GEOPHYSICS, VOL. 55, NO. 11 (NOVEMBER 1990); P. 1435–1440, 6 FIGS., 1 TABLE.

Geostatistical simulation for geophysical applications—Part I: Simulation

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ABSTRACT

Geostatistical simulation is used to create a synthetic three-dimensional geologic environment such that randomly generated values of a physical property have a required covariance and mean. We create a spatially stationary, multivariate Gaussian simulation with a Gaussian covariance. This type of simulation permits modeling of natural variations which may be an important source of noise in geologic investigations, whereas interpolation techniques such as kriging tend to smooth out those variations.

Computationally efficient frequency-domain methods allow the rapid creation of multiple scenarios, each having the required statistical distribution. For the particular problem considered, a given porosity distribution is simulated and then functionally related to physical properties needed for input into geophysical models. Additionally, megascopic cavities having random size, shape, and orientation similar to those observed in karst settings are emplaced in the physical model. Geostatistical simulation plays a particularly important role in exploring the degree to which natural variations in physical parameters lower the resolution of target anomalies that have similar signatures. In the accompanying paper, we discuss the geophysical methods tested and the results of the tests.

INTRODUCTION

Geophysical prospecting involves the use of surface or borehole measurements of some variable (e.g., gravitational acceleration, traveltime) to make inferences about the subsurface distribution of geophysical properties (e.g., density, seismic velocity). Interpretation then translates the physical property variations into a geologic framework to place constraints on the location, size, and shape of subsurface bodies and structures of interest. In the early days of geophysics, limitations on the resolution of a geophysical survey were often imposed by the sensitivity of the instrument used to measure the surface variations. In gravity prospecting, for example, initial measurements were made using the Eötvös balance. Development of the LaCoste-Romberg gravimeter in the 1930s permitted direct, highly accurate measurements of variations in the acceleration itself. Now gravity surveys may be made to microgal accuracy, and compensation for the inertial accelerations of gravimeter platforms has advanced to the point where shipboard gravity measurements are routine and airborne gravity surveys are possible (Hammer, 1983; Brozema and Peters, 1989).

Similar advances have been made in all geophysical areas, partially due to the development of new instruments with higher sensitivity. In many cases, enhanced resolution results from the ability to manipulate large amounts of data with digital computers. Whatever the reason, resolution in geophysical surveys is becoming increasingly limited not by the size of target anomalies, but by normal background variations of subsurface physical properties which may produce anomalies comparable in size to, or larger than, the anomalies due to bodies and structures of interest.

This development poses a new type of problem to the geophysicist. Rather than worrying about how to model anomalies at the limit of instrumental sensitivity, the interpreter must be concerned about proposing, on the basis of well-resolved anomalies, the existence of bodies and structures that do not exist. The best protection against such an error is to be able to evaluate, preferably in advance, whether the size and shape of target anomalies are distinguishable from anomalies produced by normal background variations of the physical properties.

We have recently been faced with a problem of this type. Our mission was to evaluate several geophysical techniques that might be used to prospect for cavities in the near subsurface (10–100 ft deep) and choose the method(s) best suited for locating and characterizing them. Our approach was to develop a technique for creating a geostatistical

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model of the subsurface, to carry out simulated geophysical surveys over these models, and to compare the resulting geophysical anomaly fields over models with and without cavities.

For this approach to be useful in practice, one must be able to create a model of subsurface physical properties that (1) preserves natural geostatistical variations to a reasonable degree, (2) resolves variations of the physical properties to a sufficiently fine detail, and (3) may be generated rapidly on digital computers of modest capabilities. In this paper, we describe the approach we used to generate relevant geostatistical models. The simulated geophysical surveys and their interpretation will then be discussed in a companion paper (Shive et al., 1990).

GEOSTATISTICAL SIMULATION

We use a frequency-domain approach to geostatistical simulation (Borgman et al., 1984) to produce three-dimensional (3-D) simulations of porosity and to introduce cavities randomly into the subsurface. Geostatistical simulation is a type of Monte Carlo method in which a large number of randomly generated scenarios are created which can be examined statistically. However, most Monte Carlo methods consider each event to occur independently. For geologic applications, independence cannot generally be assumed. Porosity, mineralization, hydraulic conductivity, and other physical properties are often spatially correlated, with high values and low values persisting over some distance. Preserving this persistence is vital for generating realistic geologic scenarios (Miller and Borgman, 1985).

