

QuickSampling v1.0: a robust and simplified pixel-based multiple-point simulation approach

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Highlights

- A new approach is proposed for pixel-based multiple-point geostatistics simulation.
- The method is flexible and straightforward to parametrize.
- It natively handles continuous and multivariate simulations.
- High computational performance with predictable simulation times.
- A free and open-source implementation is provided.

Abstract

Multiple-point geostatistics enable the realistic simulation of complex spatial structures by inferring statistics from a training image. These methods are typically computationally expensive and require complex algorithmic parametrizations. The approach that is presented in this paper is easier to use than existing algorithms, as it requires few independent algorithmic parameters. It is natively designed for handling continuous variables, and quickly implemented by capitalizing on standard libraries. The algorithm can handle incomplete training images of any dimensionality, with categorical or/and continuous variables, and stationarity is not explicitly required. It is possible to perform unconditional or conditional simulations, even with exhaustively informed covariates. The method provides new degrees of freedom by allowing kernel weighting for pattern matching. Computationally, it is adapted to modern architectures and runs in constant time. The approach is benchmarked against a state-of-the-art method. An efficient open-source implementation of the algorithm is released and can be found here (<https://github.com/GAIA-UNIL/G2S>), to promote reuse and further evolution.

Keywords

Multiple-point statistics, stochastic simulation, continuous variable, training image, cross-correlation, Fourier transform.

1. Introduction

Geostatistics is used widely to generate stochastic random fields for modeling and characterizing spatial phenomena such as Earth surface features and geological structures. Commonly used methods, such as the sequential Gaussian simulation (Gómez-Hernández and Journel, 1993) and turning bands algorithms (Matheron, 1973), are based on kriging (e.g., Graeler et al., 2016; Li and Heap, 2014; Tadić et al., 2017; 2015). This family of approaches implies spatial relations using exclusively pairs of points and expresses these relations using

37 covariance functions. In the last two decades, multiple point statistics (MPS) emerged as a
38 method for representing more complex structures using high-order nonparametric statistics
39 (Guardiano and Srivastava, 1993). To do so, MPS algorithms rely on training images, which
40 are images with similar characteristics to the modeled area. Over the last decade, MPS has been
41 used for stochastic simulation of random fields in a variety of domains such as geological
42 modeling (e.g., Barfod et al., 2018; Strebelle et al., 2002), remote sensing data processing (e.g.,
43 Gravey et al., 2019; Yin et al., 2017), stochastic weather generation (e.g., Oriani et al., 2017;
44 Wojcik et al., 2009), geomorphological classification (e.g., Vannamettee et al., 2014) and
45 climate model downscaling (a domain that has typically been the realm of kriging-based
46 methods (e.g., Bancheri et al., 2018; Jha et al., 2015; Latombe et al., 2018)).

47 In the world of MPS simulations, one can distinguish two types of approaches. The first
48 category is the patch-based methods, where complete patches of the training image are imported
49 into the simulation. This category includes methods such as SIMPAT (Arpat and Caers, 2007)
50 and DISPAT (Honarkhah and Caers, 2010), which are based on building databases of patterns,
51 and image quilting (Mahmud et al., 2014), which uses an overlap area to identify patch
52 candidates, which are subsequently assembled using an optimal cut. CCSIM (Tahmasebi et al.,
53 2012) uses cross-correlation to rapidly identify optimal candidates. More recently, Li (2016)
54 proposed a solution that uses graph-cuts to find an optimal cut between patches, which has the
55 advantage of operating easily and efficiently independently of the dimensionality of the
56 problem. Tahmasebi (2017) propose as a solution that is based on “warping” in which the new
57 patch is distorted to match the previously simulated areas. For a multivariate simulation with
58 an informed variable, Hoffmann (2017) presented an approach for selecting a good candidate
59 based on the mismatch of the primary variable, and on the mismatch rank of the candidate
60 patches for auxiliary variables. Although patch-based approaches are recognized to be fast, they
61 are typically difficult to use in the presence of dense conditioning data. Furthermore, patch-
62 based approaches often suffer from a lack of variability due to the pasting of large areas of the
63 training image, which is a phenomenon that is called verbatim copy. Verbatim copy (Mariethoz
64 and Caers, 2014) refers to the phenomenon whereby the neighbor of a pixel in the simulation
65 is the neighbor in the training image. This results in large parts of the simulation that are
66 identical to the training image.

67 The second category of MPS simulation algorithms consists of pixel-based algorithms, which
68 import a single pixel at the time instead of full patches. These methods are typically slower than
69 patch-based methods. However, they do not require a procedure for the fusion of patches, such
70 as an optimal cut, and they allow more flexibility in handling conditioning data. Furthermore,
71 in contrast to patch-based methods, pixel-based approaches rarely produce artifacts when
72 dealing with complex structures. The first pixel-based MPS simulation algorithm was
73 ENESIM, which was proposed by Guardiano and Srivastava, 1993, where for a given
74 categorical neighborhood – usually small – all possible matches in the training image are
75 searched. The conditional distribution of the pixel to be simulated is estimated based on all
76 matches, from which a value is sampled. This approach could originally handle only a few
77 neighbors and a relatively small training image; otherwise, the computational cost would
78 become prohibitive and the number of samples insufficient for estimating the conditional
79 distribution. Inspired by research in computer graphics, where similar techniques are developed

80 for texture synthesis (Mariethoz and Lefebvre, 2014), an important advance was the
81 development of SNESIM (Strebelle, 2002), which proposes storing in advance all possible
82 conditional distributions in a tree structure and using a multigrid simulation path to handle large
83 structures. With IMPALA, Straubhaar (2011) proposed reducing the memory cost by storing
84 information in lists rather than in trees. Another approach is direct sampling (DS) (Mariethoz
85 et al., 2010), where the estimation and the sampling of the conditional probability distribution
86 are bypassed by sampling directly in the training image, which incurs a very low memory cost.
87 DS enabled the first use of pixel-based simulations with continuous variables. DS can use any
88 distance formulation between two patterns; hence, it is well suited for handling various types
89 of variables and multivariate simulations.

90 In addition to its advantages, DS has several shortcomings: DS requires a threshold – which is
91 specified by the user – that enables the algorithm to differentiate good candidate pixels in the
92 training image from bad ones based on a predefined distance function. This threshold can be
93 highly sensitive and difficult to determine and often dramatically affects the computation time.
94 This results in unpredictable computation times, as demonstrated by Meerschman (2013). DS
95 is based on the strategy of randomly searching the training image until a good candidate is
96 identified (Shannon, 1948). This strategy is an advantage of DS; however, it can also be seen
97 as a weakness in the context of modern computer architectures. Indeed, random memory access
98 and high conditionality can cause 1) suboptimal use of the instruction pipeline, 2) poor memory
99 prefetch, 3) substantial reduction of the useful memory bandwidth and 4) impossibility of using
100 vectorization (Paul Shen, 2018). While the first two problems can be addressed with modern
101 compilers and pseudorandom sequences, the last two are inherent to the current memory and
102 CPU construction.

103 This paper presents a new and flexible pixel-based simulation approach, namely,
104 QuickSampling (QS), which makes efficient use of modern hardware. Our method takes
105 advantage of the possibility of decomposing the standard distance metrics that are used in MPS
106 (L^0, L^2) as sums of cross-correlations. As a result, we can use fast Fourier transforms (FFTs) to
107 quickly compute mismatch maps. To rapidly select candidate patterns in the mismatch maps,
108 we use an optimized partial sorting algorithm. A free, open-source and flexible implementation
109 of QS is available, which is interfaced with most common programming languages (C/C++,
110 MATLAB, R, and Python 3).

111 The remainder of this paper is structured as follows: Section 2 presents the proposed algorithm
112 with an introduction to the general method of sequential simulation, the mismatch measurement
113 using FFTs and the sampling approach of using partial sorting followed by methodological and
114 implementation optimizations. Section 3 evaluates the approach in terms of quantitative and
115 qualitative metrics via simulations and conducts benchmark tests against DS, which is the only
116 other available approach that can handle continuous pixel-based simulations. Section 4
117 discusses the strengths and weaknesses of QS and provides guidelines. Finally, guidelines and
118 the conclusions of this work are presented in Section 5.

119 2. Methodology and Implementation

120 2.1. Pixel-based sequential simulation

121 We recall the main structure of pixel-based MPS simulation algorithms (Mariethoz and Caers,
122 2014, p.156), which is summarized and adapted for QS in Pseudocode 1. The key difference
123 between existing approaches is in lines 3 and 4 of Pseudocode 1, when candidate patterns are
124 selected. This task is the most time-consuming in many MPS algorithms and we focus only on
125 computing it in a way that reduces its cost and minimizes the parameterization.

126

127 Pseudocode 1: QS Algorithm

128

129 Inputs:

130 T the training images

131 S the simulation grid, including the conditioning data

132 P the simulation path

133 The choice of pattern metric

134

135 1. **For** each unsimulated pixel x following the path P :

136 2. Find the neighborhood $N(x)$ in S that contains all previously simulated or conditioning
137 nodes in a specified radius

138 3. Compute the mismatch map between T and $N(x)$: [Section 2.3](#)

139 4. Select a good candidate using quantile sorting over the mismatch map: [Section 2.4](#)

140 5. Assign the value of the selected candidate to x in S

141 6. **End**

142

143 2.2. Decomposition of common mismatch metrics as sums of products

144 Distance-based MPS approaches are based on pattern matching (Mariethoz and Lefebvre,
145 2014). Here, we rely on the observation that many common matching metrics can be expressed
146 as weighted sums of the pixelwise mismatch ε . This section explores the pixelwise errors for a
147 single variable and for multiple variables. For a single variable, the mismatch metric ε between
148 two pixels is the distance between two scalars or two classes. In the case of many variables, it
149 is a distance between two vectors that are composed by scalars, by classes, or by a combination
150 of the two. Here, we focus on distance metrics that can be expressed in the following form:

151

Equation 1

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$$\varepsilon(a, b) \propto \sum_{j \in \mathcal{J}} f_j(a) \cdot g_j(b)$$

153

where a and b represent the values of two univariate pixels and f_j and g_j are functions that depend on the chosen metric. \mathcal{J} is defined by the user depending on the metric used. Here, we use the proportion symbol because we are interested in relative metrics rather than absolute metrics, namely, the objective is to rank the candidate patterns. We show below that many of the common metrics or distances that are used in MPS can be expressed as Equation 1.

158

For the simulation of continuous variables, the most commonly used mismatch metric is the L^2 -norm, which can be expressed as follows:

160

Equation 2

161

$$\varepsilon_{L^2}(a, b) = (a - b)^2 = a^2 - 2ab + b^2$$

162

Using Equation 1, this L^2 -norm can be decomposed into the following series of functions f_j and

163

g_j :

164

$$f_0: x \rightarrow x^2$$

167

$$g_0: x \rightarrow 1$$

165

$$f_1: x \rightarrow -2x$$

168

$$g_1: x \rightarrow x$$

166

$$f_2: x \rightarrow 1$$

169

$$g_2: x \rightarrow x^2$$

170

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172

173 A similar decomposition is possible for the L^0 -norm (also called Hamming distance), which is
174 commonly used for the simulation of categorical variables. The Hamming distance measures
175 the dissimilarity between two lists by counting the number of elements that have different
176 categories (Hamming, 1950). Example the dissimilarity between a,b,b,c,b,a and a,c,b,a,c,a is
177 0,1,0,1,1,0 and the associated Hamming distance is 3.

