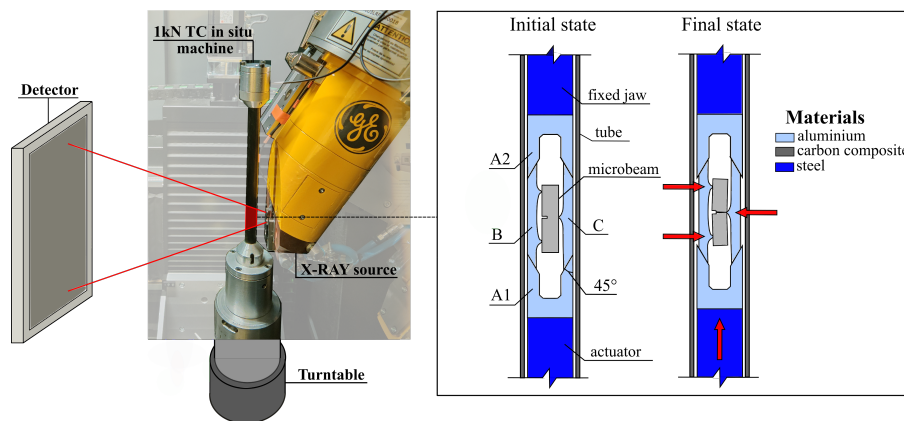


Fig. 5 Schematic and actual views of the *in situ* three-point flexural setup

161 The *in situ* test consisted of several loading steps, and CT scans were per-
 162 formed at sustained and constant load. The experimental protocol and load levels
 163 of CT scans are shown in Figure 6(a). The scans were acquired with the Phoenix
 164 v|tome|x m scanner (Table 1). First, two successive scans were performed on the
 165 undeformed specimen for uncertainty quantification. A small preload of 1 N was
 166 applied to keep the specimen stable. Second, axial displacements were applied with
 167 0.5 $\mu\text{m/s}$ rate until sample failure. The experimental configuration along with the
 168 specimen geometry did not allow for a fine control of crack initiation and propa-

169 gation. Failure was brittle, followed by substantial force drop, and very fast crack
 170 propagation on the major part of the ligament (Figure 6(b)). The second scan was
 171 carried out immediately after fracture. Third, an increment of axial displacement
 172 of 20 μm was applied to further open the crack. After each loading, a 10 min
 173 dwell was applied before the next scan (*i.e.*, force relaxation was stabilized).

174 In the reported test, the loading point was not fully aligned with the notch.
 175 This off-axis loading resulted in a bifurcation of the fractured surface into two
 176 main cracks (Figure 6(b)). The Region of Interest (ROI) was chosen to encompass
 177 all fractured surfaces while maintaining a small gap with an irregular external
 178 surface. They were observed to cross the cement paste matrix, aggregate-matrix
 179 interfaces and limestone aggregates.

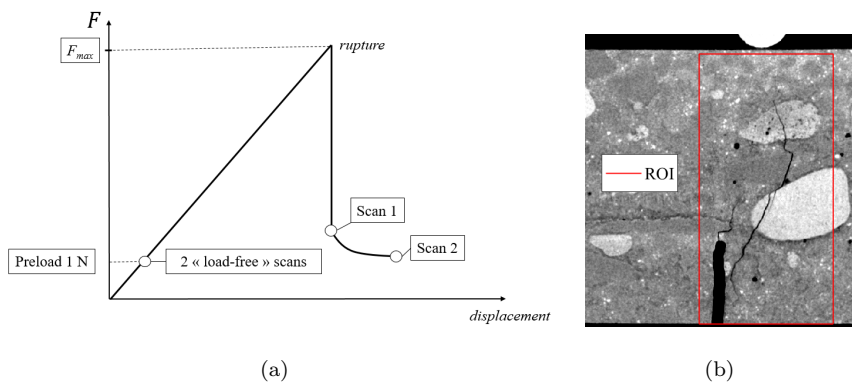


Fig. 6 (a) CT scans performed during *in situ* flexure. (b) 2D section of fractured specimen and DVC ROI

 180 2.4 Regularized DVC for Heterogeneous Materials

181 DVC measures displacement fields in the selected ROI by registering the deformed
 182 volumes g and the reference volume f assuming gray level conservation

$$f(\mathbf{x}) = g(\mathbf{x} + \mathbf{u}(\mathbf{x})) \quad (1)$$

183 where $\mathbf{u}(\mathbf{x})$ is the sought displacement field, and \mathbf{x} any voxel position within the
 184 ROI. The sought displacement field has to minimize the gap to gray level conser-
 185 vation

$$\min_{\{\mathbf{u}\}} \Phi_c^2 = \sum_{\text{ROI}} [f(\mathbf{x}) - g(\mathbf{x} + \mathbf{u}(\mathbf{x}))]^2 \quad (2)$$

186 with

$$\mathbf{u}(\mathbf{x}) = \sum_n u_n \phi_n(\mathbf{x}) \quad (3)$$

187 where $\phi_n(\mathbf{x})$ are trial displacement fields, and u_n the associated Degrees Of Free-
 188 dom (DOFs) gathered in the column vector $\{\mathbf{u}\}$. In FE-DVC, the sought DOFs
 189 are the nodal displacements of a finite element discretization, and $\phi_n(\mathbf{x})$ the cor-
 190 responding shape functions.

191 The minimization of Equation (2) is equivalent to iteratively solving a sequence
 192 of linear systems [54]

$$[\mathbf{M}]\{\delta\mathbf{u}\} = \{\mathbf{b}\} \quad (4)$$

193 where $[\mathbf{M}]$ is the DVC Hessian matrix, whose terms are products of the shape func-
 194 tions by the gradient of the reference volume, $\{\mathbf{b}\}$ the residual vector, which is a
 195 function of the difference between the reference and the corrected deformed vol-
 196 umes, and $\{\delta\mathbf{u}\}$ the corrections to the current estimate of the nodal displacement
 197 vector $\{\tilde{\mathbf{u}}\}$.

198 The gray level residual field $\varphi_c = f(\mathbf{x}) - g(\mathbf{x} + \mathbf{u}(\mathbf{x}))$ represents the difference
 199 between the volume in the reference configuration and that in the deformed con-
 200 figuration corrected by the measured displacement field. The global residual Φ_c ,
 201 which is to be minimized, is the root mean square (RMS) of the residual field φ_c
 202 and serves as indicator of the consistency of the solution, namely, a smaller RMS
 203 residual means a more trustworthy solution. Local high residual values may mark,
 204 for example, discontinuities in displacements, or in other words, cracks [48, 49,
 205 47]. Last, it is worth noting that the residual fields are, by definition, Lagrangian
 206 (*i.e.*, constructed in the reference configuration).

