GEOSTATISTICS TRÓIA '92

Volume 1

Edited by

AMILCAR SOARES

Centro de Valarizacao de Recursos Minerais,
Instituto Superior Técnico,
Lisbon, Portugal

Kluwer Academic Publishers

Dordrecht / Boston / London

SIMULATION OF RANDOM FUNCTIONS ON LARGE LATTICES

Henning Omre, Knut Sølna and Håkon Tjelmeland

Norwegian Computing Center
P.O.Box 114, Blindern
N-0314 Oslo
Norway

Abstract. Random functions are in frequent use in applications of spatial statistics. Gaussian and Gaussian intrinsic random functions are differentiated, and the screening sequential algorithm for generating realizations from them are defined. The algorithm is based on the general sequential algorithm and Markov properties for random functions. For exponential and linear variogram functions the algorithm is shown to be exact for the one-dimensional case, while empirical evaluations show that it is highly reliable also in two-dimensional cases. For fractal random functions, the screening sequential algorithm is significally more reliable than the frequently used random midpoint displacement and successive random addition algorithms. The processing requirements for the algorithm is independent of the actual variogram function and linear in number of lattice nodes — both favorable characteristics.

1 Introduction

Stochastic models are in frequent use for describing physical phenomena. In applications like geology, meteorology and pollution monitoring, spatial or spatial/temporal models must be used. Gaussian and fractal random functions have proven to be useful models. The questions being posed concerning these phenomena are usually so complex that one has to rely on stochastic simulation techniques for addressing them. The representation of these phenomena are normally on lattices in higher dimensions, lattices with up to 10^8 nodes. Hence one has to be able to generate reliable realizations of Gaussian and fractal random functions on extremely large lattices. This article addresses this problem.

The size of the lattice, and hence the dimension of the multivariate equivalent, excludes the straight forward approach of simulation from the corresponding multi-Gaussian distribution. Several other procedures for simulation have been suggested. Important references are: Matern (1963), Journel (1974), Borgman et al. (1984), Barnsley at al. (1988), Journel and Alabert (1988).

The current article concerns simulation from a stochastic model without conditioning on observations in particular locations, since the objective is to evaluate the reliability of the algorithm for reproducing a given spatial dependence structure. Moreover, the comparison with the familiar simulation algorithms for fractal random functions should be done unconditionally since the latter is defined for this case only. Extensions to the conditional case can be done by sacrificing some processing efficiency. In applications with few observations, like petroleum reservoir description for example, a two stage approach to conditioning as defined in Journel and Huijbregts (1978) can be very efficient also.

In this article the screening sequential algorithm for simulating random functions is defined and evaluated. It is based on the general sequential algorithm and Markov properties of random functions, see Ripley (1987) and Adler (1981). In spatial dimension two and higher, one has to rely on approximative exact algorithms to obtain sufficient processing efficiency. Accepting an approximation makes it even more complicated and important to: provide an intuitive justification; evaluate the properties empirically; and to constrain the class of models for which the approximation is valid. This seems often to be forgotten.

The authors do not claim that the spatially defined screening sequential algorithm is completely new, although no published work defining exactly the same algorithm has been found. Algorithms of the same flavor are numerous, however, and it is not wise to claim novelty in an area where so much trial and error has been made. The objective of the article is, however, to present a thorough justification for an algorithm we have found very reliable and processing efficient, for a relatively large class of spatial dependence structures. The class includes fractal random functions and a comparison with familiar algorithms for simulating them are done.

2 Model definition and properties

Consider a random function,

$$\{\mathcal{Z}(x)\,; x \in \mathcal{D}\}$$

with $\mathcal{Z}(\cdot)$ being a random variable with realization $z(\cdot) \in \mathcal{R}^1$; and x being a reference location in the bounded domain $D \subset \mathcal{R}^m$, with $m = 1, 2, 3$ in this study.

2.1 Model classes

Two classes of random variables will be considered:

- Gaussian random functions - defined by $\sum_{i=1}^{n} \eta_i \mathcal{Z}(x_i)$ being Gaussian for all $\{\eta_1, \eta_2, \ldots, \eta_n\}$; all location configurations $(x_1, x_2, \ldots x_n) \in \mathcal{D}$; and all integer values of n. The special case $\sum_{i=1}^{n} \eta_i = 0$ is included since constants are considered as degenerate cases of Gaussian distributions, see Mardia et al.(1979). The

Gaussian random function being considered here are stationary, homogeneous and isotropic, with,

$$\begin{aligned} E\{\mathcal{Z}(x)\} &= 0.0 \\ \mathrm{Var}\{\mathcal{Z}(x)\} &= \sigma^2 \\ \mathrm{Cov}\{\mathcal{Z}(x'), \mathcal{Z}(x'')\} &= \sigma^2 \rho(|x' - x''|) \\ \mathrm{Var}\{\mathcal{Z}(x') - \mathcal{Z}(x'')\} &= 2\sigma^2 \gamma_0(|x' - x''|) \\ &= 2\sigma^2[1 - \rho(|x' - x''|)] \end{aligned}$$

and $\rho(\cdot)$ being the correlation function; and $\gamma(\cdot)$ being the variogram function. A valid model require the correlation function, $\rho(\cdot)$, to be non-negative definite ensuring non-negative variances for all linear combinations of random variables. Consequently, $\rho(\Delta)$ has to be bounded and symmetrical around $\Delta = 0$.

- Gaussian intrinsic random functions - defined by $\sum_{i=1}^{n} \eta_i \mathcal{Z}(x_i)$ being Gaussian for $\sum_{i=1}^{n} \eta_i = 0$; for all location configurations $(x_1, x_2, \ldots, x_n) \in \mathcal{D}$; and all integer values of n. This corresponds to the IRF-0 definition in Delfiner (1979) extended by assuming Gaussianity. The Gaussian intrinsic class is larger than, and includes, the Gaussian class, since the former requires Gaussianity for a smaller set of weights $\{\eta_1, \eta_2, \ldots, \eta_n\}$ which is included in the requirement for the latter. In particular, the univariate characteristics need not be Gaussian. In this study, the term Gaussian intrinsic random function will be used for functions in the intrinsic class not being Gaussian random functions.

  The Gaussian intrinsic random functions being considered here are stationary, homogeneous and isotropic, with:

$$\begin{aligned} E\{\mathcal{Z}(x)\} &= 0.0 \\ \mathrm{Var}\{\mathcal{Z}(x') - \mathcal{Z}(x'')\} &= 2 \cdot \gamma(|x' - x''|) \end{aligned}$$

  A valid model require the negative variogram function, $-\gamma(\cdot)$, to be conditional non-negative definite, ensuring non-negative variances for all linear combinations of random variables with weights adding to zero. A consequence of this is that $\gamma(\cdot)$ need not be bounded and hence the univariate variance need not be finite.