The linear spatial persistence of a physical property can be statistically measured by the covariance (Figures 1 and 2). The covariance is defined as

$$\text{Cov}\,[V(\mathbf{x}), V(\mathbf{x}+\mathbf{h})] = E\{[V(\mathbf{x}) - \mu(\mathbf{x})] \times [V(\mathbf{x}+\mathbf{h}) - \mu(\mathbf{x}+\mathbf{h})]\} \quad (1)$$

where

E is the expectation operator,
$\mathbf{x}$ is a multicomponent spatial location,
$V(\mathbf{x})$ is the value of the property at location $\mathbf{x}$,
$\mu(\mathbf{x})$ is the expected value at location $\mathbf{x}$, and
$\mathbf{x} + \mathbf{h}$ is a location at a displacement $\mathbf{h}$ from $\mathbf{x}$.

By assuming that the stationary mean of the physical property can be estimated and removed and that the covariance is stationary (invariant in space), we can express the covariance as a function of spatial separation only:

$$C(\mathbf{h}) = E[W(\mathbf{x})W(\mathbf{x}+\mathbf{h})], \quad (2)$$

where $W(\mathbf{x}) = V(\mathbf{x}) - \mu(\mathbf{x})$. The goal of the simulation is then to produce a set of values $V(\mathbf{x})$ having the covariance relationship $C(\mathbf{h})$.

Other approaches to the production of simulations have been proposed by several authors (e.g., Journel and Huijbregts, 1981; Mantoglou, 1987; Davis, 1987b; King and Smith, 1988). The straightforward matrix approach is to decompose the covariance matrix into the form

$$\underset{\sim}{C} = \underset{\sim}{A}\underset{\sim}{A}^T, \quad (3)$$

where the matrix $\underset{\sim}{C}$ is formed of elements $C_{ij} = C(\mathbf{x}_i - \mathbf{x}_j)$, and $\mathbf{x}_i$ is the location at which a value is to be generated. Because the covariance matrix is positive semidefinite (Muirhead, 1982, p. 3), the $\underset{\sim}{A}$ matrix may be found using the Cholesky decomposition or a similar LUD decomposition algorithm (Davis, 1987a). If k values are to be estimated, the size of the resulting $\underset{\sim}{C}$ matrix is $k \times k$. Thus, doubling k

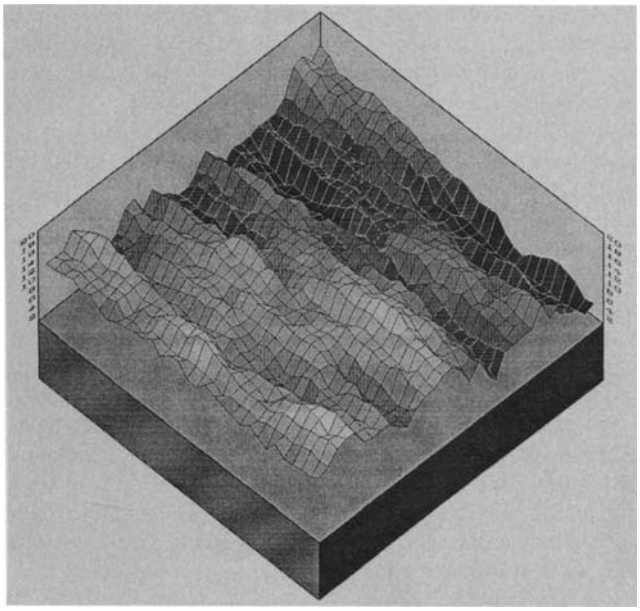

FIG. 1. Simulation of a rock property showing both strong and weak correlation, resulting from a highly anisotropic covariance. Grid spacing is 5 ft.