207 The correlation problem is ill-posed and the introduction of mechanical regu-
 208 larization is one of the ways to make it well-posed [51, 55, 52]. In regularized DVC,
 209 elasticity is enforced at a local level by the introduction of a penalty term based
 210 on the equilibrium gap

$$[\mathbf{K}_1]\{\mathbf{u}\} = \{\mathbf{f}_r\} \quad (5)$$

211 where $[\mathbf{K}_1]$ is the rectangular stiffness matrix restricted to inner nodes and traction-
 212 free surfaces, and $\{\mathbf{f}_r\}$ the nodal force vector that must vanish in the absence of
 213 body forces. The mechanical penalty term is formulated as the $L2$ -norm of the
 214 force residuals

$$\Phi_m^2 = \{\mathbf{u}\}^\top [\mathbf{K}_1]^\top [\mathbf{K}_1] \{\mathbf{u}\} \quad (6)$$

215 For other boundary (*i.e.*, Dirichlet) nodes, the fluctuations of tractions are
 216 regularized

$$\Phi_b^2 = \{\mathbf{u}\}^\top [\mathbf{K}_2]^\top [\mathbf{L}] [\mathbf{K}_2] \{\mathbf{u}\} \quad (7)$$

217 where $[\mathbf{L}]$ is based upon the Laplace-Beltrami operator [56], and $[\mathbf{K}_2]$ the rectan-
 218 gular stiffness matrix restricted to Dirichlet nodes. These additional cost functions

do not have the same physical units as Φ_c^2 . Therefore, to minimize their weighted sum, they are normalized

$$\tilde{\Phi}_m^2 = \frac{\Phi_m^2}{\{\mathbf{v}\}^\top [\mathbf{K}]^\top [\mathbf{K}] \{\mathbf{v}\}}, \tilde{\Phi}_b^2 = \frac{\Phi_b^2}{\{\mathbf{v}\}^\top [\mathbf{L}]^\top [\mathbf{L}] \{\mathbf{v}\}}, \tilde{\Phi}_c^2 = \frac{\Phi_c^2}{\{\mathbf{v}\}^\top [\mathbf{M}] \{\mathbf{v}\}} \quad (8)$$

where $\mathbf{v} = \mathbf{v}_0 \exp(i\mathbf{k}\cdot\mathbf{x})$ is the trial displacement field selected in the form of a plane wave, \mathbf{v}_0 the amplitude, and \mathbf{k} the wave vector [51,55]. The global minimization is performed on the weighted sum of the normalized cost functions

$$(1 + w_m + w_b)\Phi_t^2 = \tilde{\Phi}_c^2 + w_m\tilde{\Phi}_m^2 + w_b\tilde{\Phi}_b^2 \quad (9)$$

where Φ_t is the total cost function. The weights w_m and w_b are defined as

$$w = w_m = w_b = (2\pi k \ell_{reg})^4 \quad (10)$$

where ℓ_{reg} is the regularization length, and $k = \|\mathbf{k}\|$ the wave number. Up to now, mechanical regularization was based upon homogeneous, isotropic and linear elasticity [51,52]. If ℓ_{reg} is greater than the element size, mechanically inadmissible displacement fluctuations are filtered out over a spatial domain of size proportional to ℓ_{reg} . In the case of damage or localized plastic strains, displacement discontinuities are smeared over a domain whose size that depends on ℓ_{reg} [52,47].

As the microstructure-based mesh differentiates matrix and aggregate elements (Figure 4(c)), the proposed regularization can take into account differences in elastic properties, as already performed in 2D DIC applied to a composite material [53]. For a two-phase material, the contrast C is introduced to denote the ratio of Young's moduli of the matrix E_m and the inclusions E_i

$$C = \frac{E_i}{E_m} = \sqrt{\frac{w^i}{w^m}} = \left(\frac{\ell_{reg}^i}{\ell_{reg}^m} \right)^2 \quad (11)$$

236 where w^i and w^m denote the weight in the inclusions and in the matrix, respec-
 237 tively. In such formulation, $C > 1$ implies that inclusions are more rigid than the
 238 matrix, and more weight is put on the inclusion phase. Conversely, $C < 1$ corre-
 239 sponds to inclusions being more compliant and a larger weight is put on the matrix
 240 phase. The case $C = 1$ is equivalent to homogeneous elastic regularization.

241 Mechanically regularized DVC was implemented within the Correli 3.0 frame-
 242 work developed at LMT [57]. Table 3 gathers the DVC parameters utilized in the
 243 following analyses. For the sake of simplicity, ℓ_{reg} also denotes the regularization
 244 length in the matrix phase (*i.e.*, ℓ_{reg}^m), if heterogeneous regularization is performed
 245 since in the present case, $C < 1$ is very unlikely.

Table 3 DVC analysis parameters

DVC software	Correli 3.0 [57]
Image filtering	none
Element length ℓ (mean)	6 vx (53 μm) in <i>in situ</i> configuration
Shape functions	linear (4-noded tetrahedra)
Mesh	see Figure 4(b,c)
Matching criterion	Penalized sum of squared differences (Equation (9))
Interpolant	cubic
Displacement noise floor	see Figure 8(a)
Strain noise floor	see Figure 8(b)

246 3 DVC Results and Discussion

247 This section describes the DVC analysis workflow that begins with the mesh back-
 248 tracking procedure [58]. Then, a quantification of uncertainties for different values

249 of regularization length and contrasts was performed. Last, DVC analyses for dif-
250 ferent contrasts were carried out on the deformed (and damaged) volume.

251 3.1 Mesh Backtracking

252 The microstructure-based mesh was reconstructed on the HQ scan with a $5.3 \mu\text{m}/\text{vx}$
253 resolution acquired prior to the *in situ* test (see blue mesh in Figure 7). As men-
254 tioned above, the HQ and *in situ* (LQ) scans were acquired with different reso-
255 lutions and acquisition parameters (Table 1). Before performing DVC analyses,
256 the mesh had to be backtracked to take into account scale differences and rigid
257 body motions between the two scans (*i.e.*, initially mispositioned blue mesh in the
258 LQ configuration in Figure 7(left)). This step was important as if the mesh did
259 not match accurately the underlying microstructure, heterogeneous regularization
260 would be meaningless.