2.2 Model characteristics

The following characteristics are relevant for the study:

- Conditional random variables - defined for an unobserved arbitrary location $x_0 \in \mathcal{D}$ given observations in n arbitrary locations $(x_1, x_2, \ldots x_n) \in \mathcal{D}$. For both the Gaussian and Gaussian intrinsic random functions, the conditional distributions will be Gaussian,

$$\mathcal{Z}(x_0)|\mathcal{Z}(x_1) = z_1, \ldots, \mathcal{Z}(x_n) = z_n \rightsquigarrow \mathcal{N}(\mu_{0|1,\ldots,n}, \sigma^2_{0|1,\ldots,n})$$

with $\mathcal{N}(\mu, \sigma^2)$ indicating a Gaussian distribution with:

$$\begin{aligned} \mu_{0|1,\ldots,n} &= E\{\mathcal{Z}(x_0)|\mathcal{Z}(x_1) = z_1, \ldots, \mathcal{Z}(x_n) = z_n\} \\ \sigma^2_{0|1,\ldots,n} &= \mathrm{Var}\{\mathcal{Z}(x_0)|\mathcal{Z}(x_1) = z_1, \ldots, \mathcal{Z}(x_n) = z_n\} \end{aligned}$$

The parameters, $(\mu_\cdot, \sigma_\cdot)$, are determined differently under the two models, however. For Gaussian random functions the parameters are:

$$\begin{aligned} \mu_{0|1,\ldots,n} &= \underline{\psi}_{0n}^T \Psi^{-1} \underline{z} \\ \sigma^2_{0|1,\ldots,n} &= \sigma^2 - \underline{\psi}_{0n}^T \Psi^{-1} \underline{\psi}_{0n} \end{aligned}$$

with $\underline{\psi}_{0n}$ being $1 \times n$ -dimensional with elements $\sigma^2\rho(|x_0 - x_i|); i = 1, \ldots, n$; Ψ being $n \times n$-dimensional with elements $\sigma^2\rho(|x_i - x_j|); i, j = 1, \ldots, n$; and $\underline{z}$ being $1 \times n$-dimensional with elements $z_i; i = 1, \ldots, n$. This corresponds to the simple kriging predictor and prediction variance, see Journel and Huijbregts (1978). For Gaussian intrinsic random functions the parameters are:

$$\begin{aligned} \mu_{0|1,\ldots,n} &= \underline{\gamma}_{0n}^T \Gamma^{-1} \underline{z}^+ \\ \sigma^2_{0|1,\ldots,n} &= \underline{\gamma}_{0n}^T \Gamma^{-1} \underline{\gamma}_{0n} \end{aligned}$$

with $\underline{\gamma}_{0n}$ being $1 \times (n+1)$ -dimensional with elements $-\gamma(|x_0 - x_i|); i = 1, \ldots, n$ plus 1 in last row; Γ^{-1} being $(n+1) \times (n+1)$-dimensional with elements $-\gamma(|x_i - x_j|); i, j = 1, \ldots, n$ plus 1's in last column and row except for element $((n+1), (n+1))$ being equal to 0 ; and $\underline{z}^+$ being $1 \times (n+1)$ - dimensional with elements $z_i; i = 1, \ldots, n$ plus 0 in last row. This corresponds to the ordinary kriging predictor and prediction variance, see Journel and Huijbregts (1978).

- General simulation algorithm - defined on a lattice of nodes covering $\mathcal{D}$. Denote the set of lattice node locations $\mathcal{L}_D$, the number of nodes $\mathcal{N}_D = \#\mathcal{L}_D$: and hence the countable set of random variables representing the random function:

$$\{\mathcal{Z}(x);\ x \in \mathcal{L}_D\}$$

This can be seen as a multivariate random variable. Consider an arbitrary ordering of the random variables in the lattice, $\{\mathcal{Z}_j; j = 1, \ldots, \mathcal{N}_D\}$. The following relation follows from the definition of conditional probability:

$$\begin{aligned} &\mathrm{Prob}\{\mathcal{Z}_1 = z_1, \mathcal{Z}_2 = z_2, \ldots, \mathcal{Z}_{\mathcal{N}_D} = z_{\mathcal{N}_D}\} = \\ &\quad \mathrm{Prob}\{\mathcal{Z}_{\mathcal{N}_D} = z_{\mathcal{N}_D}|\mathcal{Z}_1 = z_1, \mathcal{Z}_2 = z_2, \ldots, \mathcal{Z}_{\mathcal{N}_D-1} = z_{\mathcal{N}_D-1}\} \\ &\quad \times \mathrm{Prob}\{\mathcal{Z}_{\mathcal{N}_D-1} = z_{\mathcal{N}_D-1}|\mathcal{Z}_1 = z_1, \mathcal{Z}_2 = z_2, \ldots, \mathcal{Z}_{\mathcal{N}_D-2} = z_{\mathcal{N}_D-2}\} \\ &\quad \times \ldots \times \mathrm{Prob}\{\mathcal{Z}_2 = z_2|\mathcal{Z}_1 = z_1\} \times \mathrm{Prob}\{\mathcal{Z}_1 = z_1\} \end{aligned}$$

The sequential simulation algorithm under a multi-Gaussian model,

$$\begin{aligned} \mathcal{Z}_1 &\rightsquigarrow \mathcal{N}(0.0, \sigma^2) \\ \mathcal{Z}_2|\mathcal{Z}_1 = z_1 &\rightsquigarrow \mathcal{N}(\mu_{2|1}, \sigma^2_{2|1}) \\ &\vdots \\ \mathcal{Z}_{\mathcal{N}_D}|\mathcal{Z}_{\mathcal{N}_D-1} = z_{\mathcal{N}_D-1}, \ldots, \mathcal{Z}_1 = z_1 &\rightsquigarrow \mathcal{N}(\mu_{\mathcal{N}_D|\mathcal{N}_D-1,\ldots,1}, \sigma^2_{\mathcal{N}_D|\mathcal{N}_D-1,\ldots,1}); \end{aligned}$$

is an immediately consequence of the decomposition above, and it is frequently used for stochastic simulation, see Ripley (1987). This entails generating z_1 from the marginal distribution; z_2 from the conditional distribution given the value obtained for z_1; etc. For generating z_i, a matrix of dimension $(i-1)\times(i-1)$must be decomposed, and the algorithm may be extremely resource requiring if $\mathcal{N}_D$ is large.