178

Equation 3

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$$\varepsilon_{L^0}(a, b) = (a - b)^0 = 1 - \sum_{j \in \mathcal{C}} (\delta_{a,j} \cdot \delta_{b,j}) \propto \sum_{j \in \mathcal{C}} \delta_{a,j} \cdot \delta_{b,j}$$

180 where $\delta_{x,y}$ is the Kronecker delta between x and y , which is 1 if x equals y and 0 otherwise,
181 and \mathcal{C} is the set of all possible categories of a specified variable. Here $\mathcal{J} = \mathcal{C}$.

182 Using Equation 1, this L^0 distance can be decomposed (Arpat and Caers, 2007) into the
183 following series of functions f_j and g_j :

184 $f_j: x \rightarrow -\delta_{xj}$

185 $g_j: x \rightarrow \delta_{xj}$

186 with a new pair of f_j and g_j for each class j of \mathcal{C} .

187 For multivariate pixels, such as a combination of categorical and continuous values, the
188 mismatch ε can be expressed as a sum of univariate pixelwise mismatches.

189

Equation 4

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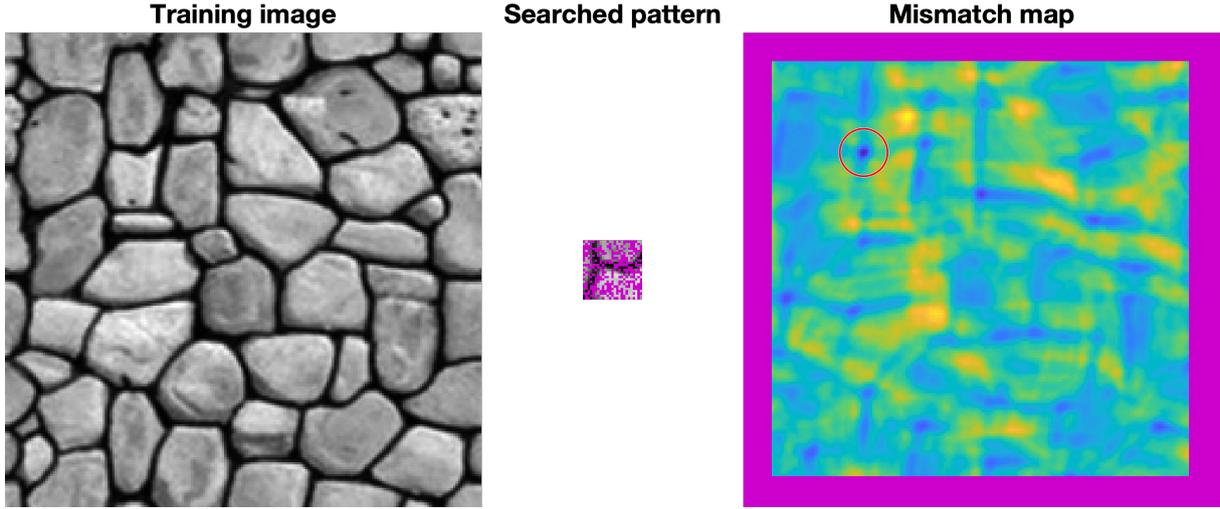
$$\varepsilon(\mathbf{a}, \mathbf{b}) \propto \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} f_j(a_i) \cdot g_j(b_i)$$

191 where \mathbf{a} and \mathbf{b} are the compared vectors and a_i and b_i are the individual components of \mathbf{a} and
192 \mathbf{b} . \mathcal{J}_i represents the set related to the metric used for the i^{st} variable, and \mathcal{J} represents the set of
193 variables.

194

195 **2.3. Computation of a mismatch map for an entire pattern**

196 The approach that is proposed in this work is based on computing a mismatch map in the TI for
197 each simulated pixel. The mismatch map is a grid that represents the pattern-wise mismatch for
198 each location of the training image and enables the fast identification of a good candidate, as
199 shown by the red circle in Figure 1.



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Figure 1 Example of a mismatch map for an incomplete pattern. Blue represents good matches, yellow bad matches and purple missing and unusable (border effect) data. The red circle highlights the minimum of the mismatch map, which corresponds to the location of the best candidate.

205

206

If we consider the neighborhood $N(s)$ around the simulated position s , then we can express a weighted dissimilarity between $N(s)$ and a location in the TI $N(t)$:

207

208

Equation 5

209

$$E(N(t), N(s)) = \sum_{l \in N(t,s)} \omega_l \varepsilon(N_l(t), N_l(s))$$

210

where $N(t, s) = \{l \mid N_l(t) \text{ and } N_l(s) \text{ exist}\}$

211

and $N_l(p)$ is the neighbors of p (p can represent either s or t) with a relative displacement l from p , therefore $N(p) = \{l \mid N_l(p)\}$, l is the lag vector that defines the relative position of each value within N , and ω_l is a weight for each pixelwise error according to the lag vector l . By extension, ω is the matrix of all weights, which we call the weighting kernel or, simply, the kernel. E represents the mismatch between patterns that are centered on s and $t \in T$, where T is the training image.

217

Some lags may not correspond to a value, for example, due to edge effects in the considered images or because the patterns are incomplete. Missing patterns are inevitable during the course of a simulation using a sequential path. Furthermore, in many instances, there can be missing areas in the training image. This is addressed by creating an indicator variable to be used as a mask, which equals 1 at informed pixels and 0 everywhere else:

222

Equation 6

223

$$\mathbb{1}_l(p) = \begin{cases} 1 & \text{if } N_l(p) \text{ is informed} \\ 0 & \text{otherwise} \end{cases}$$

224 Let us first consider the case in which for a specified position, either all or no variables are
 225 informed. Expressing the presence of data as a mask enables the gaps to be ignored because the
 226 corresponding errors are multiplied by zero.

227 Then, Equation 5 can be expressed as follows:

228 Equation 7

$$229 \quad E(N(t), N(s)) = \sum_{\mathbf{l}} \omega_{\mathbf{l}} \cdot \mathbb{1}_{\mathbf{l}}(t) \cdot \mathbb{1}_{\mathbf{l}}(s) \cdot \varepsilon(N_{\mathbf{l}}(t), N_{\mathbf{l}}(s))$$

230 . Combining Equation 4 and Equation 7, we get:

231 Equation 8

$$\begin{aligned}
 233 \quad E(N(t), N(s)) &\propto \sum_{\mathbf{l}} \omega_{\mathbf{l}} \cdot \mathbb{1}_{\mathbf{l}}(t) \cdot \mathbb{1}_{\mathbf{l}}(s) \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} f_j(N_{\mathbf{l}}(t)_i) \cdot g_j(N_{\mathbf{l}}(s)_i) \\
 234 &= \sum_{\mathbf{l}} \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \omega_{\mathbf{l}} \cdot \mathbb{1}_{\mathbf{l}}(t) \cdot \mathbb{1}_{\mathbf{l}}(s) \cdot f_j(N_{\mathbf{l}}(t)_i) \cdot g_j(N_{\mathbf{l}}(s)_i) \\
 235 &= \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \sum_{\mathbf{l}} \omega_{\mathbf{l}} \cdot \left(\mathbb{1}_{\mathbf{l}}(t) \cdot f_j(N_{\mathbf{l}}(t)_i) \right) \cdot \left(\mathbb{1}_{\mathbf{l}}(s) \cdot g_j(N_{\mathbf{l}}(s)_i) \right) \\
 236 &= \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \sum_{\mathbf{l}} \left(\mathbb{1}_{\mathbf{l}}(t) \cdot f_j(N_{\mathbf{l}}(t)_i) \right) \cdot \left(\omega_{\mathbf{l}} \cdot \mathbb{1}_{\mathbf{l}}(s) \cdot g_j(N_{\mathbf{l}}(s)_i) \right)
 \end{aligned}$$

232 .

237 After rewriting, Equation 8 can be expressed as a sum of cross-correlations that encapsulate
 238 spatial dependencies, using the cross-correlation definition $f \star g = \sum_{\mathbf{l}} f_{\mathbf{l}} \cdot g_{\mathbf{l}}$, as follows:

239 Equation 9

$$240 \quad E(N(t), N(s)) \propto \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \left(\mathbb{1}(t) \circ f_j(N(t)_i) \right) \star \left(\omega \circ \mathbb{1}(s) \circ g_j(N(s)_i) \right)$$

241 where ω and $\mathbb{1}(\cdot)$ represent the matrices that are formed by $\omega_{\mathbf{l}}$ and $\mathbb{1}_{\mathbf{l}}(\cdot)$ for all possible vectors
 242 \mathbf{l} , \star denotes the cross-correlation operator, and \circ is the element-wise product (or Hadamard-
 243 product).

244 Finally, with $T = \{T_i, i \in \mathcal{J}\}$, T_i represents the training image for the i -th variable, and by
 245 applying cross-correlations for all positions $t \in T$, we obtain a mismatch map, which is
 246 expressed as:

247 Equation 10

$$248 \quad E(T, N(s)) \propto \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \left(\mathbb{1}(T) \circ f_j(T_i) \right) \star \left(\omega \circ \mathbb{1}(s) \circ g_j(N(s)_i) \right)$$

249 . The term $\mathbb{1}(T)$ allows the consideration of the possibility of missing data in the training image
 250 T .

251 Let us consider the general case in which only some variables are informed and the weighting
 252 can vary for each variable. Equation 10 can be extended for this case by defining separate masks
 253 and weights ω_i for each variable:

254 *Equation 11*

$$255 \quad E(T, N(s)) \propto \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \left(\mathbb{1}(T_i) \circ f_j(T_i) \right) \star \left(\omega_i \circ \mathbb{1}(s_i) \circ g_j(N(s)_i) \right)$$

256 . Equation 11 can be expressed using the convolution theorem applied to cross-correlation:

257 *Equation 12*

$$258 \quad E(T, N(s)) \propto \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \mathcal{F}^{-1} \left\{ \overline{\mathcal{F}\{\mathbb{1}(T_i) \circ f_j(T_i)\}} \circ \mathcal{F}\{\omega_i \circ \mathbb{1}(s_i) \circ g_j(N(s)_i)\} \right\}$$

259 , where \mathcal{F} represents the Fourier transform, \mathcal{F}^{-1} the inverse transform, and \bar{x} the conjugate of
 260 x .