261 Backtracking consists in running a DVC analysis between the HQ scan (volume
262 f in Equation (1)) and the *in situ* scan (volume g) of the undeformed specimen to
263 find the displacement field \mathbf{u}_b linking the two configurations [58]. In the present
264 case, the HQ scan was binned to a resolution of $10.6 \mu\text{m}/\text{vx}$, and both scans
265 were converted into 8-bit volumes. An auxiliary mesh was used, consisting of a
266 rectangular hexahedral mesh composed of large T4 elements (their size was 25 vx
267 or $250 \mu\text{m}$ in the reference HQ configuration) that encompassed the volume of
268 the microstructure-based mesh (*i.e.*, $4.5 \times 4.75 \times 2.3 \text{ mm}$, see the magenta mesh
269 depicted in Figure 7).

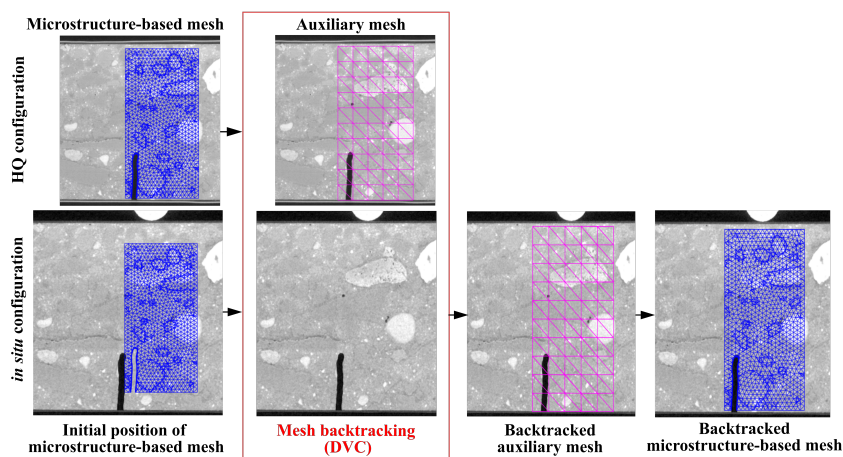


Fig. 7 Schematic view of the backtracking procedure enabling the (blue) mesh based on the HQ configuration (top) to be fitted to the *in situ* configuration (bottom) via DVC using an auxiliary (magenta)

mesh

270 The calculation was initialized with a displacement field containing scaling and
 271 rigid body degrees of freedom. After DVC convergence, the displacement field \mathbf{u}_{aux}
 272 enabled the auxiliary mesh to be positioned in the LQ configuration. The inter-
 273 polation of the displacement field \mathbf{u}_{aux} at the nodes of the meshed microstructure
 274 yielded \mathbf{u}_b , which gave the nodal coordinate corrections to fit it back to the *in situ*
 275 (LQ) configuration (*i.e.*, repositioned blue mesh in the LQ configuration shown in
 276 Figure 7(right)).

277 3.2 Uncertainty Quantification

278 Uncertainty quantifications were performed by running DVC analyses on the two
 279 scans performed on the undeformed specimen. Four different contrasts were consid-
 280 ered to investigate the effects of this parameter on the results. First, the contrast C

281 was set to 1, which implied that the elastic properties of the different phases were
 282 identical. This choice was equivalent to homogeneous mechanical regularization.
 283 Second, the contrast C was set to $E_i/E_m = 70.0/13.3 = 5.26$, which corresponds
 284 to realistic properties of mortar constituents when inclusions were more rigid than
 285 the cementitious matrix [59]. Third, the case $C = 0.5$ was considered, which im-
 286 plied that inclusions were more compliant than the matrix. Last, the contrast was
 287 set to a rather high value ($C = 20$), which was the case of highly rigid inclusions
 288 and very compliant matrix.

289 DVC analyses were run with different regularization lengths. For the first step,
 290 ℓ_{reg} was set to a high value (*i.e.*, 150 vx). Then, the displacement field at con-
 291 vergence was used to initialize the next step where the regularization length was
 292 decreased. This step-by-step (relaxation) process was continued until ℓ_{reg} reached
 293 15 vx. In this study, too small ℓ_{reg} values (*i.e.*, less than twice the element size)
 294 were observed to be ineffective for mechanical regularization. When $C = 20$, DVC
 295 calculations with $\ell_{reg} < 30$ vx could not converge.

296 Figure 8(a) shows the displacement uncertainties and Figure 8(b) the maxi-
 297 mum principal strain ϵ_1 uncertainties as functions of the regularization ℓ_{reg} . A
 298 decrease of ℓ_{reg} leads to an increase in displacement and strains fluctuations. This
 299 trend is consistent with the trade-off between spatial resolution (here controlled
 300 by the regularization length) and measurement uncertainty. Further, the more
 301 heterogeneous the regularization (*i.e.*, C departs from one), the higher the fluc-
 302 tuations since the regularization contrast increased (Equation (11)). On a more
 303 quantitative level, the strain uncertainty decay with ℓ_{reg} follows power laws that
 304 are not too far from -2.5 , which are expected when the dominant source of uncer-

305 tainty corresponds to acquisition noise on the radiographs utilized to reconstruct
 306 3D images [36].

307 Figure 8(c) shows the change of RMS residuals as functions of ℓ_{reg} . Their
 308 variation remained very limited since for any regularization length, the kinematics
 309 was very simple (essentially rigid body motions). These levels are baselines to
 310 which further analyses will be compared.