For Gaussian random functions the sequential simulation algorithm, as described above, can be used directly, since the marginal distribution is Gaussian, and so are all conditional distributions. The parameter values to be used are defined in the previous sub-section.

For Gaussian intrinsic random functions the picture is slightly more complicated, since the marginal distribution is not necessarily Gaussian. Assume that the value z_1 is generated by a suitable probability distribution centered at 0.0. Then all conditional distributions will be Gaussian and the sequential algorithm, as described above, can be used. The parameter values to be used are defined in the previous sub-section. The fact that realizations of Gaussian intrinsic random functions based on the sequential, or any other, algorithm can be said to be conditional to the value of z_1 obtained, will be ignored in the following discussion. Note also that whenever one or more observations are available, the problem will disappear. The objective of this sub-section is to define a completely general simulation algorithm, and the sequential algorithm, with the reservations made for the Gaussian intrinsic random functions, provide this.

2.3 Special cases

The two classes of random functions, Gaussian and Gaussian intrinsic, contain several sub-classes with particular characteristics. A presentation and discussion of some of the sub-classes relevant for this study follows:

- Markov property - appears as very different for the one-dimensional case, $x \in \mathcal{D} \subset \mathcal{R}^1$, and higher dimensional cases, $x \in \mathcal{D} \subset \mathcal{R}^m$ with $m = 2, 3$. This is caused by the lack of ordering in the reference space in higher dimensions.

  In one dimension with $\mathcal{D} \subset \mathcal{R}^1$, define an unobserved arbitrary location $x_0 \in \mathcal{D}$ and observations in n arbitrary locations $(x_1, x_2, \ldots, x_n) \in \mathcal{D}$. Assume, without

loss of generality, that the set of locations is ordered increasingly and that $x_i < x_o < x_{i+1}$. The one-dimensional Markov property is defined by:

$$\begin{aligned}&\text{Prob}\{\mathcal{Z}(x_0) = z|\mathcal{Z}(x_1) = z_1, \mathcal{Z}(x_2) = z_2, \ldots, \mathcal{Z}(x_n) = z_n\}\\ &= \text{Prob}\{\mathcal{Z}(x_0) = z|\mathcal{Z}(x_i) = z_i, \mathcal{Z}(x_{i+1}) = z_{i+1}\}\end{aligned}$$

Hence the conditioning is only dependent on the closest observations on each side of location x_0, and they are screening the influence of the other observations. For Gaussian and Gaussian intrinsic random functions, it is sufficient that;

$$\begin{aligned}&E\{\mathcal{Z}(x_0)|\mathcal{Z}(x_1) = z_1, \mathcal{Z}(x_2) = z_2, \ldots, \mathcal{Z}(x_n) = z_n\}\\ &= E\{\mathcal{Z}(x_0)|\mathcal{Z}(x_i) = z_i, \mathcal{Z}(x_{i+1}) = z_{i+1}\}\\ &\text{Var}\{\mathcal{Z}(x_0)|\mathcal{Z}(x_1) = z_1, \mathcal{Z}(x_2) = z_2, \ldots, \mathcal{Z}(x_n) = z_n\}\\ &= \text{Var}\{\mathcal{Z}(x_0)|\mathcal{Z}(x_i) = z_i, \mathcal{Z}(x_{i+1}) = z_{i+1}\}\end{aligned}$$

since the conditional distributions are dependent on the two first moments only. For Gaussian random functions defined on $D \subset \mathcal{R}^1$ of arbitrary size, the Markov property is present for the exponential correlation function only, see Adler (1981). The exponential correlation function is:

$$\rho(|x' - x''|) = \exp\{-\alpha|x' - x''|\}\ ;\ \alpha \geq 0$$

with α being a parameter related to extent of spatial correlation. In Adler (1981) a couple of other correlation functions with Markov property are also listed, but for them the size of $\mathcal{D}$ is linked to the extent of spatial correlation. This is considered to be too restrictive for our study. For Gaussian intrinsic random functions defined on $D \subset \mathcal{R}^1$ of arbitrary size, the Markov property is present for the linear variogram function, see Matheron (1971). The linear variogram function is;

$$\gamma(|x' - x''|) = \tau|x' - x''|\ ;\ \tau \geq 0$$

with τ being a scale parameter. Note that this variogram function is unbounded and that it is closely related to Brownian motion in one dimension.

In higher dimensions with $\mathcal{D} \subset \mathcal{R}^m$ with $m = 2, 3$, the Markov property is not uniquely defined due to the lack of ordering in the reference space $\mathcal{D}$. A natural extension of the one-dimensional definition would, however, be: The conditional probability for $\mathcal{Z}(x_0)$ given the observations on a closed surface surrounding x_0 and several other observations outside this surface, is identical to the conditional probability given the observations on the surface only. A definition along these lines will be used here, although it is recognized that the conditioning on observations on a closed surface will not be possible whenever

the representation is on a lattice $\mathcal{L}_D$. In higher dimensions approximations must be used anyhow. For Gaussian random functions defined on $D \subset \mathcal{R}^m$ with $m = 2, 3$, the Markov definition above yields only trivial results entailing no stochasticity, see Adler (1981). If, however, conditioning is done on both the value and on the derivative perpendicular to the closed surface, a meaningful Markov definition, named pseudo-Markov, can be obtained, see Adler (1981). Correlation functions having Markov properties for $D \subset \mathcal{R}^1$ tends to have pseudo-Markovian properties in higher dimensions also. For Gaussian intrinsic random functions on $\mathcal{D} \subset \mathcal{R}^2$ it can be shown that the de Wijsian variogram function, $\gamma(\Delta) = \log(|\Delta|)$, would yield Markov properties as defined here, see Matheron (1971). The fact that this variogram function is not a valid variogram function for point support causes problems, and is the reason for not evaluating it further here. For $\mathcal{D} \subset \mathcal{R}^3$ non-valid variogram functions having Markov properties may also be identified, but these are ignored here for the same reason.

- Self affine, or fractal, random functions - defined through the scaling characteristics of the random function. According to Feder (1988) the definition of self affine processes is,

$$\mathcal{Z}(cx) = c^\beta \mathcal{Z}(x)\ ;\ 0 < \beta < 1$$

with c being the enforced scaling factor; and β being a constant for all c. Contrary to the definition of self similar processes, the variability of self affine processes will change with scale. The change should be according to the model described above. For Gaussian random functions the self affine property cannot exist, since the correlation function is bounded, and hence the scaling cannot be arbitrary large. For Gaussian intrinsic random functions it is obvious that the variogram function,

$$\gamma(|x' - x''|) = \tau|x' - x''|^{2\beta}\ ;\ 0 < \beta < 1$$

defines a self affine process. If the parameter β is defined to be the Hurst exponent, H, the corresponding random function is often termed fractal random function, see Feder (1988). The self affine property holds for $D \subset \mathcal{R}^m$ with $m = 1, 2, 3$. Note that for $D \subset \mathcal{R}^1$ with $\beta = 1/2$ the special case of Brownian motion having Markov properties appear.