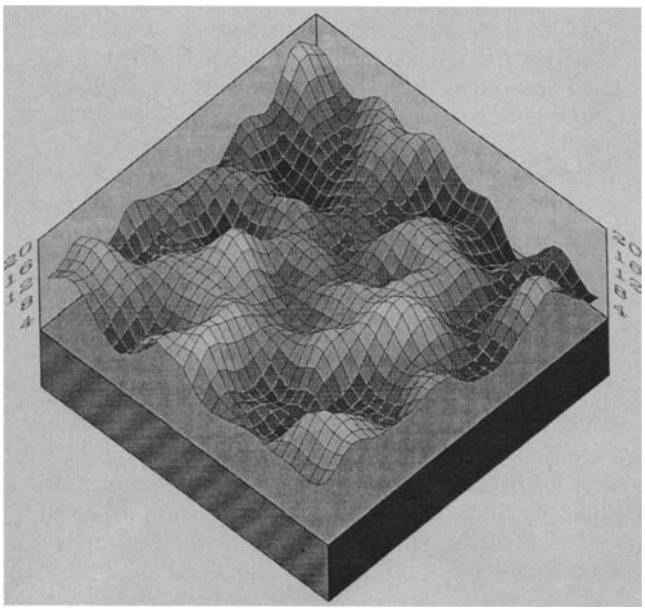

FIG. 2. Simulation of a rock property which lacks any strong directional correlation, resulting from an isotropic covariance with a short range of influence.

quadruples the size of $\underset{\sim}{C}$ and increases the solution time eightfold (Burden et al., 1978).

When points at which values are to be generated lie on a regular grid, an alternative to the matrix decomposition method is the frequency-domain method (Borgman et al., 1984). The motivation for using frequency-domain techniques rather than matrix operations comes from the speed of the fast Fourier transform (e.g., Blahut, 1985), which provides a method of rapidly converting between the discrete form of the covariance and its spectral equivalent, and from the smaller size of the matrices which are needed for storing the Fourier coefficients.

The frequency-domain method for generating simulations uses the multidimensional relationship between the covariance and the spectrum,

$$\underset{\sim}{\mathbf{C}}(\mathbf{h}) = F[S(\mathbf{f})], \tag{4}$$

where F is the Fourier transform and $S(f)$ is the spectrum, a function of frequency f.

The Fourier transform is invertible, so that the inverse transform of the covariance is the spectrum. For gridded 3-D simulations, the spectrum is given by

$$\underset{\sim}{S}_m = \Delta\mathbf{h} \sum_{\mathbf{n}} \underset{\sim}{C}_{\mathbf{n}} \times \exp\left[-i2\pi\left(\frac{m_1 n_1}{N_1} + \frac{m_2 n_2}{N_2} + \frac{m_3 n_3}{N_3}\right)\right], \tag{5}$$

where

$\underset{\sim}{C}_{\mathbf{n}} = C(n_1\Delta h_1, n_2\Delta h_2, n_3\Delta h_3)$,

$\underset{\sim}{S}_{\mathbf{m}} = S(m_1\Delta f_1, m_2\Delta f_2, m_3\Delta f_3)$,

N_i = the number of grid points in the i direction, i

$$= 1,2,3,$$

$$\Delta f_i \Delta h_i = 1/N_i, \text{ and } 0 \le m_i, n_i < N_i.$$

To accelerate the generation of simulations, we further assume a Gaussian covariance relationship

$$\underset{\sim}{C}(\mathbf{h}) = \sigma^2 \exp\left[-\mathbf{h}^T\underset{\sim}{E}\mathbf{h}/2\right], \tag{6}$$

where $\underset{\sim}{E}$ is an invertible matrix describing size and orientation of the covariance ellipsoid for a multivariate normal distribution (e.g., Anderson, 1958). The resulting analytical form of the spectrum is

$$\underset{\sim}{S}(\mathbf{f}) = \frac{(2\pi)^{3/2}\sigma^2}{\underset{\sim}{E}} \exp\left[-2\pi^2\mathbf{f}^T\underset{\sim}{E}^{-1}\mathbf{f}/2\right]. \tag{7}$$

The zero-mean, stationary Gaussian covariance is real and symmetric about lag $h = 0$. The resulting spectrum is also Gaussian, real, and symmetric about zero (Borgman, 1973, p. 4.4). The complex Fourier coefficients in frequency space, A_m (defined below), are weighted according to the magnitude of the spectrum and the choice of grid spacing and size. The frequency-domain weights and symmetry relations for the one- and two-dimensional simulations were presented by Borgman et al. (1984). For 3-D simulations, let $T_i = N_i\Delta h_i$. The weights for coefficients where $0 < m_i < N_i/2$, for all values of i, are

$$A_m = R_m + iI_m,$$

$$R_m = \sqrt{\frac{T_1T_2T_3}{2}\,\underset{\sim}{S}_m}, \tag{8}$$

and

$$I_m = \sqrt{\frac{T_1T_2T_3}{2}\,\underset{\sim}{S}_m}.$$

The weights for coefficients where $m_i = 0$ or $m_i = N_i/2$, for any value of i, are

$$R_m = \sqrt{T_1T_2T_3\,\underset{\sim}{S}_m} \tag{9}$$

and

$$I_m = 0.$$

The remaining coefficients are determined by complex conjugate symmetry relations with the weights listed above. These relationships are