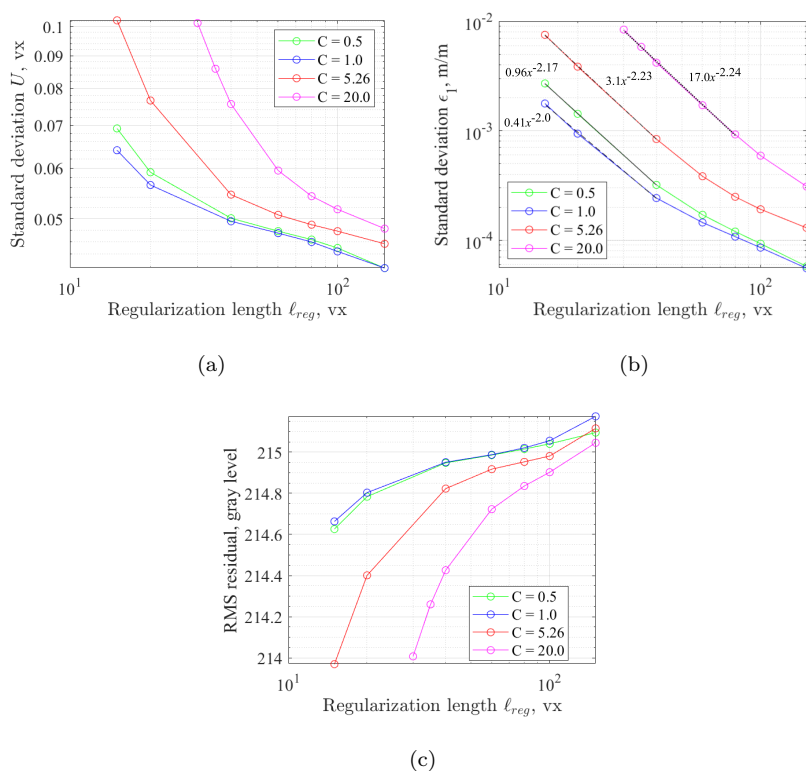


Fig. 8 (a) Displacement and (b) maximum principal strain uncertainties as functions of the regularization length for different contrasts. (c) Corresponding RMS residuals (note their small dynamic range)

311 3.3 DVC Analysis of Crack Propagation

312 The scan acquired right after specimen failure revealed that the crack had prop-
313 agated on most of the ligament height. Therefore, DVC was run between the
314 undeformed scan and this first scan. For the first DVC step, the regularization
315 length was set to 100 vx, and gradually decreased down to 15 vx. The converged
316 solution for higher ℓ_{reg} was used as initialization for the next step with less weight
317 put on the mechanical part. The gradual relaxation of mechanical regularization
318 allowed most of the long wave displacement components to be captured, and then
319 iteratively converged to a better solution with short wave length fluctuations that
320 were gradually restored. This iterative process was carried out for $C = 5.26$.

321 3D renderings of thresholded Lagrangian residual fields are shown in Figure 9.
322 The maximum RMS level for $\ell_{reg} = 100$ vx was less than 1.4 times (287 gray level)
323 the baseline RMS residual (215 gray level). The highest absolute levels correspond
324 to the fractured surfaces, which were continuous and well defined. The absence of
325 high residuals in the intact zones proves a good overall registration quality and
326 efficient mechanical regularization of DVC. It is worth noting that when using the
327 gray level residuals, the detection of the cracks was straightforward as all other
328 heterogeneities, some of which had similar gray levels as the cracks, were no longer
329 visible.

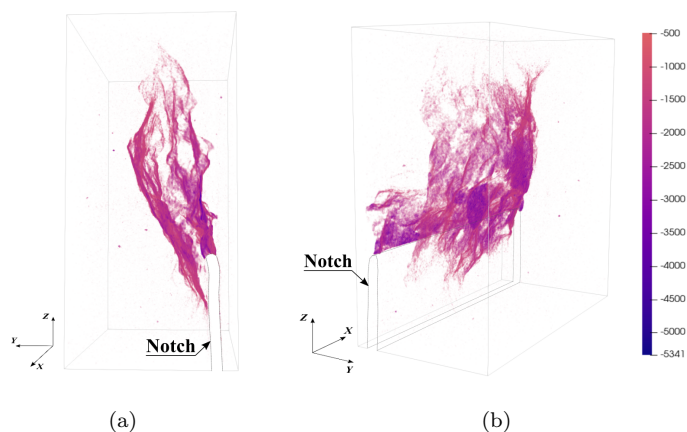


Fig. 9 Thresholded Lagrangian residual field showing the fractured surfaces ($\ell_{reg} = 15$ vx and $C = 5.26$). (a) Face and (b) side views

330 In terms of displacements, cracks induce discontinuities that mechanical regu-
 331 larization tends to spread over a zone whose size depends on ℓ_{reg} [47]. The followed
 332 relaxation procedure led to displacement jumps localized in a smaller domain.
 333 Consequently, the corresponding strains were higher and more concentrated (Fig-
 334 ure 10).

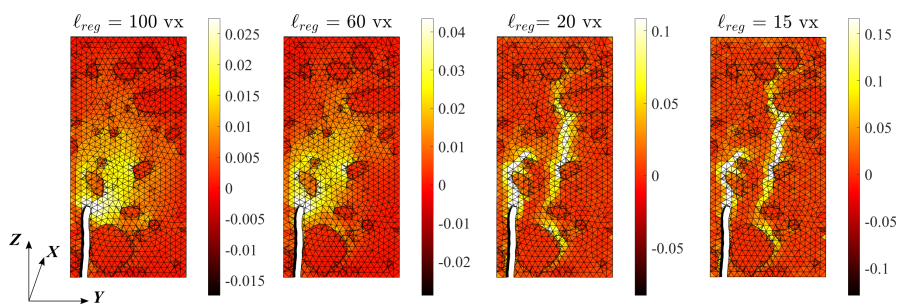


Fig. 10 Front face views of maximum principal strain ϵ_1 fields for different regularization lengths expressed in voxels ($C = 5.26$)

335 Figure 11(a) shows that the gray level residuals were essentially concentrated
 336 along the crack path. Very high maximum principal strains are observed in the
 337 zones where cracks were located. The differences in mechanical regularization per-
 338 formance in matrix and inclusions is visible in Figure 11(b). The crack crossed
 339 limestone aggregates (white in Figure 11(c)) where l_{reg} was $\sqrt{C} = \sqrt{5.26} \approx 2.3$
 340 times greater than in the matrix, which led to more diffuse strains with lower
 341 values.