3 Screening sequential simulation algorithm

The random function $\{\mathcal{Z}(x); x \in \mathcal{D}\}$ will be represented by random variables on a lattice covering $\mathcal{D}$, $\{\mathcal{Z}(x); x \in \mathcal{L}_D\}$, with $\mathcal{L}_D$ being the set of locations of lattice nodes; and $\mathcal{N}_D = \#\mathcal{L}_D$ being the number of nodes. The algorithm will be defined in an unconditional setting given the spatial correlation or variogram function, hence without available observations.

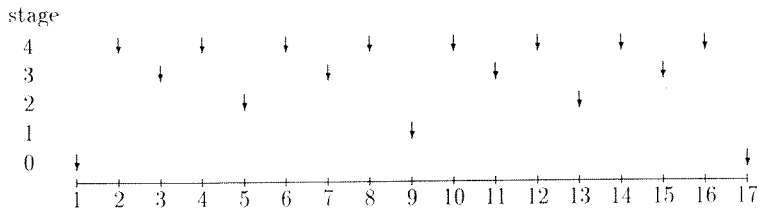

Figure 1: Sketch of halfing procedure used in the simulation algorithm

The justification of the algorithm appears from the sequential simulation algorithm and the Markov properties for $D \subset \mathcal{R}^1$, both defined in the previous section. Consider a Markovian Gaussian or Gaussian intrinsic random function for $D \subset \mathcal{R}^1$, and denote the set of random variables on the lattice $\{\mathcal{Z}_i; i = 1, \ldots, \mathcal{N}_D\}$. Without loss of generality, assume that the set is ordered increasingly in location on $D \subset \mathcal{R}^1$ and that $\mathcal{N}_D = 2^n + 1$ with n being an arbitrary integer. It follows immediately from the assumptions above and the discussion in the previous section that the following holds and fills the lattice;

$$\begin{aligned} \mathcal{Z}_1 &\rightsquigarrow \mathcal{N}(0, \sigma^2) \\ \mathcal{Z}_{\mathcal{N}_D} &\rightsquigarrow \mathcal{N}(\mu_{\mathcal{N}_D|1}, \sigma^2_{\mathcal{N}_D|1}) \end{aligned}$$

$$\mathcal{Z}_{(2k+1)2^{n-i}+1} | \mathcal{Z}_{k2^{n-i+1}+1} = z_\cdot, \mathcal{Z}_{(k+1)2^{n-i+1}+1} = z_\cdot \rightsquigarrow \mathcal{N}(\mu_{\cdot|\cdot}, \sigma^2_{\cdot|\cdot})$$
$$\text{for } k = 0, \ldots, 2^{i-1} - 1 \text{ and } i = 1, \ldots, r$$

with the dot sub-scripts being obvious from the context. The recursive expression above defines a halfing procedure as sketched in Figure 1. Firstly, at the initiation stage, the two end values are generated by the sequential algorithm. At stage one, the value half way between is generated by conditioning on the end values. At stage two, values half way between the assigned values are generated conditioned on the two closest values. At stage three, another halfing takes place and so on. The Markov property entails that conditioning on the closest two values is sufficient and this screening effect gives name to the algorithm. The algorithm can be considered as a zooming procedure with the conditioning values on each side getting increasingly closer with increasing stages.

From the assumptions made, it is clear that this is an exact simulation algorithm for a Gaussian random function on $D \subset \mathcal{R}^1$ with exponential covariance function, $\rho(\Delta) = \sigma^2 \exp\{-\alpha|\Delta|\}$. For Gaussian intrinsic random functions on $D \subset \mathcal{R}^1$ with linear variogram function, $\gamma(\Delta) = \tau|\Delta|$, it is also exact, except for the initiation

problem discussed in relation to the sequential algorithm in the previous section. The screening sequential algorithm in one dimension, as described above, is of course extremely efficient since conditioning on only the two closest values is required. Moreover, the identical configuration appearing on each stage of the generation procedure makes it necessary to determine $\underline{\psi}_{0_n} \Psi^{-1}$ and $\underline{\gamma}_{0_n} \Gamma^{-1}$ only once on each stage. Finally, for the linear variogram function it is known that the weights are scale invariant hence their values are known a priori to be equal to 0.5 on each conditioning value. This is recognized as the familiar simulation procedure for Brownian motions and for fractal random functions with $H = 0.5$, corresponding to the linear variogram function, see Feder (1988).

Note that exactness is obtained only for the one-dimensional case, $D \subset \mathcal{R}^1$, and Gaussian and Gaussian intrinsic random functions with exponential covariance functions and linear variogram functions respectively. In particular, the fractal random functions, being self affine, with Hurst exponent different from 0.5 will not be exactly simulated not even in one dimension. This is of course a far too restrictive class of random functions to be useful in practice. The sequential simulation algorithm presented in the previous section is exact also for higher dimensions for all random functions considered here, but it is far too resource consuming for practical applications. Hence one has to rely on approximatively correct simulation algorithms. The remainder of this article is devoted to definition and evaluation of the screening sequential algorithm in higher dimensions and for models for which it is not exact. The objective is to identify an algorithm providing a reasonable trade off between conceptual and implementation simplicity, processing efficiency, and precision.

The screening sequential simulation algorithm for higher dimensions, $D \subset \mathcal{R}^m; m = 2, 3$, and for an arbitrary covariance or variogram function is defined as follows:

- Define a set of directions $\{\phi_i; i = 1, \ldots, \mathcal{N}_\phi\}$ in the lattice $\mathcal{L}_D$. These directions should span the space reasonably uniformly, and will intersect any surrounding surface.

- Initiate the values $\mathcal{Z}(\cdot)$ in the border area of $\mathcal{L}_D$, defined as the set of lattice locations on the border and its neighbors, by the sequential simulation algorithm. Recall that this algorithm is exact, but for higher dimensional cases not the entire border area need be initiated.

- Step for $t = 1, 2, \ldots, n$:
  Use a halfing procedure for densifying the lattice for each dimension of $D \subset \mathcal{R}^m$ in each step. Determine the pdf $\mathcal{N}(\mu_{\cdot|\cdot}, \sigma^2_{\cdot|\cdot})$ for the actual lattice node by conditioning on the two closest available values in each of the directions $\{\phi_i; i = 1, \ldots, \mathcal{N}_\phi\}$. Assign the actual lattice node a value by simulation from $\mathcal{N}(\mu_{\cdot|\cdot}, \sigma^2_{\cdot|\cdot})$. Recall that pseudo-Markov properties in higher dimensions require conditioning both on the value and the derivative on the surrounding surface, hence the two closest values are used.