261 By linearity of the Fourier transform, the summation can be performed in Fourier space, thereby
 262 reducing the number of transformations:

263 *Equation 13*

$$264 \quad E(T, N(s)) \propto \mathcal{F}^{-1} \left\{ \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{J}_i} \overline{\mathcal{F}\{\mathbb{1}(T_i) \circ f_j(T_i)\}} \circ \mathcal{F}\{\omega_i \circ \mathbb{1}(s_i) \circ g_j(N(s)_i)\} \right\}$$

265 . Equation 13 is appropriate for modern computers, which are well-suited for computing FFTs
 266 (Cooley et al., 1965; Gauss, 1799). Currently, FFTs are well implemented in highly optimized
 267 libraries (Rodríguez, 2002). Equation 13 is the expression that is used in our QS implementation
 268 because it reduces the number of Fourier transforms, which are the most computationally
 269 expensive operations of the algorithm. One issue with the use of FFTs is that the image T is
 270 typically assumed to be periodic. However, in most practical applications, it is not periodic.
 271 This can be simply addressed by cropping the edges of $E(T, N(s))$ or by adding a padding
 272 around T .

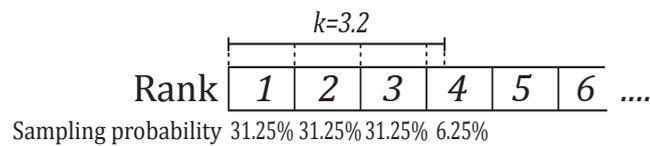
273 The computation of the mismatch map (Equation 13) is deterministic; as a result, it incurs a
 274 constant computational cost that is independent of the pixel values. Additionally, Equation 13
 275 is expressed without any constraints on the dimensionality. Therefore, it is possible to use the
 276 n -dimensional FFTs that are provided in the above libraries to perform n -dimensional
 277 simulations without changing the implementation.

278 **2.4. Selection of candidates based on a quantile**

279 The second contribution of this work is the k -sampling strategy for selecting a simulated value
 280 among candidates. The main idea is to use the previously calculated mismatch map to select a
 281 set of potential candidates that are defined by the k smallest (i.e. a quantile) values of E . Once
 282 this set has been selected, we randomly draw a sample from this pool of candidates. This differs

283 from strategies that rely on a fixed threshold, which can be cumbersome to determine. This
 284 strategy is highly similar to the ϵ -replicate strategy that is used in image quilting (Mahmud et
 285 al., 2014) in that we reuse and extend to satisfy the specific requirements of QS. It has the main
 286 advantage of rescaling the acceptance criterion according to the difficulty; i.e. the algorithm is
 287 more tolerant of rare patterns while requiring very close matches for common patterns.

288 In detail, the candidate selection procedure is as follows: All possible candidates are ranked
 289 according to their mismatch and one candidate is randomly sampled among the k best. This
 290 number k can be seen as a quantile over the training dataset. However, parameter k has the
 291 advantage of being an easy representation for users, who can associate $k = 1$ with the best
 292 candidate, $k = 2$ with the two best candidates, etc. For fine-tuning parameter k , the sampling
 293 strategy can be extended to non-integer values of k by sampling the candidates with
 294 probabilities that are not uniform. For example, if the user sets $k = 1.5$, the best candidate has
 295 a probability of $2/3$ of being sampled and the second best a probability of $1/3$. For $k = 3.2$,
 296 (Figure 2) each of the 3 best candidates are sampled with an equal probability of 0.3125 and
 297 the 4th best with a probability of 0.0625. This feature is especially useful for tuning k between
 298 1 and 2 and for avoiding a value of $k = 1$, which can result in the phenomenon of verbatim
 299 copy.



300

301 *Figure 2 Illustration of the k -sampling strategy*

302 An alternative sampling strategy for reducing the simulation time is presented in Appendix A.3.
 303 However, this strategy can result in a reduction in the simulation quality.

304 The value of non-integer k -values is not only in the fine tuning of parameters. It also allows
 305 direct comparisons between QS and DS. Indeed, under the hypothesis of a stationary training
 306 image, using DS with a given max fraction of scanned training image (f) and a threshold (t) of
 307 0 is statistically similar to using QS with $k=1/f$. In both situations, the best candidate is
 308 sampled in a fraction f of the training image.

309

310 **2.5. Simplifications in the case of a fully informed training image**

311 In many applications, spatially exhaustive TIs are available. In such cases, the equations above
 312 can be simplified by dropping constant terms from Equation 1, thereby resulting in a simplified
 313 form for Equation 13. Here, we take advantage of the ranking to know that a constant term will
 314 not affect the result.

315 As in Tahmasebi (2012), in the L^2 -norm, we drop the squared value of the searched pattern,
 316 namely, b^2 , from Equation 2. Hence, we can express Equation 4 as follows:

317

Equation 14

318

$$\varepsilon(\mathbf{a}, \mathbf{b}) = \sum_{i \in \mathcal{J}} a_i^2 - 2 \sum_{i \in \mathcal{J}} a_i \cdot b_i$$

319

320

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The term a^2 , which represents the squared value of the candidate pattern in the TI, differs among training image locations and, therefore, cannot be removed. Indeed, the assumption that $\sum a^2$ is constant is only valid under a strict stationarity hypothesis on the scale of the search pattern. While this hypothesis might be satisfied in some cases (as in Tahmasebi et al., 2012), we do not believe it is generally valid. Via the same approach, Equation 3 can be simplified by removing the constant terms; then, we obtain the following for the L^0 -norm:

325

Equation 15

326

$$\varepsilon(\mathbf{a}, \mathbf{b}) = - \sum_{i \in \mathcal{J}} \sum_{j \in \mathcal{C}} \delta_{a_i, j} \cdot \delta_{b_i, j}$$

327

328

2.6. Efficient Implementation

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An efficient implementation of QS was achieved by 1) performing precomputations, 2) implementing an optimal partial sorting algorithm for selecting candidates and 3) optimal coding and compilation. These are described below.

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According to Equation 13, $\overline{\mathcal{F}\{\mathbb{1}(T_i) \circ f_j(T_i)\}}$ is independent of the searched pattern $N(s)$. Therefore, it is possible to precompute it at the initialization stage for all i and j . This improvement typically reduces the computation time for an MPS simulation by a factor of at least 2.

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In the QS algorithm, a substantial part of the computation cost is incurred in identifying the k best candidates in the mismatch map. In the case of non-integer k , the upper limit $\lceil k \rceil$ is used. Identifying the best candidates requires sorting the values of the mismatch map and retaining the candidates in the top k ranks. For this, an efficient sorting algorithm is needed. The operation of finding the k best candidates can be implemented with a partial sort, in which only the elements of interest are sorted, while the other elements remain unordered. This results in two sets: \mathfrak{S}_s with the k smallest elements and \mathfrak{S}_l with the largest elements. The partial sort guarantees that $x \leq y \mid (x, y) \in \mathfrak{S}_s \times \mathfrak{S}_l$. More information about our implementation of this algorithm is available in Appendix A.1. Here, we use a modified vectorized online heap-based partial sort (Appendix A.1). With a complexity of $O(n \cdot \ln(k))$, it is especially suitable for small values of k . Using the cache effect, the current implementation yields results that are close to the search of the best value (the smallest value of the array). The main limitation of standard partial sort implementations is that in the case of equal values, either the first or the last element is sampled. Here, we develop an implementation that can uniformly sample a position among similar values with a single scan of the array. This is important because systematically selecting the same position for the same pattern will reduce the conditional probability density function to a unique sample, thereby biasing the simulation.

353 Due to the intensive memory access by repeatedly scanning large training images, interpreted
354 programming languages, such as MATLAB and Python, are inefficient for a QS
355 implementation and, in particular, for a parallelized implementation. We provide a NUMA-
356 aware (Blagodurov et al., 2010) and flexible C/C++/OpenMP implementation of QS that is
357 highly optimized. Following the denomination of Mariethoz (2010), we use a path-level
358 parallelization with a waiting strategy, which offers a good trade-off between performance and
359 memory requirements. In addition, two node-level parallelization strategies are available: if
360 many training images are used, a first parallelization is performed over the exploration of the
361 training images; then, each FFT of the algorithm is parallelized using natively parallel FFT
362 libraries.

363 The FFTw library (Frigo and Johnson, 2018) provides a flexible and performant architecture-
364 independent framework for computing n -dimensional Fourier transformations. However, an
365 additional speed gain of approximately 20% was measured by using the Intel MKL library (Intel
366 Corporation, 2019) on compatible architectures. We also have a GPU implementation that uses
367 cIFFT for compatibility. Many Fourier transforms are sparse and, therefore, can easily be
368 accelerated in n -dimensional cases with “partial FFT” since Fourier transforms of only zeros
369 result in zeros.