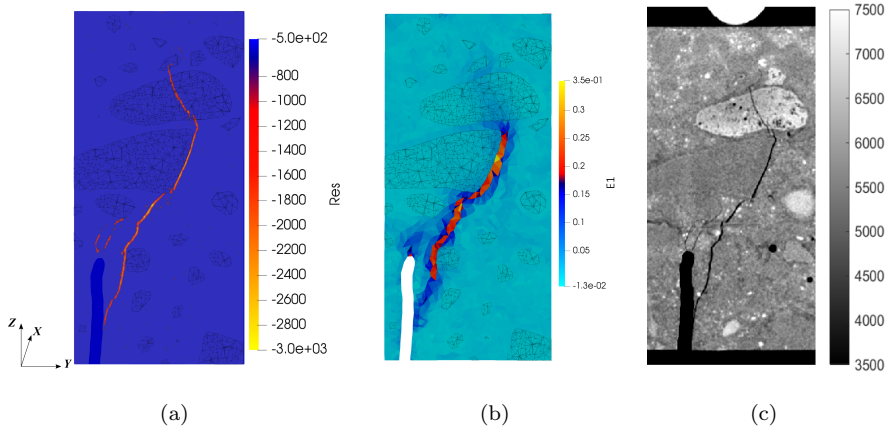


Fig. 11 Midsections of (a) gray level residuals ($l_{reg} = 15 \text{ vx}$), (b) maximum principal strain ϵ_1 , and (c) deformed volume

342 3.4 Contrast Influence

343 The relaxation process was also carried out for $C = 1.0$ (*i.e.*, homogeneous regular-
 344 ization), and the results are compared with the previous calculations. Figure 12(a)
 345 shows the RMS residual history during the relaxation process for the two con-
 346 sidered contrasts. For $C > 1$, the RMS residuals were systematically lower, and
 347 dropped to 273 gray levels, while for $C = 1.0$ the minimum level was 279 gray
 348 levels. These levels are rather close to the baselines (*i.e.*, 214-5 gray levels). This

349 observation shows that the regularization used herein was not too strong and did
 350 not induce significant deviations.

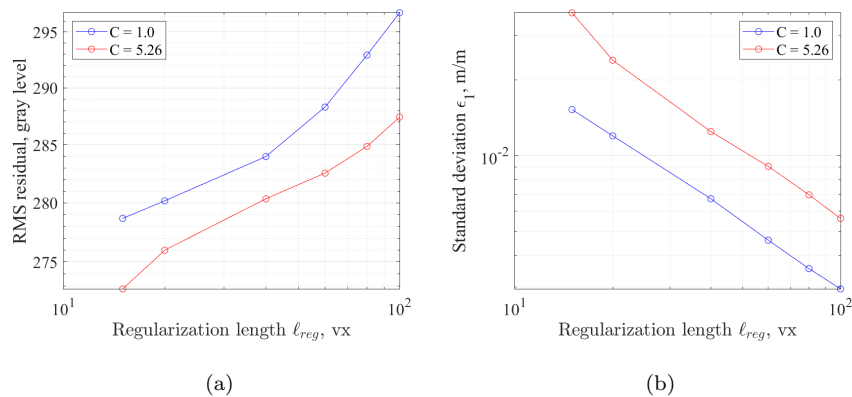


Fig. 12 (a) RMS gray level residuals, and (b) maximum principal strain ϵ_1 fluctuations as functions of the regularization length ℓ_{reg} and contrast C

351 For the maximum principal strains (Figure 12(b)), their standard deviation
 352 was systematically larger for higher contrast, which allowed for more fluctuations
 353 especially at the interfaces between aggregates and the matrix to be captured.
 354 Moreover, the growth of strain fluctuations was more progressive for $C = 5.26$
 355 along with the relaxation of mechanical regularization.

356 To further investigate the influence of contrast, the regularization length ℓ_{reg}
 357 was set to 20 vx, and the contrast C was varied between 0.5 and 20. The maximum
 358 principal strain fields (Figure 13) demonstrate how elastic contrast contributed to
 359 crack localization. The higher C , the less regularization was put on the matrix and
 360 the crack localized in fewer elements. In heterogeneous cementitious materials, the
 361 difference in mechanical properties of phases causes matrix-aggregate interfaces to

362 debond. This mechanism as well as damage in the matrix are better captured with
 363 heterogeneous regularization.

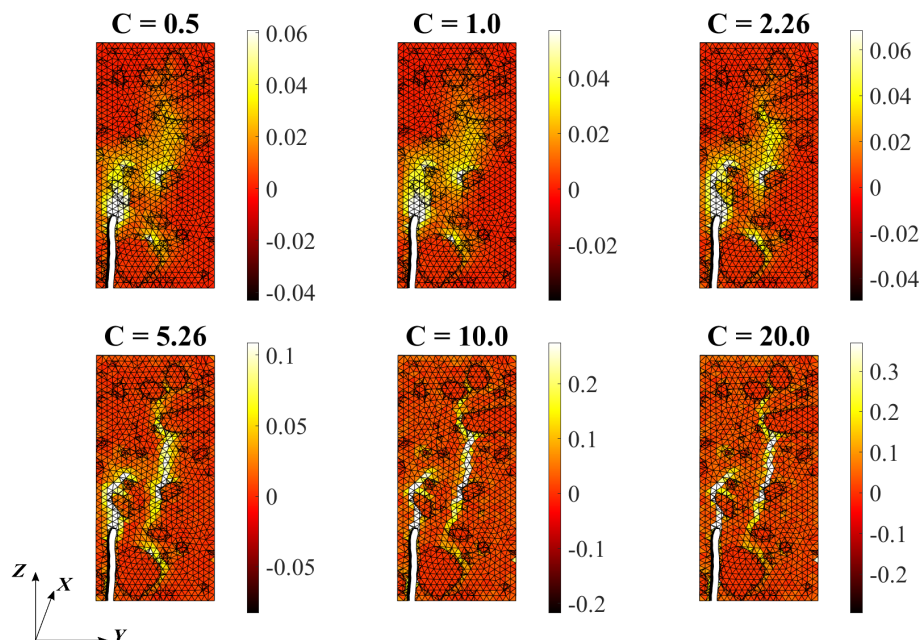


Fig. 13 Front face views of the maximum principal strain fields ϵ_1 for different contrasts ($\ell_{reg} = 20 \text{ vx}$)

364 Figure 14(a) shows that higher contrasts resulted in lower residuals since they
 365 allowed for more localized strains due to the presence of cracks. It is also reflected
 366 in the increase of standard deviation of maximum principal strains (Figure 14(b)).
 367 Although it may seem that taking a high value for C is a good option, the mean
 368 of maximum principal strains grows as well with an increase of C . It is a signal
 369 that too high contrasts result in "undeformed" aggregates and unphysical large
 370 strains in the totality of the matrix. Therefore, taking a contrast value greater than
 371 that based on physical properties of the constituents may result in displacement

372 fields that are no longer physically correct. Therefore, in further calculations the
 373 contrast was set to 5.26.