- The values in the $(2^n + 1)_1 \times \ldots \times (2^n + 1)_m$ lattice is generated.

The screening sequential algorithm draws on the properties of the sequential simulation algorithm and the insight in pseudo-Markov properties in higher dimensions. The screening sequential algorithm is of course only approximative in higher dimensions since the surrounding surface is represented by the $\mathcal{N}_\phi$ intersections with the directions only. A clever implementation, using the high symmetry of the algorithm, requires a few matrix decompositions on each step only. Hence the algorithm will appear as extremely processing efficient. Note in particular that the processing requirements will be independent of the correlation structure since the screening effect is assumed.

The screening sequential algorithm is based on the sequential Gaussian algorithm and the Markov properties. The algorithms used in Alabert (1989) and the SIS-algorithm defined in Journel and Alabert (1988) are developed for the conditional case, and are also based on the sequential algorithm. These algorithms run through the lattice in a random path however, and the dimensionality of the conditioning is reduced by using only the closest conditioning values. This is done in line with the 'local' kriging tradition justified through robustness with regard to local departure from stationarity. The screening sequential algorithm differs from the ones above by efficiently using the screening effect provided by the Markov properties. The values are generated in a sequence which reproduces the same configurations of conditioning values and zoom into smaller scales. The justification of the algorithm from approximate Markov properties simplifies the identification of models for which the algorithm is acceptably reliable. The screening sequential algorithm should rather be seen as an extension of the random midpoint displacement algorithm used for generating self affine, or fractal, random functions, see Barnsley et al. (1988). This algorithm is also based on the sequential algorithm and it draws on the Markov properties for justifying conditioning on only the closest values. Moreover, it is defined such that the configuration of conditioning values remain unchanged during the procedure. The random midpoint displacement algorithm appears as somewhat ad hoc, however. This will be more thoroughly discussed in the next section. It is worth noting that the screening sequential algorithm is extended to cover not only fractal random functions, but also classes of Gaussian random functions.

4 Empirical evaluations and discussion

The empirical evaluation is performed along two directions:

- generalization to higher dimensions. For Gaussian and Gaussian intrinsic random functions with exponential and linear variogram functions respectively, the presence of approximate Markov properties for $\mathcal{R}^2$ are evaluated.

- extension of the class of correlation and variogram functions. The generalization will be to other commonly used correlation functions and to other fractal dimensions for the Gaussian intrinsic model. The study is performed for $\mathcal{D} \subset \mathcal{R}^2$. For self affine, or fractal, random functions, a comparison with the commonly used random midpoint displacement algorithm is also included.

Two different simulation algorithms are involved in the study:

- screening sequential algorithms is used in most of the cases. It is defined in the previous section. In the study the directions denoted ϕ are $\{i\pi/4; i = 1, \ldots, 8\}$. Hence 16 observations are used in the conditioning in the two dimensional case.

- random midpoint displacement algorithm as described in Barnsley et al. (1988), frequently used in practice, is used as a comparison for fractal cases. This algorithm can be considered as a simplified version of the screening sequential algorithm in the sense that only the four or six main directions for ϕ are used in two and three dimensions respectively. Moreover, only the closest values in each direction is used and the same weights are assigned to each of the values to obtain the conditional distribution for all stages in the procedure. To avoid severe anisotropy effects, the directions used are rotated $\pi/4$ in two dimensions, and correspondingly in three dimensions, for certain configurations. The initiation described in Barnsley et al. (1988) appears as arbitrary. The initiation step is crucial when simulating fractal random functions since correlation appear for all distances. The initial values have considerable impact through the conditioning on values later to be generated. To provide anything like a fair comparison, the initiation procedure presented in Barnsley et al. (1988) is replaced by the sequential algorithm.

The study in two dimensions are done on a regular lattice of $\mathcal{L}_D \in \{x_{ij} | i, j = 1, \ldots, 129\}$. The shortest distance between two lattice nodes is used as the unit. For each case 100 realizations are generated. The traditional variogram estimator is used:

$$\hat{\gamma}(h) = \frac{1}{2\mathcal{N}_h} \sum_{(i,j)(k,l) \in E_h} (\mathcal{Z}(x_{ij}) - \mathcal{Z}(x_{kl}))^2$$

with $E_h : \{(i,j),(k,l) | |x_{ij} - x_{kl}| = h\}$ and $\mathcal{N}_h = \#E_h$ Recall that the correlation function, $\rho(h)$, can be expressed as a variogram function $\gamma_0(h) = (1 - \rho(h))$.

The empirical results are presented in quantile-plots, for example Figure 3. The horizontal axis is the lag in the variogram function and the vertical one is the variogram value. For each lag the variogram value along one of the main directions is estimated for each of the realizations. The hatched line indicates the average of the estimates of the variogram for each lag. The dotted lines indicates the 0.2, 0.4, 0.6 and 0.8 quantiles for the estimates for each lag. At lag 20, 60 and 100, the histograms for the estimates of the variogram values at the respective lags are displayed. The target variogram function is presented by a solid line.

In Figure 3 and 4, the results from the empirical study of the screening sequential algorithm on Gaussian random functions for $\mathcal{D} \subset \mathcal{R}^2$ are displayed. The exponential variogram function with $\alpha = 0.2$ and $\alpha = 0.02$ are used in the two figures. The former represents a random function with correlation structure having much shorter extent than $\mathcal{D}$, while the latter has long correlation structure. There appears to be no significant bias for any of the cases. The estimation variance seems to increase considerably with increasing correlation structure. This is not surprising since then higher correlation between values in the lattice nodes appear and this redundancy causes the total information content to be less. From plots not reported here, the estimates appear as almost perfectly isotropic. Recall that for exponential variogram functions, the screening sequential algorithm is exact for $D \subset \mathcal{R}^1$, although sampling uncertainty will occur of course. The results in Figure 3 and 4 suggest that the screening sequential algorithm is, practically spoken, exact for $\mathcal{D} \subset \mathcal{R}^2$ also, at least for relatively short correlation structures.

In Figure 5, the results from the empirical study of the screening sequential algorithm on Gaussian intrinsic random functions for $\mathcal{D} \subset \mathcal{R}^2$ are displayed. The linear variogram function is used in the figure. There appears to be no significant bias, but the estimation variance is relatively large. This is, as previously discussed, caused by the long, or in this case infinite, correlation structure. The slight anisotropy in the estimates is considered to be sampling uncertainty only. Recall that for linear variogram functions the screening sequential algorithm is exact for $D \subset \mathcal{R}^1$. The algorithm seems highly reliable for $\mathcal{D} \subset \mathcal{R}^2$ also.

