CONDITIONAL SIMULATION AND ESTIMATION OF GAUSS-MARKOV RANDOM FIELDS USING THE BAYESIAN NEAREST NEIGHBOR METHOD

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Abstract

In this paper a specialized method for generating Markovian random fields, with or without conditioning, is presented. Here, the prior fields are assumed to be stationary second-order Gauss-Markov random fields in N-dimensional (N-D) euclidian space. The unconditional Markov fields are generated as numerical solutions of white-noise driven PDEs, for the solution of which finite difference or finite volume discretization on a regular grid yields an algorithm commonly known as the Nearest Neighbor Method (NNM). In addition, starting with the continuous space PDE-driven field, we develop a generalization of the NNM algorithm for the generation and optimal interpolation (estimation) of conditional random fields in the Bayesian sense. This generalized NNM algorithm is called Bayesian-NNM, or B-NNM, and is essentially similar to the classical NNM-type algorithms. The B-NNM method can be used for conditional simulation of random fields, as well as the optimal estimation of spatial fields assuming Markovian prior statistics, based on a collection of measurements or data. These data may be defined either at points or, more importantly, on continuous subdomains of various sizes and shapes, such as lineaments, faults, layers, boreholes, etc. In this paper, we also present exact closed form relations for linear estimation of 1-D Markovian fields, and this without recourse to space discretization. The complete analytical results are used for testing the multi-dimensional B-NNM code in the 1-D case.

1. Introduction and Overview

Geologic media are known to be heterogeneous when examined in detail but their detailed structure is rarely observed on a sufficiently large domain in the field. Nonetheless, a stochastic representation of spatial variability can be used for representing, based on available information, the unobserved fluctuations of material properties. More precisely, the medium is represented as a statistical continuum, with fluctuations that are random but, in a certain statistical sense, continuous. The statistical continuum approach has been used in a number of hydrogeologic studies, and there is today an increasing amount of experimental results and field data that supports the usefulness of the stochastic postulate (Gelhar, 1986; King and Smith, 1988; Baker, 1984).

We examine here a more specialized, but powerful, method for generating random fields with or without conditioning. Here, the prior fields are assumed to be stationary second-order Gauss-Markov random fields in N-dimensional euclidian space. Briefly, the unconditional Markov fields are generated as the numerical solutions of white noise-driven Partial Differential Equations (PDEs). A finite difference (FD) or finite volume discretization of this equation on a regular grid yields an algorithm commonly known as the Nearest Neighbor Method (NNM) (Whittle, 1962; King and Smith, 1988; Smith and Freeze, 1979 a,b; Smith and Schwartz, 1980). However, it is important to keep in mind that the random field model at hand is the continuous-space, PDE-driven process, rather than the discrete NNM model itself. Thus, it will be shown that, contrary to early applications of the method, certain strict restrictions need to be imposed on the parameters of the NNM model in order to obtain physically realizable and accurate approximations of the random fields. In addition, starting with the continuous space PDE-driven field, we develop a generalization of the NNM algorithm for the generation and optimal interpolation (estimation) of conditional random fields in the Bayesian sense. This generalized NNM algorithm is called Bayesian-NNM, or B-NNM and is similar to the classical NNM-type algorithms. The B-NNM method can be used for conditional simulation of random fields, as well as the optimal estimation of spatial fields assuming Markovian prior statistics, based on a collection of measurements or data. These data may be defined either at points or on continuous subdomains of various sizes and shapes, such as lineaments, faults, layers, boreholes, etc. While we only illustrate 1-D point conditioning in this paper, the more general case of subdomain conditioning will be important in future geological applications. When no data are provided the conditional B-NNM generator reduces to the unconditional NNM generator. We have also developed exact closed form relations for linear estimation of 1-D Markovian fields, and this without recourse to space discretization. The complete analytical results are used for testing purposes in the 1-D case.

2. Markov Fields and the Klein-Gordon Equation

2.1. ONE-DIMENSIONAL TIME

A discrete-time Markov process, $F(t_n)$, is such that the probability density function of the future state, $F(t_{n+1})$, depends only on the present state, $F(t_n)$, and not on the past states, $\{F(t_{n-1})...F(t_1)\}$:

$$P_{F(t)}\left(t_{n+1} \mid t_n, t_{n-1} \dots t_1\right) = P_{F(t)}\left(t_{n+1} \mid t_n\right) \tag{1}$$