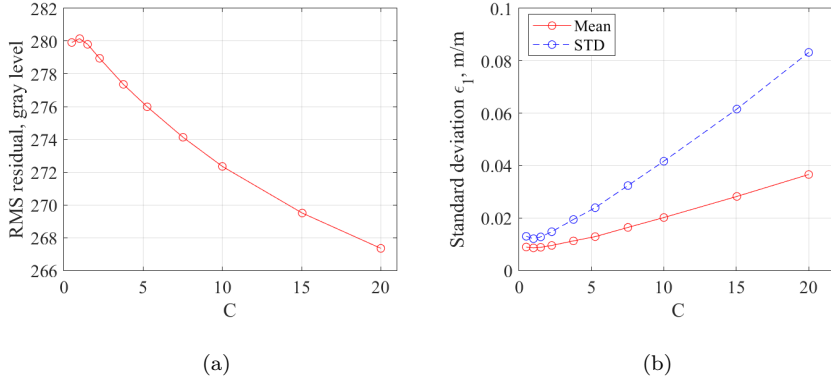


Fig. 14 (a) Change of RMS residual with contrast and regularization length. (b) Mean and standard deviation of the maximum principal strains ϵ_1 as functions of contrast ($l_{reg} = 20$ vx)

374 4 Damage Quantification

375 After adding elastic contrast for heterogeneous mechanical regularization, the anal-
 376 ysis was continued with the introduction of damage into mechanical regularization.
 377 A study of crack opening displacements and crack morphology at the mesoscale is
 378 finally proposed.

379 4.1 Damage Introduction into Mechanical Regularization

380 In the first stage, the heterogeneous regularization was taking into account the
 381 difference in mechanical behavior of different phases. In the present stage, damage
 382 can be considered in a similar manner [47]. The weight of mechanical regularization
 383 can be significantly reduced in the fractured zone, thereby allowing for large local
 384 strains. The damaged elements were selected based on two criteria, namely, the

385 average residual per element and Crack Opening Displacement (COD) $\llbracket u_I \rrbracket$, which
 386 is estimated as

$$\llbracket u_I \rrbracket = \epsilon_1 \ell \quad (12)$$

387 by neglecting the regular contribution to mean strains [60]. To study the effect
 388 of damage in mechanical regularization, two contrasts C were considered, namely,
 389 1.0 and 5.26. The results of previous analyses with $\ell_{reg} = 20$ vx were chosen to
 390 initialize calculations and select damaged elements. The thresholds and number of
 391 selected damaged elements for both cases are listed in Table 4. For the gray level
 392 residuals, the baseline levels were observed to be equal to 214-5 (Figure 8(a)).
 393 Consequently, the thresholds were selected as about two times this level to avoid
 394 false cracks. For the COD, their uncertainties were observed to be less than 0.1 vx
 395 with the evaluated strain uncertainties (Figure 8(b)). Consequently, the threshold
 396 COD for detecting damaged elements was set to 0.1 vx. The number of selected
 397 damaged elements for the two contrasts were very close. It is concluded that the
 398 selected criteria allowed for a reproducible description of the damaged zones. For
 399 a higher contrast (*i.e.*, $C = 5.26$), the maximum principal strains in the damaged
 400 zones were higher (Figure 13), and consequently the crack opening displacement.
 401 The number of detected damaged elements was also slightly higher.

Table 4 Damaged element selection

Thresholds	$C = 1$	$C = 5.26$
RMS residual, gray level	400	
COD , vx	0.1	
Number of damaged elements	18,076	18,206

402 The detected damaged elements for $C = 5.26$ are presented in Figure 15. The
 403 damaged zone is continuous and replicates well the residual fields corresponding
 404 to fractured surfaces (Figure 9), thereby validating the choice of residual and
 405 COD criteria. The thickness of damaged zone consists of several elements since
 406 the mesh does not describe explicitly the fracture surface and, as a consequence,
 407 high residual values corresponding to the crack span over several elements in its
 408 vicinity.

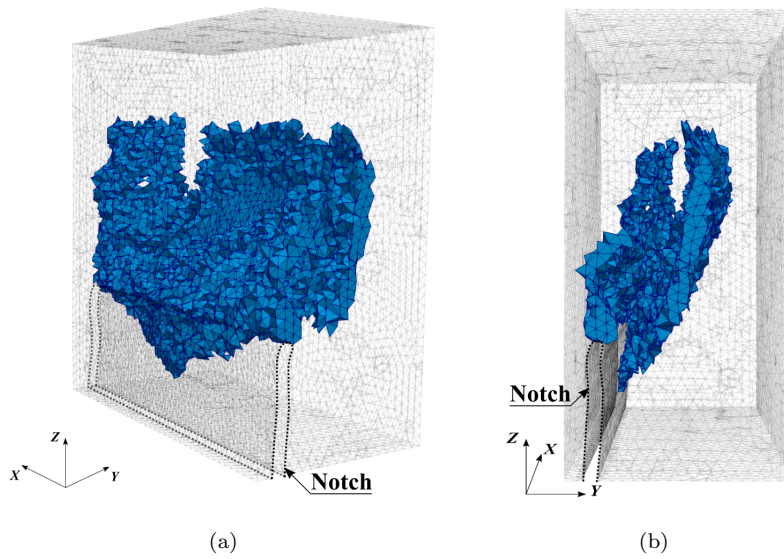


Fig. 15 3D renderings of damaged elements (corresponding to cracks) in the mechanical regularization ($\ell_{reg} = 20 \text{ vx}$, $C = 5.26$). (a) Side and (b) face views

409 Introducing a lower stiffness in damaged elements will help localize the in-
 410 elastic strains due to cracks. Thus the weight of mechanical regularization in the
 411 remainder of the volume could be increased. In the following calculations, the reg-
 412 ularization length was set to $\ell_{reg} = 60 \text{ vx}$ in order to increase the weight put on
 413 mechanical regularization in undamaged elements for which heterogeneous elastic-

414 ity is a very good approximation. Three different values were considered for the
 415 Young's modulus of the damaged elements E_d , namely, $0.2E_m$, $0.1E_m$ and $0.05E_m$.
 416 Figure 16 shows the maximum principal strain fields for different Young's moduli
 417 of damaged elements. Lower mechanical weight put in the damaged zones does
 418 allow for a better localization of strains in the cracked zones.