The screening sequential algorithm is considered to be reliable for Gaussian and Gaussian intrinsic random functions with exponential and linear variogram functions for $\mathcal{D} \subset \mathcal{R}^m$ with $m = 1, 2$. This is interpreted to be caused by the Markov property being present for $\mathcal{D} \subset \mathcal{R}^1$, playing approximately over to the two-dimensional case also. Preliminary empirical evaluations for $\mathcal{D} \subset \mathcal{R}^3$ leaves the same impression for that case as well.

In Figure 6 and 7, the results for Gaussian random functions with correlation functions being non-Markovian for even $D \subset \mathcal{R}^1$ are displayed. Two variogram functions are evaluated: the spherical model,

$$\gamma_o(\Delta) = \begin{cases} \frac{3}{2}(\frac{\Delta}{r}) - \frac{1}{2}(\frac{\Delta}{r})^3 & ; \quad 0 < \Delta < r \\ 1.0 & ; \quad r < \Delta \end{cases} \quad ; r = 20$$

and the second-order exponential model

$$\gamma_o(\Delta) = 1 - \exp\{-\alpha|\Delta|^2\} \; ; \; \alpha = 0.005$$

The former is frequently used and appears as exact for a three-dimensional spherical moving average operator on a white noise lattice. The latter constitutes an extreme case for Gaussian random functions, resulting in an infinitely times derivable realization. The results for $\mathcal{D} \subset \mathcal{R}^2$ for the spherical model in Figure 6, suggests a fairly distinct downward bias and relatively large estimation variance in the estimates. The

results display no anisotropy. It appears as the screening sequential algorithm creates realizations according to the exponential variogram model closest to the spherical one specified. The spherical model can of course be reasonably well represented by linearly combining realizations of exponential models. Direct simulation is not possible since linear combination of exponential models do not exhibit Markov properties, even for $\mathcal{D} \subset \mathcal{R}^1$. The results for the second-order exponential model for $\mathcal{D} \subset \mathcal{R}^2$ in Figure 7, seem promising without noticeable bias although with relatively large estimation variance. No anisotropy can be identified. The experience from other tests is, however, that whenever the correlation structure is extended, the correlation between neighboring values in the lattice increases, and this will cause numerical instability. All algorithms based on the sequential algorithm will face these problems.

In Figure 8 and 9, the results for $\mathcal{D} \subset \mathcal{R}^2$ for Gaussian intrinsic random functions with variogram functions being non-Markovian for even $D \subset \mathcal{R}^1$ are displayed. The following class of self affine, or fractal, random functions are evaluated:

$$\gamma(\Delta) = \tau|\Delta|^{2H} \; ; \; H = 0.2 \; ; \; H = 0.8$$

The former represents a fairly erratic random function, while the latter represents a fairly smooth one. The results in Figure 8 and 9, suggest that no bias is present, although the estimation variance is fairly large. This is caused by the long correlation structure as previously discussed. No anisotropy can be identified. These results are considered to be encouraging.

In Figure 10 through 12, the results from applying the random midpoint displacement algorithm for $\mathcal{D} \subset \mathcal{R}^2$ on the fractal model for $H = 0.5, H = 0.2$ and H=0.8 are displayed. The results in Figure 10 through 12 should be compared to the results in Figure 5, 8 and 9, displaying the corresponding results for the screening sequential algorithm. The random midpoint displacement algorithm seems to provide severely biased results which are significantly less reliable than the ones from the screening sequential algorithm. Moreover, the initiation step in the random midpoint displacement algorithm was improved from what is usually done, not doing so would have provided even more striking differences. Other reasons for the difference are: the random midpoint displacement algorithm only relying on the four major directions in the lattice makes it vulnerable; and the fact that it assigns the same weights to all values makes it vulnerable for non-symmetric patterns in border areas.

In practical applications, the processing requirements are of major concern when representations on large lattices are needed. The screening sequential algorithm has processing requirements being independent of the actual variogram function and linear in the number of lattice nodes. These are favorable characteristics. In Figure 2 the processing requirement of the screening sequential and the random midpoint displacement algorithms, are displayed in a log-log plot. The latter algorithm is considered to be immensely fast. Note that the screening sequential algorithm has similar properties as the random midpoint displacement algorithm, although multiplied by a factor of approximately 1.75. The fact that the screening sequential algorithm is

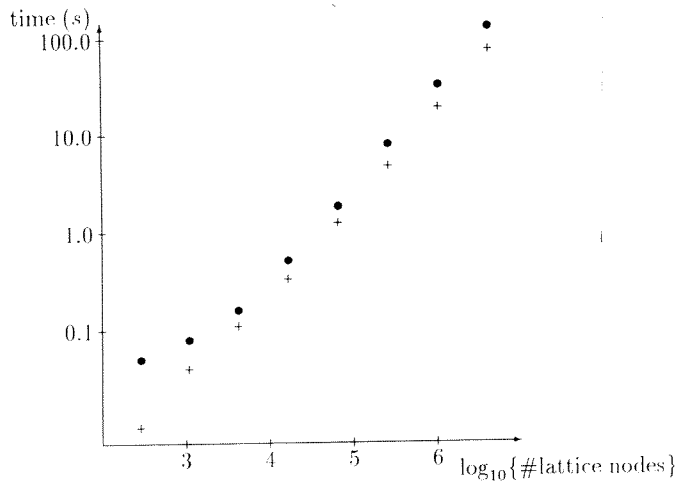

Figure 2: Processing requirements for the screening sequential algorithm (•) and for the random midpoint displacemant algorithm (+) for different grid sizes

both more general and considerably more reliable should justify the additional processing time in practical applications. Note that a two dimensional lattice of size $2049 \times 2049 = 4198401$ can be generated in 2 min. 8 sec. on a IBM Risc 6000/320. A lattice of size approximately 10^9 would require 8 h. 30 min., and considerable memory, of course, on the same computer.