Corners: no symmetry

Edges:

$$\begin{aligned} &m_1 = 0 \text{ or } m_1 = N_1/2 \\ &m_1 = 0 \text{ or } m_2 = N_2/2 \end{aligned}, \quad A_{m_1,m_2,m_3} = \bar{A}_{m_1,m_2,N_3-m_3},$$

$$\begin{aligned} &m_1 = 0 \text{ or } m_1 = N_1/2 \\ &m_3 = 0 \text{ or } m_3 = N_3/2 \end{aligned}, \quad A_{m_1,m_2,m_3} = \bar{A}_{m_1,N_2-m_2,m_3}, \tag{10}$$

$$\begin{aligned} &m_2 = 0 \text{ or } m_2 = N_2/2 \\ &m_3 = 0 \text{ or } m_3 = N_3/2 \end{aligned}, \quad A_{m_1,m_2,m_3} = \bar{A}_{N_1-m_1,m_2,m_3}.$$

Faces:

$$\begin{aligned} &m_1 = 0 \text{ or } m_1 = N_1/2, \quad A_{m_1,m_2,m_3} = \bar{A}_{m_1,N_2-m_2,N_3-m_3} \\ &m_2 = 0 \text{ or } m_2 = N_2/2, \quad A_{m_1,m_2,m_3} = \bar{A}_{N_1-m_1,m_2,N_3-m_3} \\ &m_3 = 0 \text{ or } m_3 = N_3/2, \quad A_{m_1,m_2,m_3} = \bar{A}_{N_1-m_1,N_2-m_2,m_3}. \end{aligned} \tag{11}$$

Interior:

$$A_{m_1,m_2,m_3} = \bar{A}_{n_1-m_1,N_2-m_2,N_3-m_3}. \tag{12}$$

By multiplying each weight by a standard normally distributed random number Z, the weights are randomly apportioned between the real and imaginary parts of the Fourier coefficients:

$$\underset{\sim}{A}_m = \begin{bmatrix} R'_{\mathbf{m}} \\ I'_{\mathbf{m}} \end{bmatrix} = \begin{bmatrix} R_{\mathbf{m}}Z \\ I_{\mathbf{m}}Z' \end{bmatrix}, \tag{13}$$

which has mean

$$E[\underset{\sim}{A}_m] = E\begin{bmatrix} R'_{\mathbf{m}} \\ I'_{\mathbf{m}} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{14}$$

and covariance

$$E[\underset{\sim}{A}_{\mathbf{m}}\underset{\sim}{A}_{\mathbf{m}}^{T\prime}] = \begin{cases} \underset{\sim}{B}_{\mathbf{m}}, & \text{if } \mathbf{m} = \mathbf{m}' \\ \text{matrix of zeroes}, & \text{if } \mathbf{m} \neq \mathbf{m}' \end{cases}, \tag{15}$$

where $\underset{\sim}{\mathbf{B}}_m$ is a 2×2 matrix whose components are defined by (Borgman, 1973)

$$\text{Cov}\,(R'_{\mathbf{m}} I'_{\mathbf{m}}) = 0, \tag{16}$$

$$\text{Var}\,(R'_{\mathbf{m}}) = \begin{cases} T_1 T_2 T_3 S_{\mathbf{m}} \text{ for zero \& Nyquist frequencies,} \\ T_1 T_2 T_3 S_{\mathbf{m}}/2 \text{ otherwise,} \end{cases} \tag{17}$$

$$\text{Var}\,(I'_{\mathbf{m}}) = \begin{cases} 0 \text{ for zero and Nyquist frequencies,} \\ T_1 T_2 T_3 S_{\mathbf{m}}/2 \text{ otherwise.} \end{cases} \tag{18}$$

Simulations with the desired covariance relationships are then rapidly generated by inverse Fourier transformation. The resulting simulations have zero mean and have a multivariate Gaussian distribution and covariance. A mean can then be added to the simulations as needed.