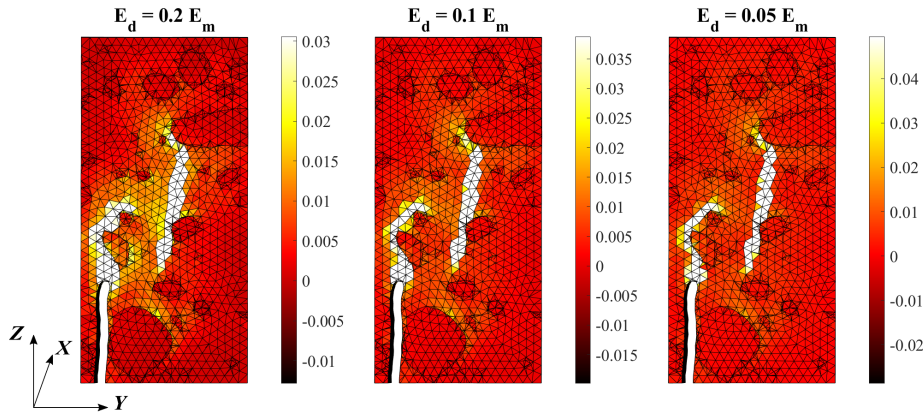


Fig. 16 Front face views of the maximum principal strain fields ϵ_1 for different elastic moduli of damaged elements ($\ell_{reg} = 60$ vx, $C = 5.26$)

419 Higher damage levels also led to lower global residuals (Figure 17), meaning
 420 convergence to a better solution, as well as higher strain fluctuations. Last, setting
 421 the damaged stiffness to values closer to zero (*i.e.*, $E_d < 0.05E_m$ in this study)
 422 resulted in the divergence of the DVC calculations. The elastic modulus of the
 423 damaged area E_d should be therefore set to the lowest possible value to allow for
 424 localized strains to occur, while retaining proper convergence of the DVC compu-
 425 tations. Based on these results, in further calculations the Young's modulus of the
 426 damaged elements was set to 5% of the matrix modulus (*i.e.*, $E_d = 0.05 E_m$).

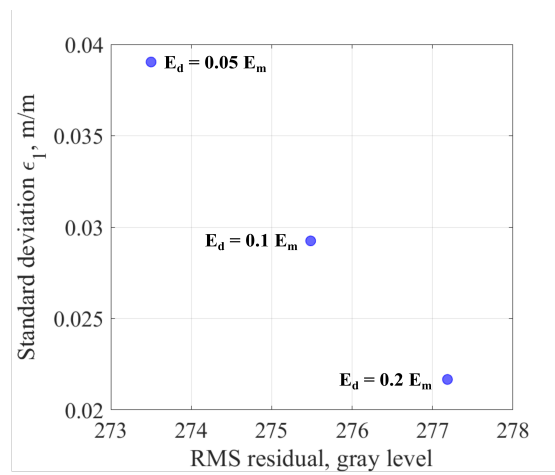


Fig. 17 Standard deviation of the maximum principal strain ϵ_1 compared to the RMS residual for different elastic moduli of damaged elements ($\ell_{reg} = 60$ vx, $C = 5.26$)

427 Figure 18 shows the maximum principal strain field for different contrasts and
 428 damage configurations. The introduction of damage into mechanical regulariza-
 429 tion was more effective for crack localization than the consideration of mechanical
 430 contrast between different phases (Figure 13). With the highest contrast, damage
 431 could also be better described at interfaces between the matrix and the aggregates.

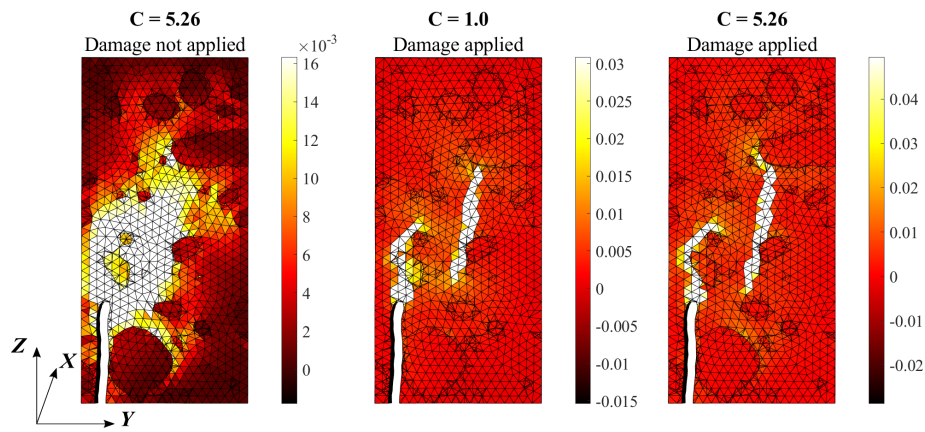


Fig. 18 Front face views of the maximum principal strain fields ϵ_1 for different contrasts and damage ($l_{reg} = 60$ vx)

432 Figure 19 displays the change of RMS residual and fluctuations of ϵ_1 fields
 433 characterized by their standard deviation. In terms of residual, the introduction of
 434 damage lowered their overall levels. The combination of both methods (*i.e.*, con-
 435 trast and damage) gives a better solution in terms of residual levels and strain
 436 localization, which indicates a more correct description of the physical mecha-
 437 nisms. These results were kept for further damage quantification.

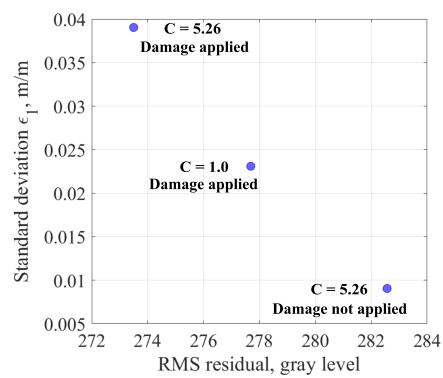


Fig. 19 Standard deviation of the maximum principal strain ϵ_1 compared to the RMS residual for different contrasts and damage implementations ($\ell_{reg} = 60$ vx)

438 4.2 Characterization of CODs

439 The dominant crack was observed to cross the cement paste matrix, aggregate-
 440 matrix interfaces and limestone aggregates. Once the DVC analysis was performed
 441 and the damaged elements detected, the damaged elements belonging to the ma-
 442 trix, interphases and aggregates were quantified (Figure 20). In cementitious mate-
 443 rials, matrix-aggregate interfaces have different chemical compositions along with
 444 higher porosity. It is considered that due to the lower properties and mismatch of
 445 mechanical properties, damage initiates preferably in such interfacial zones, which
 446 lead to debonding [61]. Experimental evidence shows that the interfacial zone
 447 width varies in the 10-50 μm range [62,63]. Since the average element size was
 448 ≈ 50 μm , the matrix elements adjacent to aggregates were considered as interphase
 449 elements for further analysis (Table 2).