5 Conclusions

The screening sequential algorithm for simulation of random functions is defined and evaluated. It is based on the general sequential simulation algorithm and approximate Markov properties in random functions. For Gaussian and Gaussian intrinsic random functions with exponential and linear variogram functions respectively, i.e. $\gamma_o(\Delta) = 1 - \exp\{-\alpha|\Delta|\}$ and $\gamma(\Delta) = \tau|\Delta|$, the screening sequential algorithm is exact in one dimension. This is due to the Markov properties for these models in one dimension. In higher dimensions, the Markov property is not present exactly, and the reliability of the algorithm must be evaluated empirically. The empirical study shows that the screening sequential algorithm is reliable also in the two-dimensional case for the models mentioned above. Moreover, for self affine, or fractal, models, $\gamma(\Delta) = \tau|\Delta|^{2H}$ with $0.2 \leq H \leq 0.8$ the screening sequential algorithm does also appear as reliable. Consequently, the simulation algorithm is reliable for models with

variogram functions being both bounded and unbounded - or "with and without sill". Empirical evaluations of the same variogram functions in three dimensions seem to provide similar conclusions. This provides good opportunities for modeling many real phenomena.

For Gaussian random functions with spherical variogram functions, the algorithm provides relatively strongly downward biased results, and the general shape is not reproduced. It appears like the closest exponential variogram function is reproduced. With second-order exponential variogram functions, the algorithm appears as reasonably reliable, unless the correlation structure is long and numerical instability occurs. The screening sequential algorithm should for both these cases, be used with care.

The random midpoint displacement algorithm, frequently used for generation of fractal random functions, is also empirically evaluated. The results are significantly less reliable than for the screening sequential algorithm. In applications concerning scientific computing, the random midpoint displacement algorithm is not considered to be sufficiently reliable. The authors' experience is that the successive random addition procedure, frequently used in the fractal community, is even less reliable than the random midpoint displacement algorithm, and hence should be used with care. Procedures in the frequency domain tend to be very processing requiring in higher dimensions.

The processing requirements for the screening sequential algorithm are independent of the correlation structure and linear in the number of lattice nodes. The algorithm has processing characteristics similar to the random midpoint displacement algorithm, although with a constant 1.75 times higher. The latter is considered to be an immensely processing efficient simulation algorithm. The screening sequential algorithm required 2 min. 8 sec. to generate a lattice of size $2049 \times 2049 = 4198401$ on an IBM Risc 6000/320.

6 Acknowledgment

The study is financed by Norsk Hydro a.s., Statoil a.s. and Norwegian Computing Center.

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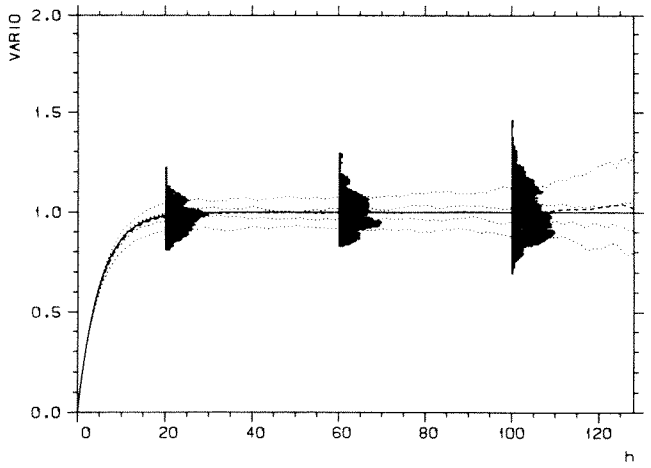

Figure 3: Screening sequential algorithm in two dimensions; exponential variogram function with $\alpha = 0.2$

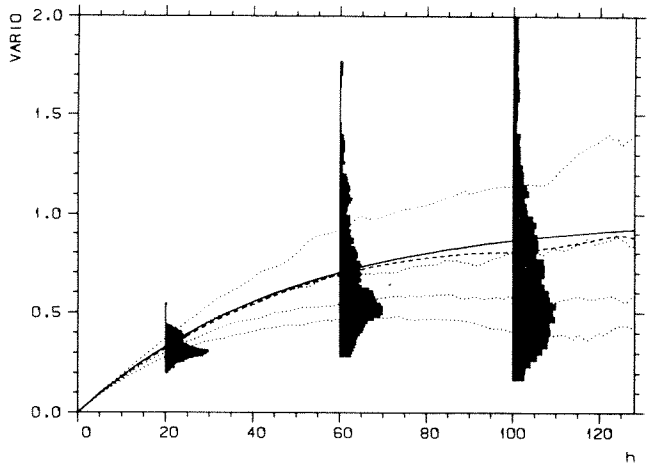

Figure 4: Screening sequential algorithm in two dimensions; exponential variogram function with $\alpha = 0.02$

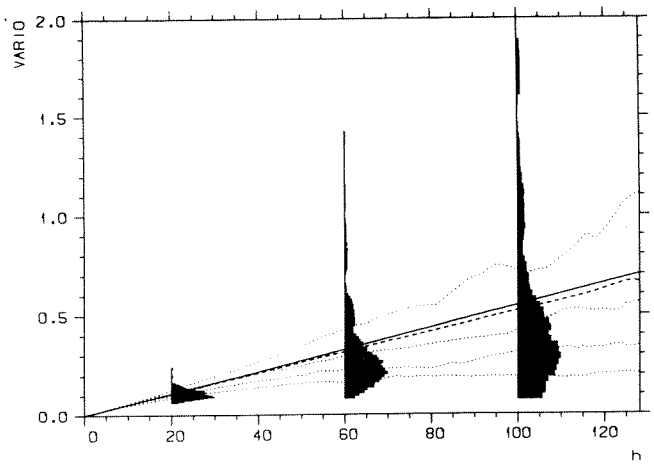

Figure 5: Screening sequential algorithm in two dimensions; fractal variogram function with $H = 0.5$; linear variogram function

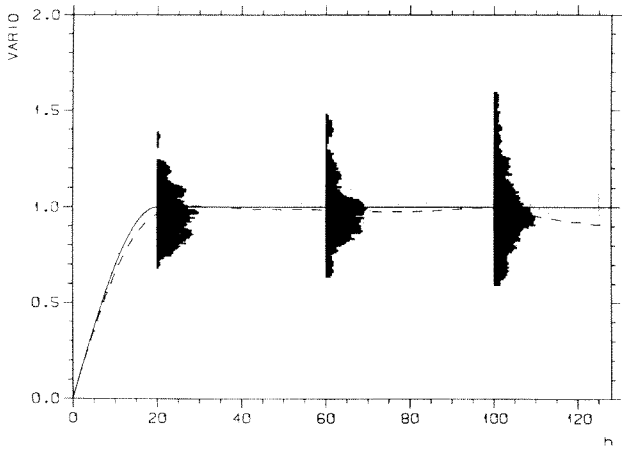

Figure 6: Screening sequential algorithm in two dimensions; spherical variogram function with $r = 20$