370 **3. Results**

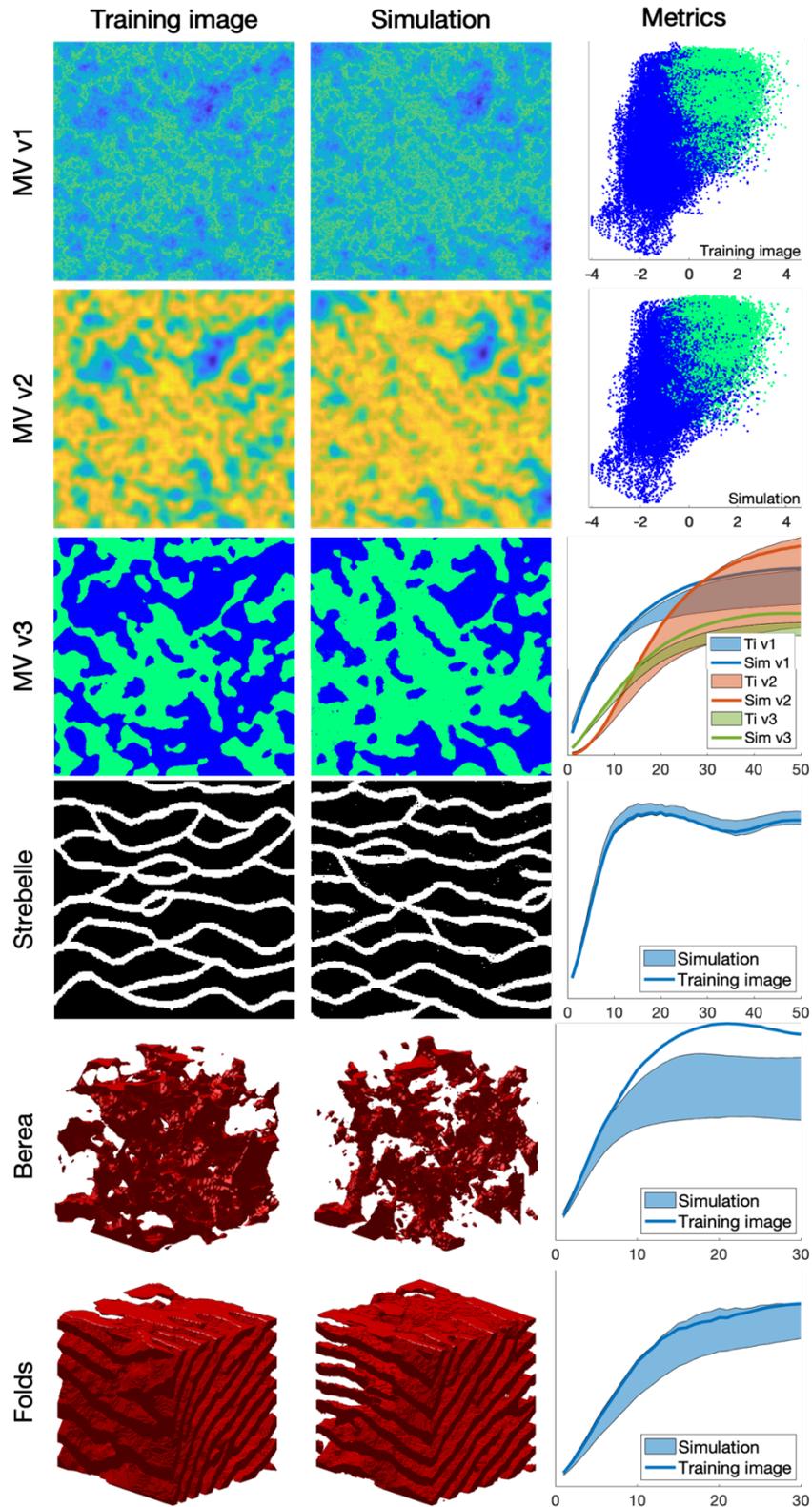
371 **3.1. Simulation examples**

372 This section presents illustrative examples for continuous and categorical case studies in 2D
373 and in 3D. Additional tests are reported in Appendix 0. The parameters that are used for the
374 simulations of Figure 3 are reported in Table 1.

375 The results show that simulation results are consistent with what is typically observed with
376 state-of-the-art MPS algorithms. While simulations can accurately reproduce TI properties for
377 relatively standard examples with repetitive structures (e.g., MV, Strebelle, and Folds), training
378 images with long-range features (typically larger than the size of the TI) are more difficult to
379 reproduce, such as in the Berea example. For multivariate simulations, the reproduction of the
380 joint distribution is satisfactory, as observed in the scatterplots (Figure 3). More examples are
381 available in Annex A4, in particular the Figure A2 for 2D examples and the Figure A3 for 3D
382 examples.

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Figure 3 Examples of unconditional continuous and categorical simulations in 2D and 3D and their variograms. The first column shows the training images that were used, the second column one realization, and the third column quantitative quality metrics. MVs v1, v2 and v3 represent a multivariate training image (and the corresponding simulation) using 3 variables. The first two metrics are scatter plots of MV v1 vs. MV v2 of the training image and the simulation, respectively. The third metric represents the reproduction of the variogram for each of MVs v1, v2 and v3.

	MVs v1, v2, v3	Strebelle	Berea	Folds
Source	(Mariethoz and Caers, 2014)	(Strebelle, 2002)	Doi:10.6084/m9.figshare.1153794	(Mariethoz and Caers, 2014)
Size of the training image (px)	490 × 490	250 × 250	100 × 100 × 100	180 × 150 × 120
Size of the simulation (px)	490 × 490	250 × 250	100 × 100 × 100	180 × 150 × 120
Computation time (s)	1456	54	1665	76270
k	1.2			
N	80		125	

394 *Table 1 Parameters that were used for the simulations in Figure 3. Times are specified for*
395 *simulations without parallelization.*

396 **3.2. Comparison with direct sampling simulations**

397 QS simulations are benchmarked against DS using the “Stone” training image (Figure 4). The
398 settings that are used for DS are based on optimal parameters that were obtained via the
399 approach of Baninajar et al. (2019), which uses stochastic optimization to find optimal
400 parameters. In DS, we use a fraction of scanned TI of $f = 1$ to explore the entire training image
401 via the same approach as in QS and we use the L^2 -norm as in QS. To avoid the occurrence of
402 verbatim copy, we include 0.1% conditioning data, which are randomly sampled from a rotated
403 version of the training image. The number of neighbors N is set to 20 for both DS and QS and
404 the acceptance threshold of DS is set to 0.001.

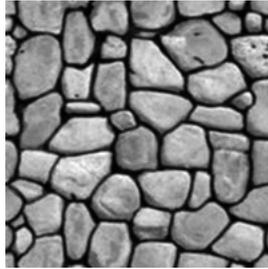
405 The comparison is based on qualitative (Figure 5) and quantitative (Figure 6) metrics, which
406 include directional and omnidirectional variograms, along with the connectivity function, the
407 Euler characteristic (Renard and Allard, 2013) and cumulants (Dimitrakopoulos, 2010). The
408 connectivity represents the probability for 2 random pixels to be in the same connected
409 component. This metric is suited to detect broken structures. The Euler characteristic represents
410 the number of objects subtracted by the number of holes of the objects, and is particularly
411 adapted to detect noise in the simulations such as salt and pepper. Cumulants are high order
412 statistics and therefore allow considering the relative positions between elements. The results
413 demonstrate that the simulations are of a quality that is comparable to DS. With extreme settings
414 (highest pattern reproduction regardless of the computation time), both algorithms perform
415 similarly, which is reasonable since both are based on sequential simulation and both directly
416 import data from the training image. The extra noise present in the simulation is shown in the
417 Euler characteristic. Furthermore, it demonstrates that the use of a kernel can reduce this noise
418 to get better simulations.

419 With QS, kernel weighting allows fine tuning of the parametrization to improve the results, as
420 shown in Figure 5. In this paper, we use an exponential kernel:

421 *Equation 16*

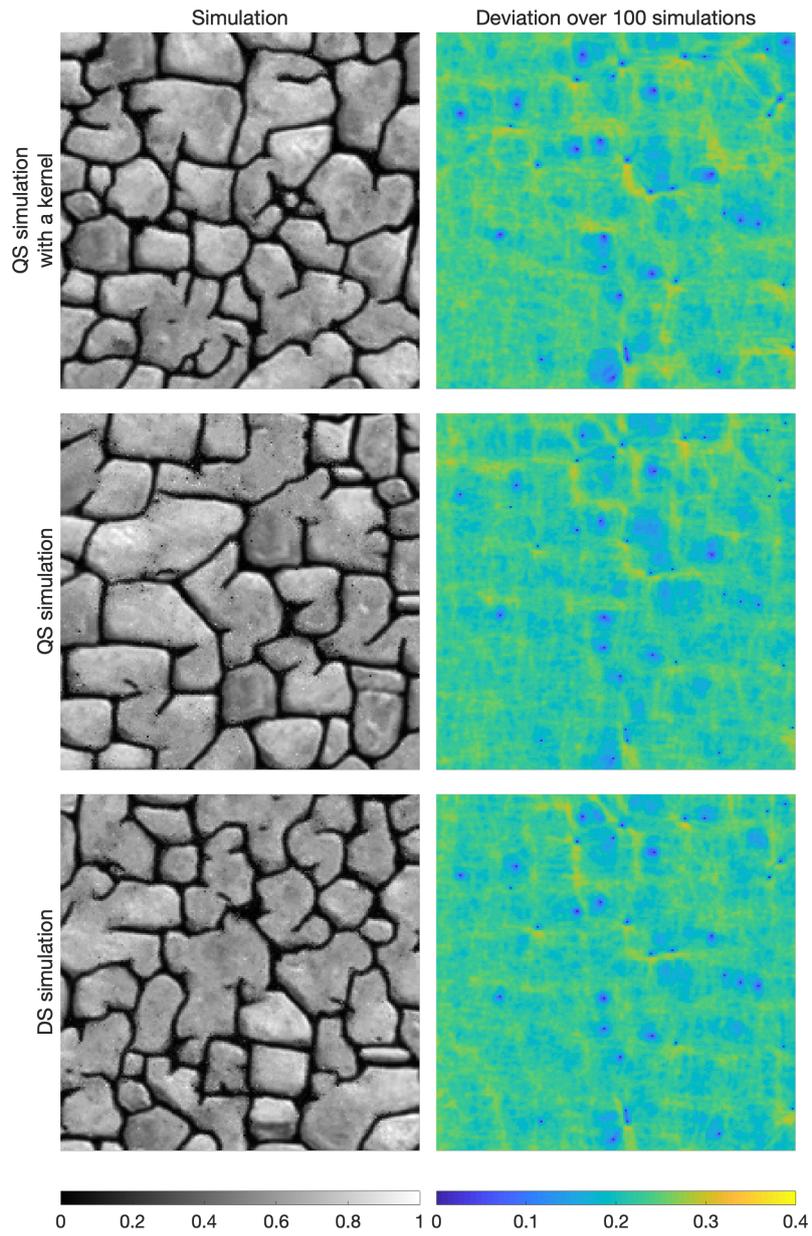
422
$$\omega_l = e^{-\alpha \|l\|_2}$$

423 where α is a kernel parameter and $\|\cdot\|_2$ the Euclidean distance. The validation metrics of Figure
424 6 show that both QS and DS tend to slightly underestimate the variance and the connectivity.
425 Figure 6 shows that an optimal kernel improves the results for all metrics, with all training
426 image metrics in the 5-95% realization interval, except for the Euler characteristic.



427

428 *Figure 4 Training image that was used for benchmarking and sensitivity analysis.*