CONVERSION OF POROSITY SIMULATIONS

For a task in which only one geophysical method is evaluated, it would make sense to simulate the relevant physical property directly. However, if several methods are compared, direct simulation of all properties may become tedious or be a poor use of computer time. For example, if we wish to evaluate gravity, seismic refraction, dc resistivity, and radar in a scenario that includes five different rock types, we require 20 simulations (a simulation for density, velocity, electrical conductivity, and dielectric constant for each rock type). This task may be considerably simplified in cases for which functional relationships exist between different physical properties.

Study of physical property measurements (e.g., Dobrin, 1960; Grant and West, 1965; Telford et al., 1976) indicates that the factors which most strongly influence the above physical properties are porosity and water content. Our approach is to simulate only one variable for each rock type—the variable is porosity Φ. The creation of a Gaussian distribution for porosity is supported in the univariate case by various researchers, as listed by Freeze (1975). Therefore, our choice of the Gaussian covariance model is provisional, awaiting the collection of field data. Hewitt (1986) analyzed geophysical well logs to obtain estimates for the vertical covariance. He proposed that, in the absence of data for horizontal covariance estimation, the vertical covariance be used as a best guess. Given that changes in sediment type usually occur over much shorter distances vertically than laterally, this initially seems quite suspect. However, because we are simulating porosity only within a given rock type and not across formation boundaries, the covariance model may be adequate, assuming the initial vertical covariance estimation was within the given rock type.

After using the covariance estimates to create the porosity simulations, we establish the location of the water table. Any physical property for a given rock type is then calculated from its functional relationship with porosity and by the content (air or water) of the pores. In the following equations relating physical properties to porosity, the subscript b refers to the property of the rock (with no pores) and subscript f to the property of the fluid in the pores (either air or water); the porosity Φ is a fraction between 0 and 1. The equations should return the bulk property of the rock when $\Phi = 0$, the property of the fluid when $\Phi = 1$, and bear a reasonable relationship to observed property variations.

For density ρ, we use

$$\rho = \rho_b(1 - \Phi) + \rho_f \Phi \quad \begin{cases} \rho_f = 0 \text{ g/cm (air)} \\ \rho_f = 1 \text{ g/cm (water),} \end{cases} \tag{19}$$

and for velocity v,

$$\frac{1}{v} = \frac{(1 - \Phi)}{v_b} + \frac{\Phi}{v_f} \quad \begin{cases} v_f = 1000 \text{ ft/s (air)} \\ v_f = 5000 \text{ ft/s (water).} \end{cases} \tag{20}$$

The velocity function is the well-known time average equation (Telford et al., 1976, p. 257) used in well-log interpretation. Archie's law (Telford et al., 1976, p. 775) gives the resistivity r, an approximately inverse square relationship to porosity. We use

$$\frac{1}{r} = \frac{(1 - \Phi^2)}{r_b} + \frac{\Phi^2}{r_f} \quad \begin{cases} r_f = 10^5\ \Omega \cdot \text{m (air)} \\ r_f = 3\ \Omega \cdot \text{m (water).} \end{cases} \tag{21}$$

The finite value for r_f (air) may be adjusted to acknowledge the role of moisture above the water table; it also protects against computational overflow. The value of 3 for r_f (water) is a representative value for natural waters in sediments (Telford et al., 1976, p. 452).

Fewer measurements of dielectric constant k exist than for the other physical properties. Knight and Nur (1987) show an approximate linear relationship between k and Φ. We use

$$k = k_b(1 - \Phi) + k_f \Phi \quad \begin{cases} k_f = 1 \text{ (air)} \\ k_f = 80 \text{ (water).} \end{cases} \tag{22}$$

It remains to establish the values for k_b for different rock types. Table 1 shows the values used to convert porosity simulations to physical property models. These are derived from a variety of sources (e.g., Dobrin, 1960; Clark, 1966;

Table 1. Representative bulk properties of common rock types.

Rock type	Density (g/cm^3)	Velocity (ft/s)	Resistivity (Ω·m)	Dielectric constant	Porosity mean	Porosity variance
Alluvium	2.75	10 000	800	4.0	0.44	0.005
Clay	2.60	9 000	100	7.0	0.51	0.005
Sandstone	2.75	14 000	10 000	4.0	0.11	0.004
Limestone	2.72	20 000	10 000	8.0	0.40	0.005
Shale	2.75	14 000	1 000	6.0	0.30	0.001
Metamorphic	2.72	20 000	10 000	7.0	0.30	0.0005
Igneous rock	2.70	20 000	10 000	6.0	0.30	0.0005
Silt	2.75	10 000	500	5.0	0.50	0.005

Telford et al., 1976). The user chooses a rock type, simulates porosity, and specifies the water table level. The formulas then establish the physical properties.