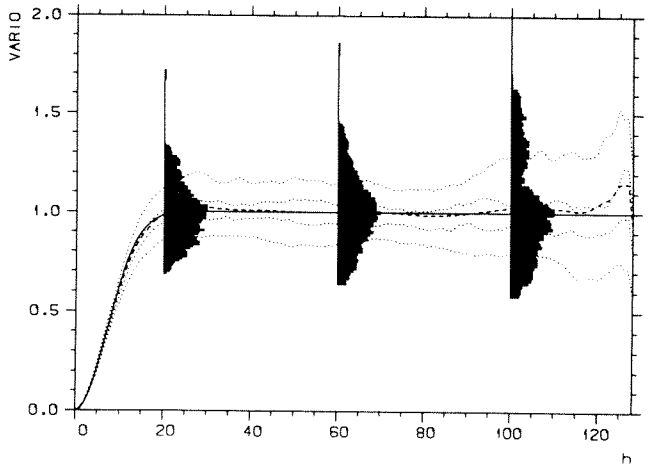

Figure 7: Screening sequential algorithm in two dimensions; second-order exponential variogram function with $\alpha = 0.005$

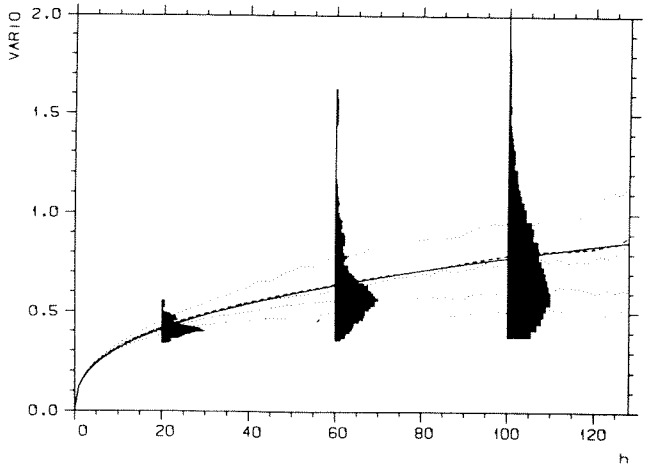

Figure 8: Screening sequential algorithm in two dimensions; fractal variogram function with $H = 0.2$

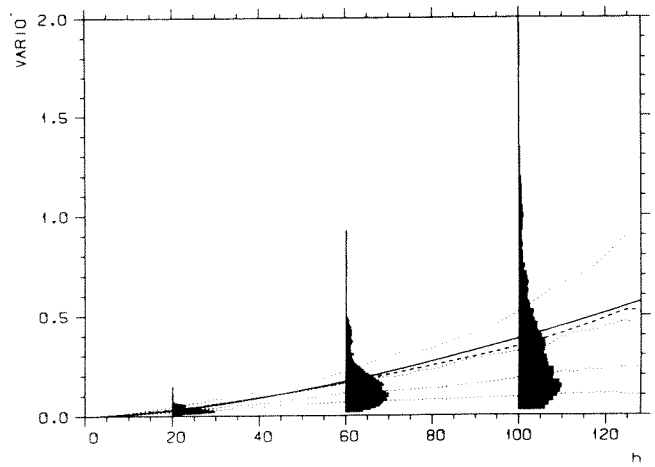

Figure 9: Screening sequential algorithm in two dimensions; fractal variogram function with $H = 0.8$

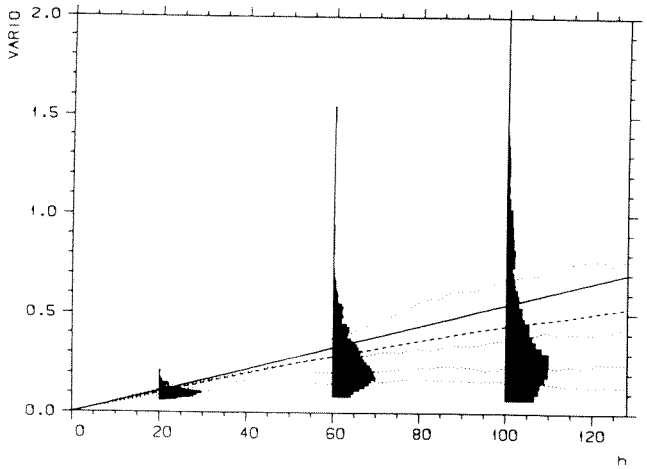

Figure 10: Random midpoint displacement algorithm in two dimensions; fractal variogram function with $H = 0.5$; linear variogram function

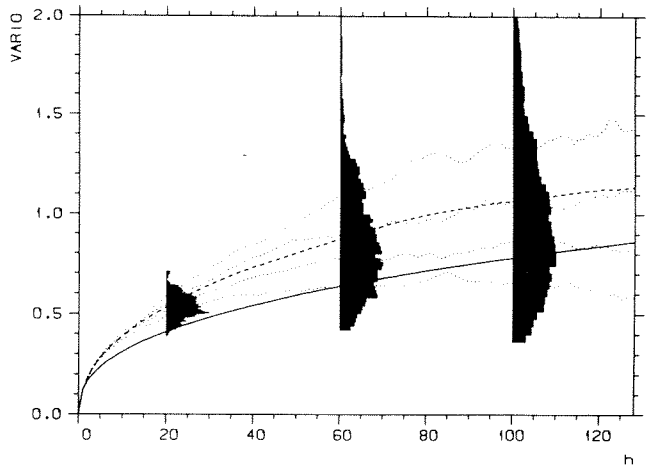

Figure 11: Random midpoint displacement algorithm in two dimensions; fractal variogram function with $H = 0.2$

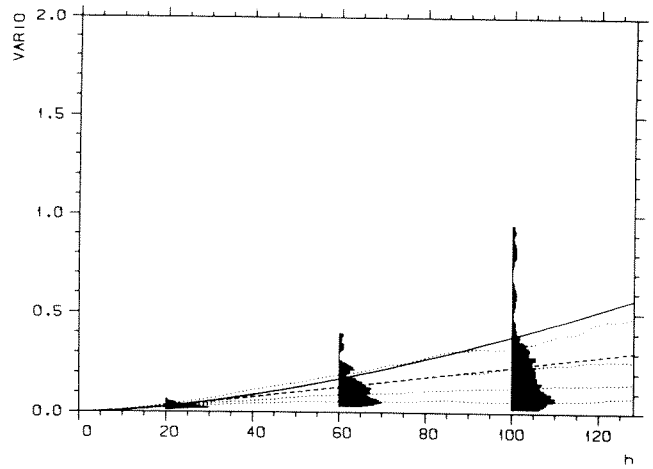

Figure 12: Random midpoint displacement algorithm in two dimensions; fractal variogram function with $H = 0.8$