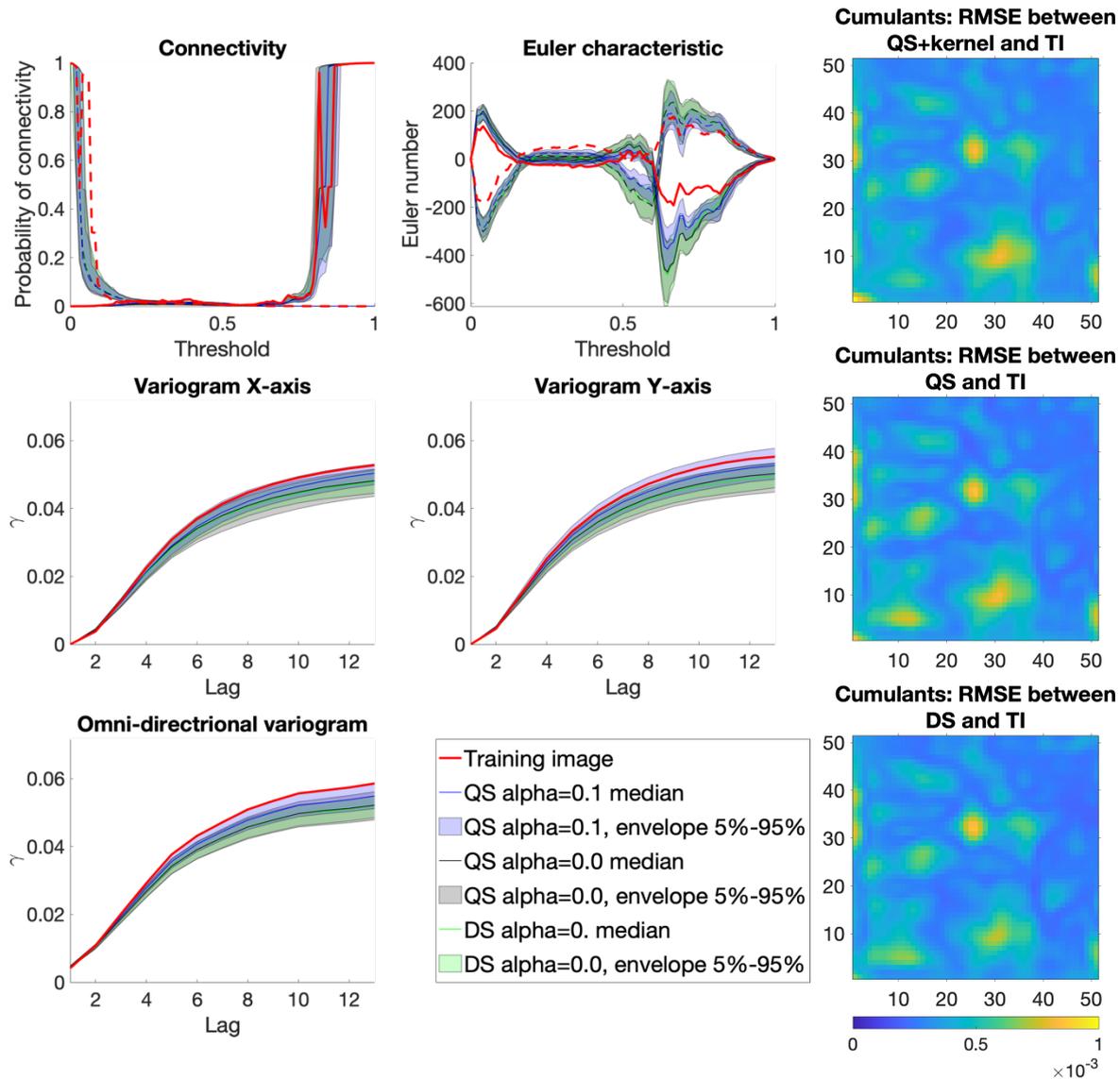
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Figure 5 Examples of conditional simulations and their standard deviation over 100 realizations that are used in the benchmark between QS and DS.



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Figure 6 Benchmark between QS (with and without kernel) and DS over 6 metrics Using each time 100 unconditional simulation.

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3.3. Parameter sensitivity analysis

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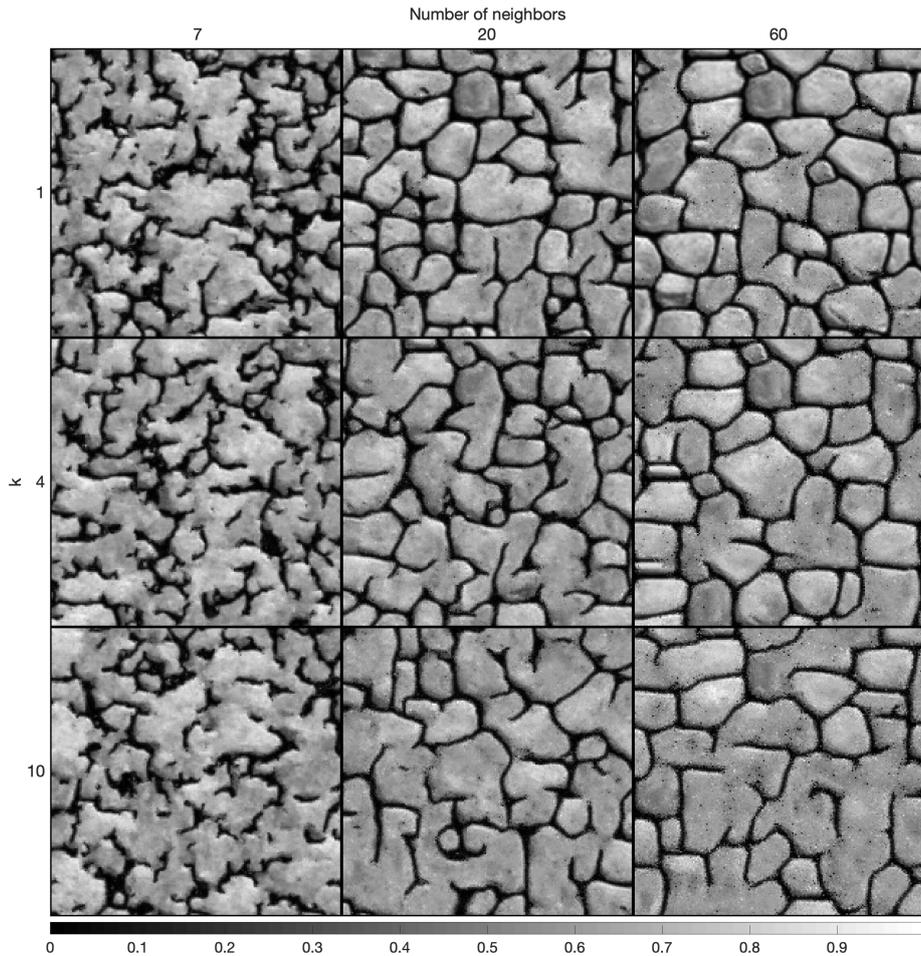
In this section, we perform a sensitivity analysis on the parameters of QS using the training image in Figure 4. Only essential results are reported in this section (Figure 7 and Figure 8); more exhaustive test results are available in Appendix 0 (Figure A 4 and Figure A 5). The two main parameters of QS are the number of neighbors N and the number of used candidates k .

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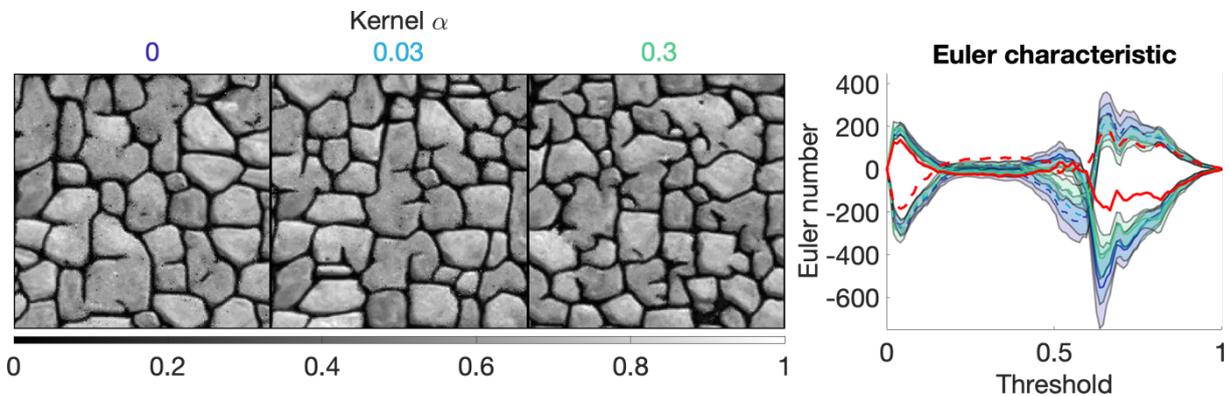
Figure 7 (and Appendix 0 Figure A 4) shows that large N values and small k values improve the simulation performance; however, tend to induce verbatim copy in the simulation. Small values of N result in noise with good reproduction of the histogram.



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Figure 7 Sensitivity analysis on one simulation for the two main parameters of QS using a uniform kernel.

447 ω can be a very powerful tool, typically using the assumption that the closest pixels are more
448 informative than remote pixels. The sensitivity analysis of the kernel value α are explored in
449 Figure 8 and Figure A 5. They show that α provides a unique tool for improving the simulation
450 quality. In particular, using a kernel can reduce the noise in simulations, which is clearly visible
451 by comparing the Euler characteristic curves. However, reducing too much the importance of
452 distant pixels results in ignoring them altogether, therefore damaging long-range structures.



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Figure 8 Sensitivity analysis on the kernel parameter α , with fixed parameters $k=1.5$ and $N=40$. The values of the kernels are shown in colors that correspond to the Euler characteristic lines (red is the training image).

457

3.4. Computational efficiency and scalability

458 In this section, we investigate the scalability of QS with respect to the size of the simulation
 459 grid, the size of the training image grid, the number of variables, incomplete training images,
 460 and hardware. According to the test results, the code will continue to scale with new-generation
 461 hardware.

462 As explained in Section 2.3 and 2.4, the amounts of time that are consumed by the two main
 463 operations of QS (finding candidates and sorting them) are independent of the pixel values.
 464 Therefore, the training image that is used is not relevant (here, we use simulations that were
 465 performed with the TI of Figure 4 and its classified version for categorical cases). Furthermore,
 466 the computation time is independent of the parametrization (k and N). However, the
 467 performance is affected by the type of mismatch function that is used; here, we consider both
 468 continuous (Equation 2 and Equation 14) and categorical cases (Equation 3 and Equation 15).

469 We also test our implementation on different types of hardware, as summarized in Table 2. We
 470 expect Machine (2) to be faster than Machine (1) for medium-sized problems due to the high
 471 memory bandwidth requirement of QS. Machine (3) should also be faster than Machine (1)
 472 because it takes advantage of a longer vector computation (512-bit VS. 256-bit instruction set).

Name of the machine	Machine (1)	Machine (2)	Machine (3)
CPU	-2x Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80 GHz	-Xeon Phi, Intel(R) Xeon Phi (TM) CPU 7210 @ 1.30 GHz	-2x Intel(R) Xeon(R) Gold 6128 Processor @ 3.40 GHz
Memory type	- DDR3	- MCDRAM / DDR4	- DDR4
OS, compiler and compilation flags	Linux, Intel C/C++ compiler 2018 with -xhost		