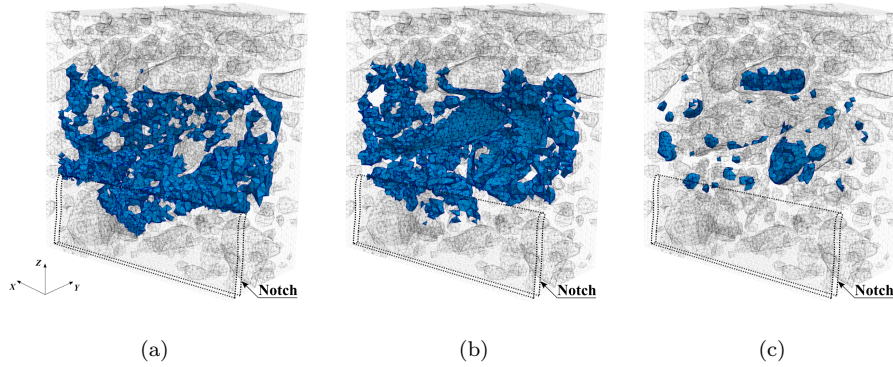


Fig. 20 Damaged elements belonging to (a) the matrix, (b) interphases, and (c) aggregates

450 The distribution of damaged zones between the three phases is reported in Ta-
 451 ble 5. The volume fraction of damaged elements was mostly in the matrix (>90%)
 452 with almost equal partitioning between interphases and matrix bulk. The maxi-
 453 mum average COD is in interphases (7.3 μm), and the minimum is in the matrix
 454 bulk (6.2 μm). The highest COD fluctuations, which were characterized by their
 455 standard deviation, was in the aggregates (5.6 μm). For the other phases, the COD
 456 fluctuations were similar.

Table 5 Damaged zone characteristics

Parameters	Total	Bulk matrix	Interphases	Aggregates
Number of elements in damaged zone	18,206	8,340	8,329	1,537
Percentage of elements in damage zone	100%	46%	46%	8%
Damaged volume, mm^3	2.42	1.10	1.09	0.23
Average COD, μm	6.8	6.2	7.3	7.2
COD standard deviation, μm	4.6	4.2	4.7	5.6

457 The crack opening displacement was averaged over the total width of the sam-
 458 ple and over its height with a 0.132 mm step. Figure 21(a) shows the COD field in

459 the specimen. Figure 21(b) reports the averaged crack opening displacement along
 460 the specimen height for the entire crack, and Figure 21(c) for each individual phase.

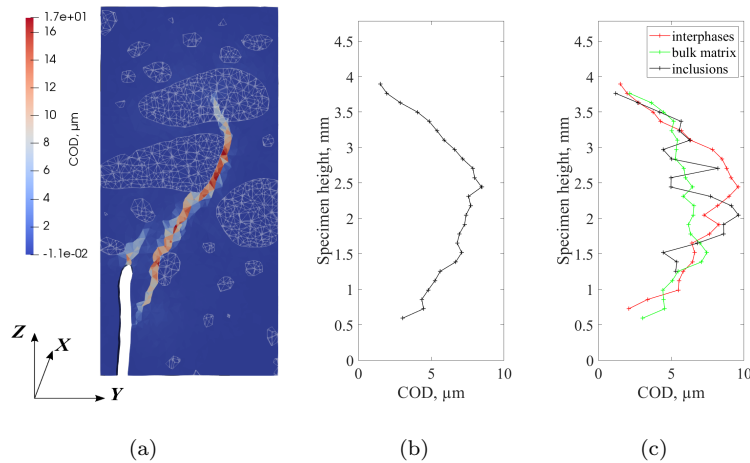


Fig. 21 (a) Cross-section (at $x = 2.5$ mm) of the COD field. (b) Average COD and (c) average COD per phase along the specimen height

461 The crack started below the notch root at 3.0 μm width and its opening in-
 462 creased significantly up to 7.1 μm when it reached the notch root. Then the COD
 463 grew slowly until it reached its maximum level of 8.5 μm at the mid-ligament
 464 height, where a large aggregate with a vertical interface was located. Beyond the
 465 mid-ligament, the COD decreased down to 1.5 μm at 3.9 mm specimen height. The
 466 COD in the matrix bulk peaked at the notch root (7.4 μm) and then gradually
 467 decreased as it propagated upward. The COD at interphases was higher than in
 468 the matrix bulk over a significant part of the ligament with a maximum opening of
 469 9.6 μm . The COD in aggregates was fluctuating considerably along the specimen
 470 height. This effect was due to the relatively small number of cracked aggregates

471 and their sparse distribution in the volume (Figure 20(c)). However, locally the
472 COD could reach 9.6 μm .

473 5 Conclusion and Perspectives

474 In the present study, an *in situ* three-point flexural test was carried out in an
475 X-ray CT scanner on a small-scale mortar microbeam. A realistic 3D mesh was
476 built consistently with the imaged underlying microstructure (based on a 5.3 μm
477 resolution tomographic scan acquired prior to the *in situ* test). Mechanically reg-
478 ularized FE-DVC was adapted to heterogeneous materials by taking into account
479 the difference between the elastic properties of the different phases of mortar. The
480 introduction of elastic contrast C allowed the strain heterogeneities related to the
481 underlying microstructure to be better described, and the inelastic strains to be
482 better captured in the damaged zones. The contrast study showed that prescribing
483 contrast levels above the expected properties of phases could result in unrealistic
484 strains in the matrix. It is worth emphasizing that realistic Young's moduli of
485 the various phases are needed to obtain trustworthy strain fields, especially when
486 stronger mechanical regularization is enforced.

487 Furthermore, the damaged elements were selected based on previous compu-
488 tations for the introduction of damage in the regularization scheme. The Young's
489 modulus in damaged elements was set to 5% of that in the undamaged matrix,
490 which allowed displacement measurements to be more localized in the fractured
491 zone. The estimation of crack opening displacements and crack morphology was
492 carried out and gave more insight into the damage mechanisms at the mesoscale.
493 The study thus demonstrated the potential of mechanically regularized FE-DVC

494 enriched with microstructure-based features for the quantification of damage at
495 lower scales.

496 In future studies, the construction of 3D meshes consistent with fractured
497 surfaces may improve the estimation of crack opening displacements [64,65]. The
498 test reported herein may also be used to calibrate numerical models accounting
499 for the various damage mechanisms discussed herein.

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502 **Conflict of interest**

503 The authors declare that they have no conflict of interest.

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