EMPLACEMENT OF CAVITIES

A simulation method similar to that for generating porosity is used to generate cavities. A simulation is generated with a given covariance structure. All values above a given threshold value are then considered as lying within a cavity. Because of the inherent linearity of the covariance function and the ellipsoidal multidimensional form assumed in equation (5), this "truncation process" (Lawton, 1985) produces ellipsoidal cavities (Figure 3) whose locations are independent of porosity values near the cavities. Thus, this is not the final answer in the generation of cavities (see, for example, Journel and Isaaks, 1984) but offers a computationally efficient method of generation of ellipsoidal cavities. Furthermore, most of the same software used for generating the physical property simulations may also be used for simulating the cavities.

The cavities thus generated are placed within the physical model. Equivalently, porosity is set at 100 percent at grid locations which lie within the cavity. The values of physical properties within the cavity are therefore that of the fluid only.

CREATION OF THE GEOLOGIC ENVIRONMENT

The final step in the creation of the simulations is the merging of the physical property data for each rock type into a model of the subsurface. We assume that a certain amount of information is known about the subsurface: (1) the rock types present, (2) the boundaries between these rock types, and (3) the location of the water table. Within the boundaries for a rock type, the data from the previous independent simulations of physical properties for that rock type are used. For example, if limestone is overlain with alluvium containing clay lenses, we specify the location of the top of the limestone, the thickness of the alluvium, the location of the clay lenses, and the level of the water table (Figure 4). We then combine the physical property simulations for limestone, alluvium, and clay and produce a data base of physical properties to use as input to a geophysical model for that particular geologic configuration. The cavities are simulated separately and superimposed on the data base, as discussed above.

Figures 5 and 6 show density values for horizontal and vertical slices through a resulting density simulation for the physical system shown in Figure 4. In the lower section of the figure, density within the limestone varies slowly over distance. Above the limestone, Figure 4 shows three elements: (1) the contact between the limestone and the overlying alluvium and clay; (2) the presence of the clay lens near the top center of the plot; and (3) the water table, at about 15 ft beneath the surface.

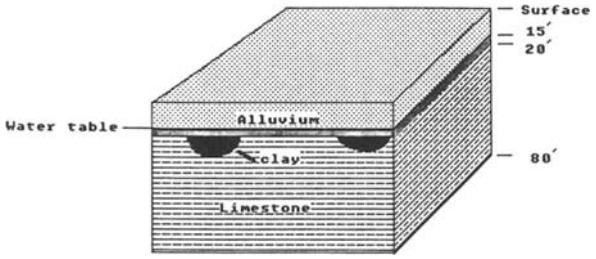

FIG. 4. Diagram of the physical system to be simulated. The rock types and boundaries and the water table are determined by the user. Properties are then simulated independently within each rock type.

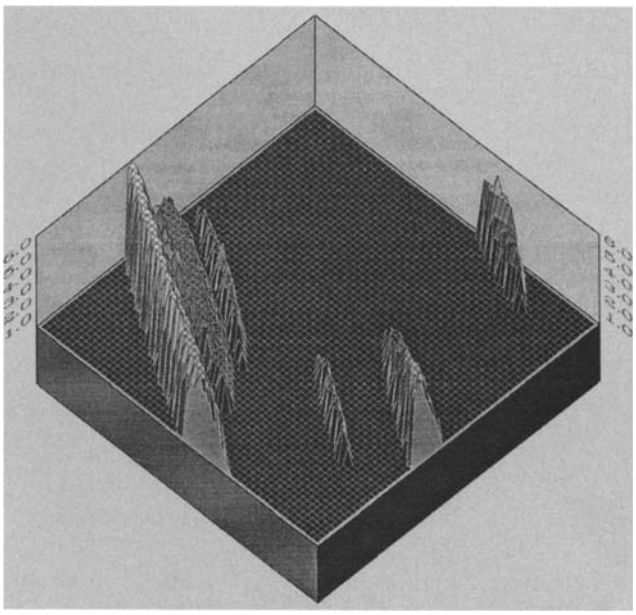

FIG. 3. Projection of cavities onto the surface plan. Plot height indicates cavity thickness.