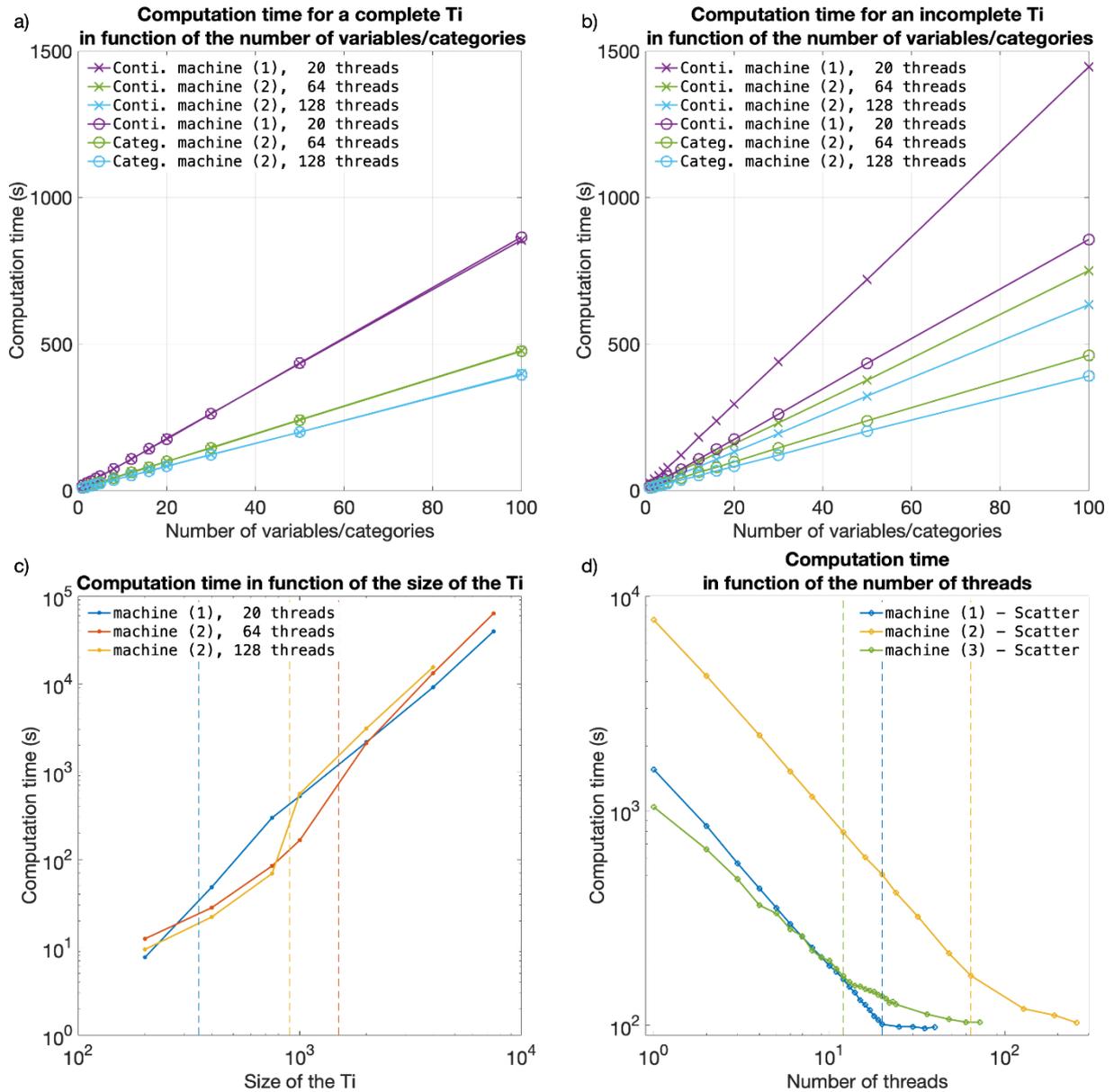
473

Table 2 Hardware that was used in the experiments

474 Figure 9 plots the execution times on the 3 tested machines for continuous and categorical cases
 475 and with training images of various sizes. Since QS has a predictable execution time, the
 476 influence of the parameters on the computation time is predictable: linear with respect to the
 477 number of variables (Figure 9a, Figure 9b), linear with respect to the size of the simulation grid
 478 and following a power function of the size of the training image (Figure 9c). Therefore, via a
 479 few tests on a set of simulations, one can predict the computation time for any other setting.

480 Figure 9d shows the scalability of the algorithm when using the path-level parallelization. The
 481 algorithm scales well until all physical cores are being used. Machine (3) has a different scaling
 482 factor (slope). This suboptimal scaling is attributed to the limited memory bandwidth. Our
 483 implementation of QS scales well with an increasing number of threads (Figure 9d), with an
 484 efficiency above 80% using all possible threads. The path-level parallelization strategy that was
 485 used involves a bottleneck for large number of threads due to the need to wait for neighborhood
 486 conflicts to be resolved (Mariethoz 2010). This effect typically appears for large values of N or

487 intense parallelization (>50 threads) on small grids. It is assumed that small grids do not require
 488 intense parallelization; hence, this problem is irrelevant in most applications.



489
 490 *Figure 9 Efficiency of QS with respect to all key parameters. a) and b) are the evolution of the*
 491 *computation time for complete and incomplete training images, respectively, with continuous*
 492 *and categorical variables. c) shows the evolution of the computation time as the size of the*
 493 *training image is varied; the dashed lines indicate that the training image no longer fits in the*
 494 *CPU cache. d) shows the evolution of the computation time as the number of threads is*
 495 *increased. The dashed lines indicate that all physical cores are used.*

496

497 4. Discussion

498 The parameterization of the algorithm (and therefore simulation quality) has almost no impact
 499 on the computational cost, which is an advantage. Indeed, many MPS algorithms impose trade-

500 offs between the computation time and the parameters that control the simulation quality,
501 thereby imposing difficult choices for users. QS is comparatively simpler to set up in this
502 regard. In practice, a satisfactory parameterization strategy is often to start with a small k value
503 (say 1.2) and a large N value (> 50) and then gradually change these values to increase the
504 variability if necessary (Figure 6 and Figure A 4).

505 QS is adapted for simulating continuous variables using the L^2 -norm. However, a limitation is
506 that the L^1 -norm does not have a decomposition that satisfies Equation 1 and, therefore, cannot
507 be used with QS. Another limitation is that for categorical variables, each class requires a
508 separate FFT, which incurs an additional computational cost. This renders QS less
509 computationally efficient for categorical variables (if there are more than 2 categories) than for
510 continuous variables. For accelerated simulation of categorical variables, a possible alternative
511 to reduce the number of required operations is presented in Appendix A.2. The strategy is to
512 use encoded variables, which are decoded in the mismatch map. While this alternative yields
513 significant computational gains, it does not allow the use of a kernel weighting and is prone to
514 numerical precision issues.

515 Combining multiple continuous and categorical variables can be challenging for MPS
516 approaches. Several strategies have been developed to overcome this limitation, using either a
517 different distance threshold for each variable, or a linear combination of the errors. Here we use
518 the second approach, taking advantage of the linearity of the Fourier transform. The relative
519 importance can be set in f_i and g_i functions in Equation 1. However, it is computationally
520 advantageous to use the kernel weights in order to have standard functions for each metric.
521 Setting such variable-dependent parameters is complex. Therefore in order to find optimal
522 parameters, stochastic optimization approaches (such as Baninajar et al., 2019) are applied to
523 QS. The computational efficiency of QS is generally advantageous compared to other pixel-
524 based algorithms: for example, in our tests it performed faster than DS. QS requires more
525 memory than DS, especially for applications with categorical variables with many classes and
526 with a path-level parallelization. However, the memory requirement is much lower compared
527 to MPS algorithms that are based on a pattern database, such as SNESIM.

528 There may be cases where QS slower than DS, in particular when using a large training image
529 that is highly repetitive. In such cases, using DS can be advantageous as it must scan only a
530 very small part of the training image. For scenarios of this type, it is possible to adapt QS such
531 that only a small subset of the training image is used; this approach is described in Appendix
532 A3. In the cases of highly repetitive training images, this observation remains true also for
533 SNESIM and IMPALA.

534 Furthermore, QS is designed to efficiently handle large and complex training images (up to 10
535 million pixels), with high variability of patterns and few repetitions. Larger training images
536 may be computationally burdensome, which could be alleviated by using a GPUs
537 implementation allowing gains up to two orders of magnitude.

538 QS can be extended to handle the rotation and scaling of patterns by applying a constant rotation
539 or affinity transformation to the searched patterns (Strebelle, 2002). However, the use rotation-
540 invariant distances and affinity-invariant distances (as in Mariethoz and Kelly, 2011), while
541 possible in theory, would substantially increase the computation time. Mean-invariant distances

542 can be implemented by simply adapting the distance formulation in QS. All these advanced
543 features are outside the scope of this paper.

544 **5. Conclusions**

545 QS is an alternative approach for performing n -dimensional pixel-based simulations, which
546 uses an L^2 -distance for continuous cases and an L^0 -distance for categorical data. The framework
547 is highly flexible and allows other metrics to be used. The simple parameterization of QS
548 renders it easy to use for nonexpert users. Compared to other pixel-based approaches, QS has
549 the advantage of generating realizations in constant and predictable time for a specified training
550 image size. Using the quantile as a quality criterion naturally reduces the small-scale noise
551 compared to DS. In terms of parallelization, the QS code scales well and can adapt to new
552 architectures due to the use of external highly optimized libraries.

553 The QS framework provides a complete and explicit mismatch map, which can be used to
554 formulate problem-specific rules for sampling or even solutions that take the complete
555 conditional probability density function into account, for example, such as a narrowness
556 criterion for the conditional pdf of the simulated value (Gravey et al., 2019; Rasera et al., 2019),
557 or to use the mismatch map to infer the optimal parameters of the algorithm.

558 **6. Code availability**

559 The source code and documentation of the QS simulation algorithm are available as part of the
560 G2S package at: <https://github.com/GAIA-UNIL/G2S> under GPLv3 license. Or permanently
561 at <https://doi.org/10.5281/zenodo.3546338>

562 Platform: Linux / macOS / Windows 10 Language: C/C++

563 Interfacing functions in MATLAB, Python3, R

564 A package is available with our unbiased partial sort at:
565 <https://github.com/mgravey/randomKmin-max>

566 **7. Author contribution**

567 MG proposed the idea, implemented and optimized the QS approach and wrote the manuscript.
568 GM provided supervision, methodological insights and contributed to the writing of the
569 manuscript.

570 8. Appendices

571 A.1. Partial sorting with random sampling

572 Standard partial sorting algorithms resolve tie ranks deterministically, which does not accord
573 with the objective of stochastic simulation with QS, where variability is sought. Here, we
574 propose an online heap-based partial sort. It is realized with a single scan of the array of data
575 using a heap to store previously found values. This approach is especially suitable when we are
576 interested in a small fraction of the entire array.

577 Random positions of the k best values are ensured by swapping similar values. If $k = 1$, the
578 saved value is switched with a smaller value each time it is encountered. If an equal value is
579 scanned, a counter c is increased for this specific value and a probability of $1/c$ of switching to
580 the new position is applied. If $k > 1$, the same strategy is extended by carrying over the counter
581 c .

582 This partial sort outperforms random exploration of the mismatch map. However, it is difficult
583 to implement efficiently on GPUs. A solution is still possible for shared-memory GPUs by
584 performing the partial sort on the CPU. This is currently available in the proposed
585 implementation.

586 k : the number of values of interest

587 D : the input data array

588 S : the array with the k smallest values (sorted)

589 Sp : the array with the positions that are associated with the values of S

590

591 1. **for** each value v of D

592 2. **if** v is smaller than the smallest value of S

593 3. search in S for the position p at which to insert v and insert it

594 4. **if** $p = k$ // last position of the array

595 5. reinitialize the counter c to 0

596 6. insert v at the last position

597 7. **else**

598 8. increment c by one

599 9. swap the last position with another of the same value

600 10. insert the value at the expected position p

601 11. **end**

602 12. **else if** v is equal to the smallest value of S

603 13. increment c by one

604 14. change the position of v to one of the n positions of equal value with a probability of
605 $n/(n + c)$

606 15. **end**

607 16. **end**

608 **A.2. Encoded categorical variables**

609 To handle categorical variables, a standard approach is to consider each category as an
 610 independent variable. This requires as many FFTs as classes. This solution renders it expensive
 611 to use QS in cases with multiple categories.

612 An alternative approach is to encode the categories and to decode the mismatch from the cross-
 613 correlation. It has the advantage of only requiring only a single cross-correlation for each
 614 simulated pattern.

615 Here, we propose encoding the categories as powers of the number of neighbors, such that their
 616 product is equal to one if the class matches. In all other cases, the value is smaller than one or
 617 larger than the number of neighbors.

618
$$\varepsilon_{L^0}(a, b) = \psi((a - b)^0 \propto -(N + 1)^{-p(a)} \cdot (N + 1)^{-p(b)})$$

619 where N is the largest number of neighbors that can be considered and $p(c)$ is an arbitrary
 620 function that maps index classes of \mathcal{C} , $c \in \mathcal{C}$.

621 In this scenario, in Equation 1 this encoded distance L_e^0 can be decomposed into the following
 622 series of functions f_j and g_j :

623 $f_0: x \rightarrow -(N + 1)^{p(x)}$

624 $g_0: x \rightarrow (N + 1)^{-p(x)}$

625 and the decoding function is

626
$$\psi(x) = \lfloor x \rfloor \bmod N$$

627 Table A 1 describes this process for 3 classes, namely, a, b , and c , and a maximum of 9
 628 neighbors. Then, the error can be easily decoded by removing decimals and dozens.

Products	$g_0(a) = 1$	$g_0(b) = 0.1$	$g_0(c) = 0.01$
$f_0(a) = 1$	1	0.1	0.01
$f_0(b) = 10$	10	1	0.1
$f_0(c) = 100$	100	10	1

629 *Table A 1 Example of encoding for 3 classes and 9 neighbors and their associated products*

630 Consider the following combination:

631 $f_0(a, b, a, c, c, b, a, a, b)$

632 $\times g_0(c, b, b, a, a, b, c, a, a)$

633 $-(0.01, 1, 0.1, 100, 100, 1, 0.01, 1, 10) = -213.12$

634 The decoding $\lfloor -213.12 \rfloor \bmod 10 = -213 \bmod 10 = -3$ yields 3 matches (in green).

635 This encoding strategy provides the possibility of drastically reducing the number of FFT
636 computations. However, the decoding phase is not always implementable if a nonuniform
637 matrix ω is used. Finally, the test results show that the method suffers quickly from numerical
638 precision issues, especially with many classes.

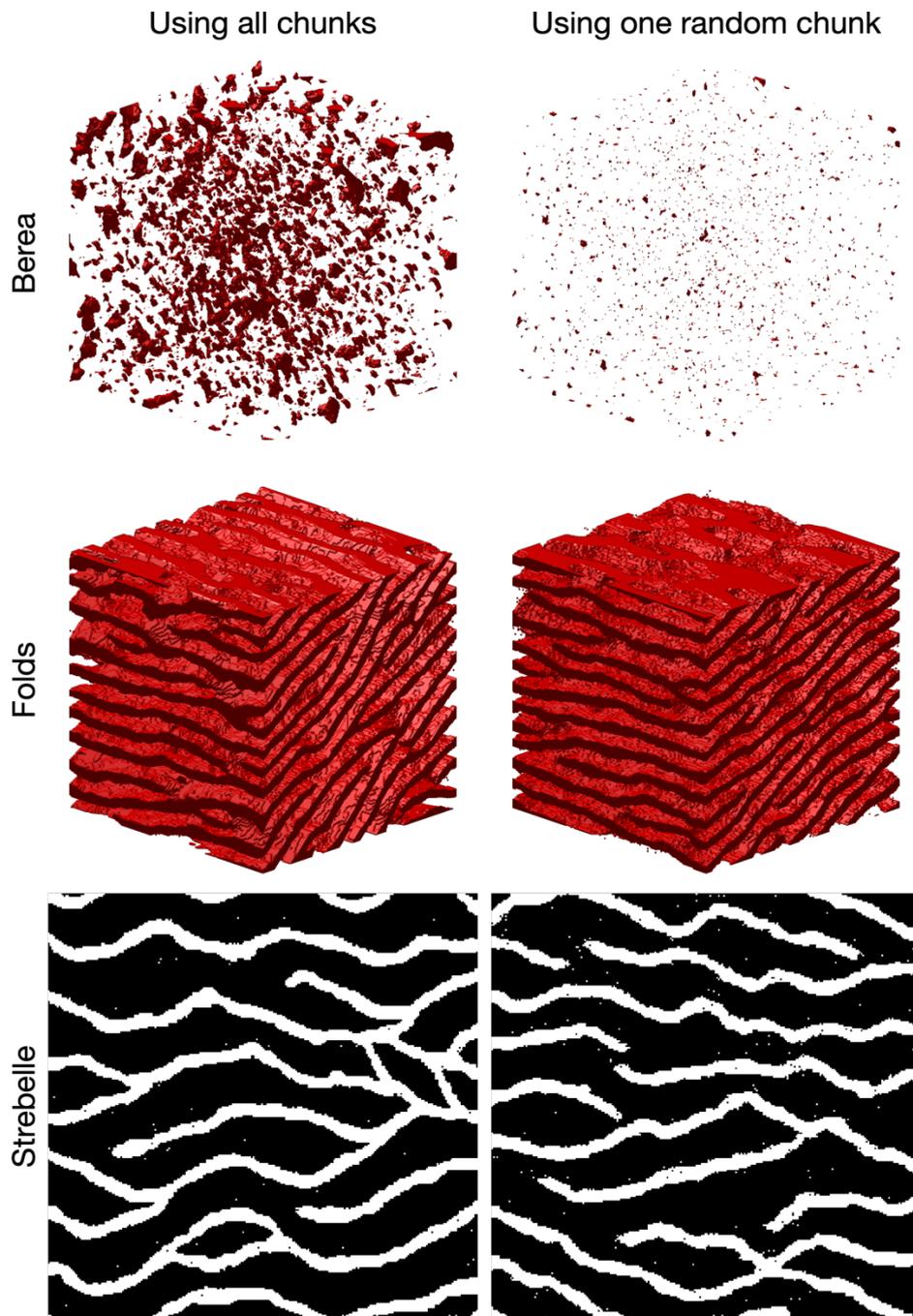
639 **A.3. Sampling strategy using training image splitting**

640 The principle of considering a fixed number of candidates can be extended by instead of taking
641 the k^{th} best candidate, sampling the best candidate in only a portion $\frac{1}{k}$, of the TI. For instance,
642 as an alternative to considering $k = 4$, this strategy searches for the best candidate in one fourth
643 of the image. This is more computationally efficient. However, if all the considered candidates
644 are contiguous (by splitting the TI in k chunks), this approximation is only valid if the TI is
645 completely stationary and all k equal subdivisions of the TI are statistically identical. In
646 practice, real-world continuous variables are often nonstationary. However, in categorical
647 cases, especially in binary ones, the number of pattern replicates is higher and this sampling
648 strategy could be interesting.

649 The results of applying this strategy are presented in Table A 2 and Figure A 1. The
650 experimental results demonstrate that the partial exploration approach that is provided by
651 splitting substantially accelerates the processing time. However, Figure A 1 shows that the
652 approach has clear limitations when dealing with training images with complex and

653 nonrepetitive patterns. The absence of local verbatim copy can explain the poor-quality
654 simulation results.

655



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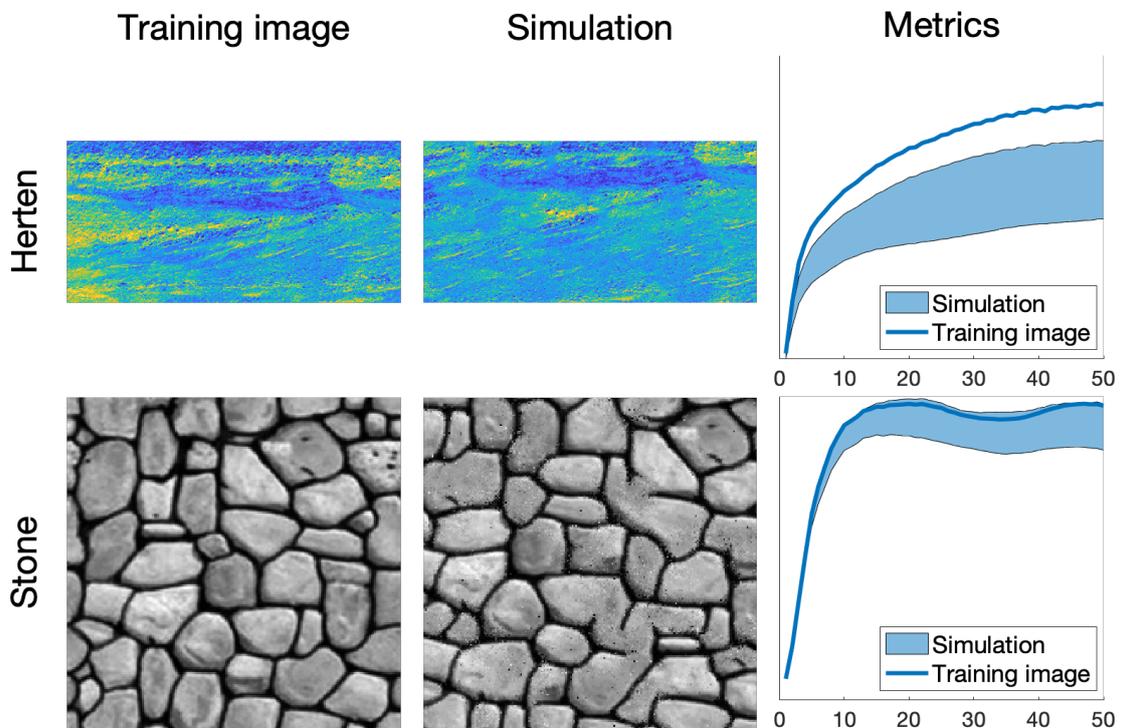
657 *Figure A 1 Comparison of QS using the entire training image and using training image*
658 *splitting. In these examples, the training image is split into two images over each dimension.*
659 *The original training images are presented in Figure 2.*

660

Training image	Using all chunks	Using one random chunk	Speedup
Berea	11 052 s	1 452 s	7.61x
Folds	35 211 s	4 063 s	8.66x
Strebelle	7.95 s	3.16 s	2.51x

661 *Table A 2 Computation times and speedups for the full and partial exploration approaches.*
662 *Times are specified for simulations with path level parallelization.*