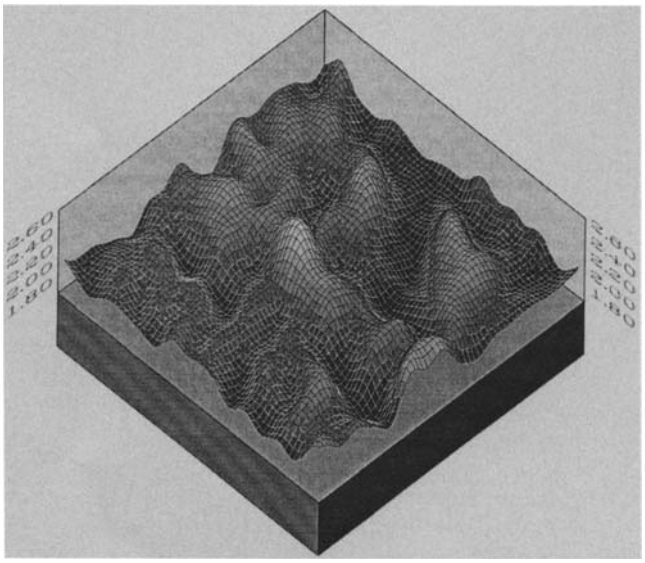

FIG. 5. Density for a horizontal cross-section through the physical model shown in Figure 4 in alluvium below the water table.

For this particular example, the range of influence of the Gaussian covariance model is tied not to physical data but to producing a scenario with more variability among some rock types (e.g., alluvium) than others (e.g., limestone). The absolute magnitude of the range of influence is not so important as the ratio of the range of influence to grid spacing and cavity size. For example, doubling both the range of influence and the grid spacing simultaneously would not alter nodal porosity values for a given simulation.

DISCUSSION AND CONCLUSIONS

Creating realistic geologic scenarios requires that simulations maintain the spatial persistence of high and low values. Frequency-domain simulation offers a means of rapidly computing many such simulations. The Fourier coefficients are computed once and then stored. All subsequent use of computer time results from generating standard normally distributed random numbers, multiplying the coefficients by them, and fast Fourier transforming the product.

For comparison of several geophysical prospecting methods, generating a single physical property (porosity) and functionally relating it to other properties needed for input to models greatly speeds the creation of simulations and eases tedious bookkeeping.

The most serious departures of these simulations from reality will be due to (1) statistical variations in the bulk properties which we have not taken into account, (2) the effects of capillary and absorbed water above the water table on the resistivity values, (3) the existence of cavities which are not ellipsoidal in form, (4) the multi-Gaussian distribution of porosity, which is not determined from field data, (5) independence of porosity values across rock type boundaries, and (6) pseudoperiodicity due to limited grid size and random weighting of individual spectral frequencies. Nevertheless, we feel that the simulations we produce in this way are effective, in the sense that they provide reasonable geophysical data. Readers may evaluate this point for themselves by reading Part II of this paper (Shive et al., 1990). In any case, most of the above difficulties can be minimized by use of more powerful hardware than was available to us.

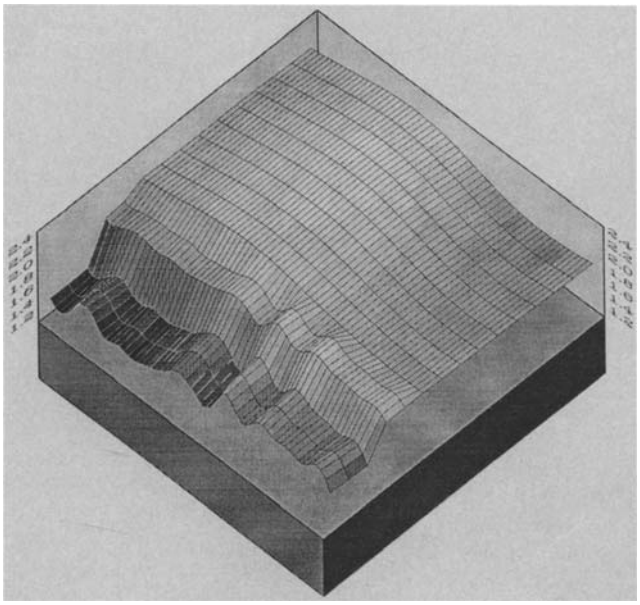

FIG. 6. Density for a vertical cross-section through the physical models shown in Figure 4.

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