663 **A.4. Additional results**

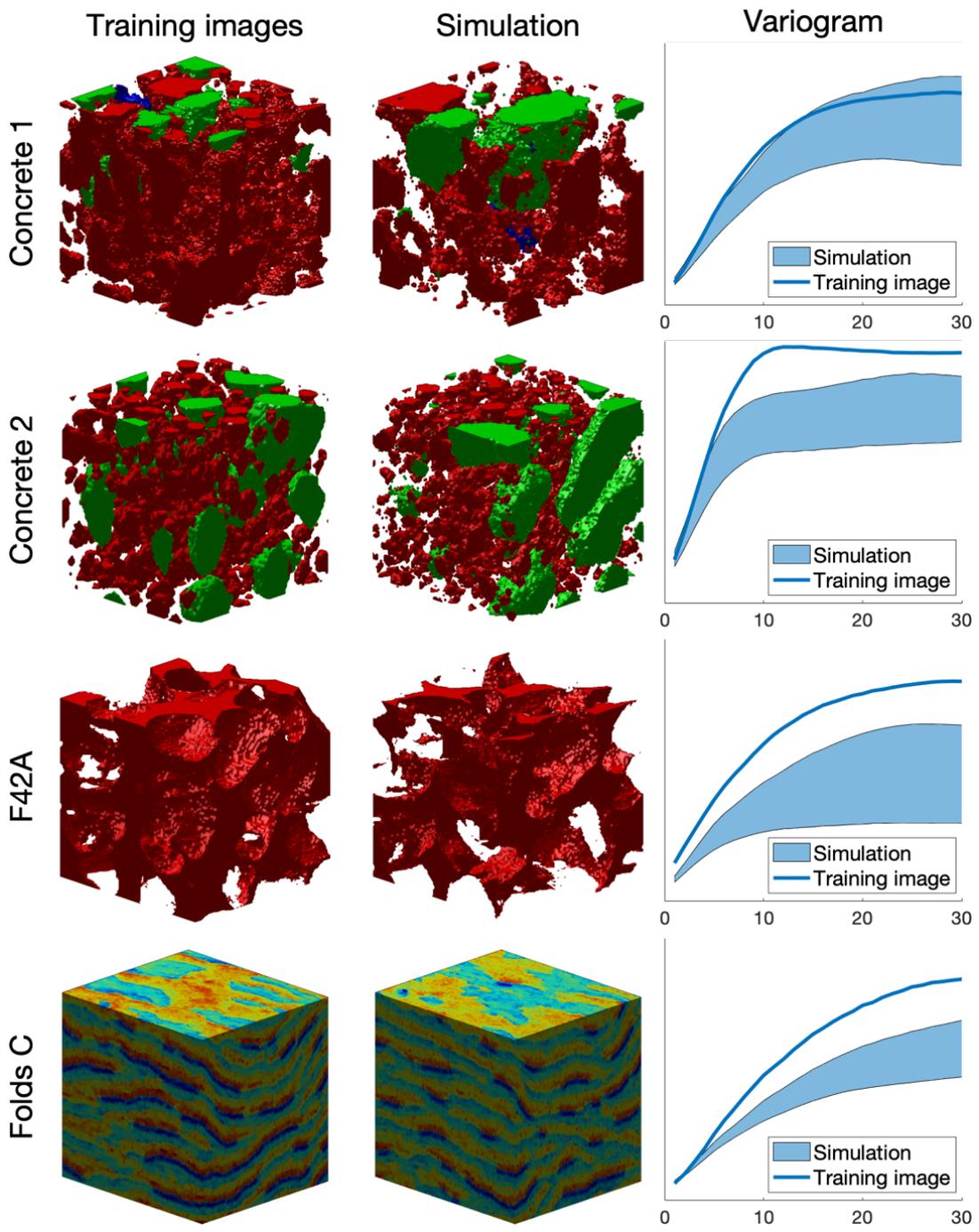


664 *Figure A 2 Examples of 2D simulations: the first 3 rows represent 3 variables of a single*
665 *simulation. Parameters available in Table A 3*
666

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Figure A 3 Examples of 3D simulation results. Parameters available in Table A 4

	Herten	Stone
Source	(Mariethoz and Caers, 2014)	(Mariethoz and Caers, 2014)
Size of the training image (px)	716 × 350	200 × 200
Size of the Simulation (px)	716 × 350	200 × 200
Computation time (s)	1133	21
k	1.2	
N	80	

672
673

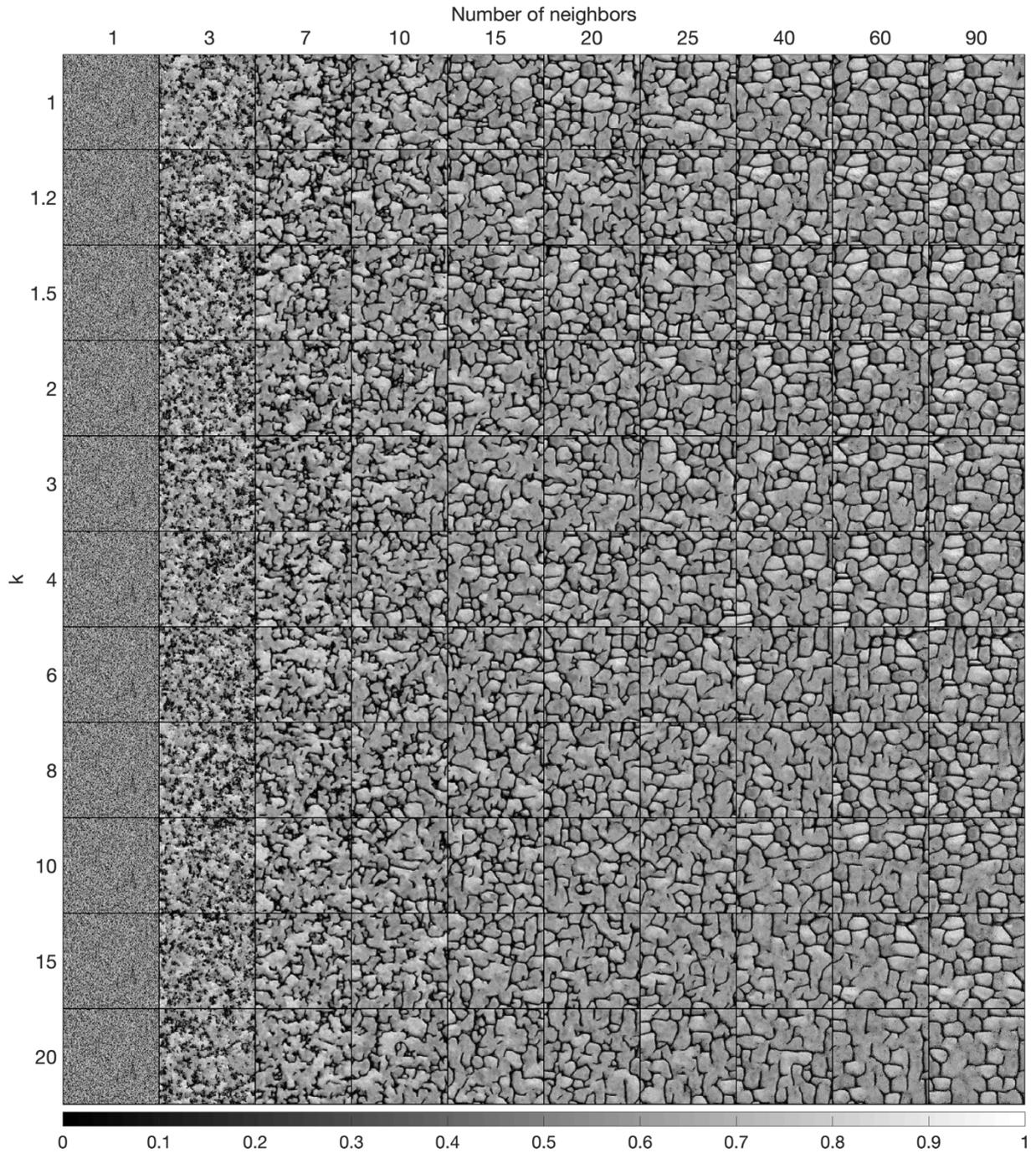
Table A 3 Simulation parameters for Figure A 2. Times are specified for simulations without parallelization.

674

	Concrete 1	Concrete 2	F42A	Folds continues
Source	(Meerschman et al., 2013)	(Meerschman et al., 2013)	Doi:10.6084/m9.fig share.1189259	(Mariethoz and Caers, 2014)
Size of the training image (px)	150 × 150 × 150	100 × 90 × 80	100 × 100 × 100	180 × 150 × 120
Size of the simulation (px)	100 × 100 × 100	100 × 100 × 100	100 × 100 × 100	180 × 150 × 120
Computation time (s)	11436	1416	1638	7637
k	1.2			
N	50		125	

675
676

Table A 4 Simulation parameters for Figure A 3. Times are specified for simulations without parallelization.

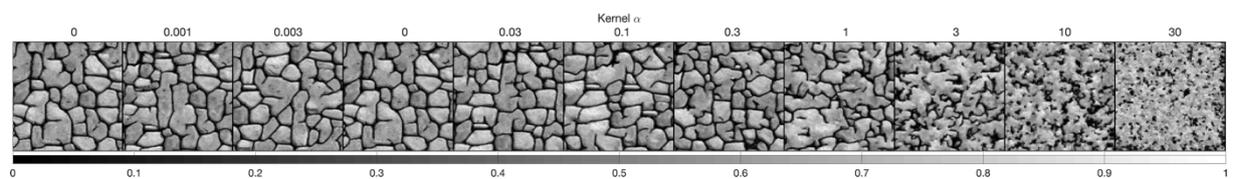


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Figure A 4 Complete sensitivity analysis, with one simulation for the two main parameters of QS.



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Figure A 5 Complete sensitivity analysis, with one simulation for each kernel with $k=1.5$ and $N=40$

683 **A.5. Mathematical derivation**

684 The convolution theorem (Stockham, 1966; Krant, 1999; Li et al., 2019) can be easily extended
685 to cross-correlation (Bracewell, 2000). The following derivation shows the validity of the theorem
686 for any function f and g .

$$\begin{aligned} 687 \quad \mathcal{F}\{f \star g\} &= \int (f \star g)(t) e^{it \cdot \xi} dt = \int \int \overline{f(s)} g(s+t) ds e^{it \cdot \xi} dt \\ 688 \quad &= \int \int \overline{f(s)} e^{i(-s) \cdot \xi} ds \cdot g(s+t) ds e^{i(t+s) \cdot \xi} dt \\ 689 \quad &= \int \int \overline{f(s)} e^{i(s) \cdot \xi} ds \cdot g(s+t) ds e^{i(t+s) \cdot \xi} dt = \overline{\mathcal{F}\{f\}} \cdot \mathcal{F}\{g\} \end{aligned}$$

690 The discretization of this property can be obtained using two piecewise continuous functions
691 associated to each discrete representation.

692 **9. Acknowledgments**

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697 optimization method, which improved the reliability of the benchmarks; and to all the early
698 users of QS for their useful feedback and their patience in waiting for this manuscript. A
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700 the paper and provided constructive comments which significantly improved the quality of the
701 paper.

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