For instance, the velocity $v(t)$ of a particle with mass m in a liquid follows a continuous Gauss-Markov process that is stationary:

$$\frac{dv}{dt} + \alpha v = \varepsilon(t) \tag{2}$$

where $\alpha = \beta/m$, β is a friction coefficient, and $\varepsilon(t)$ is a random (white) noise of intensity σ_0^2 (due to molecular shocks on the particle). Parameter α is the inverse of a correlation time $\alpha = 1/\tau$, with τ serving as an indicator of the *memory* of the stochastic process. The process $v(t)$ is entirely characterized as follows:

$$v(t) = v(0)\,\exp(-t/\tau) + \int_0^t \exp\left[\frac{-(t-s)}{\tau}\right]\varepsilon(s)\,ds \tag{3}$$

Given that $v(0) = 0$ or $t \to \infty$, this process satisfies:

$$\begin{aligned} E\,[v(t)] &= 0 \\ R_{vv}(t,s) &= \sigma_v^2\,\exp\left(\frac{|t-s|}{\tau}\right) \\ \sigma_v^2 &= \sigma_0^2 \end{aligned} \tag{4}$$

A Green's function representation of (2) suggests a direct method for generating $v(t)$ based only on the white-noise process $\varepsilon(t)$. It is worth noting the following: (i) as the correlation time $\tau = 1/\alpha$ goes to zero, $v(t)$ tends to a white noise of vanishing intensity (stationary); and (ii) as the correlation time $\tau = 1/\alpha$ goes to infinity, $v(t)$ tends to a non-stationary Wiener process, that is the integral of a white noise. The latter case is the most interesting; in case of zero-friction, the velocity process is a Wiener process with an infinite correlation scale in time. This process is non-stationary:

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$$\frac{dW}{dt} = \varepsilon(t) \tag{5}$$

$$\begin{aligned} E\left[W(t)\right] &= 0 \\ \sigma_w^2(t) &= \sigma_0^2\, t \\ W(t) &= W(0) + \int_0^t \varepsilon(s)\, ds \end{aligned} \tag{6}$$

2.2. ONE-DIMENSIONAL SPACE

A natural way to generalize the Markov property in the non-oriented $\mathbb{R}^1$ space is as follows. For a discrete-space process $F(X_i)$, the Markov property corresponds to the independence of the future state, $F(X_{i+1})$, and the past state, $F(X_{i-1})$, given the present state, $F(X_i)$:

$$P_{F,F}\left(X_{i-1}, X_{i+1} \mid X_i\right) = P_F\left(X_{i-1} \mid X_i\right) \cdot P_F\left(X_{i+1} \mid X_i\right) \tag{7}$$

Similar to the time Gauss-Markov process, one obtains a 1-D space Gauss-Markov process that is stationary and satisfies:

$$\frac{d^2F}{dx^2} - \alpha^2 F(x) = \sigma_o\, U(x) \tag{8}$$

where $U(x)$ is a white noise with unit intensity, and α is inversely proportional to the integral correlation scale λ of the process $F(x)$:

$$\begin{aligned} R_{uu}(\xi) &= \delta(\xi) \\ \alpha &= 2/\lambda \end{aligned} \tag{9}$$

The integral correlation scale is defined by a one-sided integral as:

$$\lambda = \int_0^\infty P_{FF}(\xi)\, d\xi \tag{10}$$

Note that the right hand side (RHS) of (8) can be replaced by:

$$\sigma_o \frac{dW}{dx} \tag{11}$$

where $W(x)$ is a Wiener process defined in (6). The covariance structure of a zero-mean process satisfying (8) is as follows:

$$\begin{aligned} E\left[F(x)\right] &= 0 \\ R_{FF}(\xi) &= \sigma_F^2\left(1 + \alpha|\xi|\right)\exp\left(-\alpha|\xi|\right) \\ \sigma_F^2 &= \frac{1}{4\alpha^3}\sigma_0^2 \end{aligned} \tag{12}$$

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Note that the spatial Gauss-Markov process defined in (8) has the following characteristics: (i) it is stationary, and (ii) imposes a covariance structure that is dependent on dimensionality.

We may now investigate a Green's function representation of the process satisfying (8). Remember that for the time process, this was given by (2) for a given initial condition. Now we need boundary conditions (BCs) rather than an initial condition. In order to obtain an infinite domain representation, the boundaries should be taken at infinity $(x = \pm\infty)$. By specifying deterministic homogeneous BCs:

$$F(\pm\infty) = 0 \tag{13}$$

we obtain the Green's function representation:

$$F(x) = \left(-\frac{\sigma_0}{2\alpha}\right) \int_{-\infty}^{+\infty} \exp\left(-\alpha|x-\xi|\right) U(\xi)\, d\xi \tag{14}$$

As a result, we have obtained an explicit representation for the zero-mean, stationary Markov process characterized by the covariance function (12). Note again that $U(\xi) = \frac{dW}{d\xi}$ is in the integral of (14), so this integral exists only because the Wiener process $W(\xi)$ exists.

2.3. MULTI-DIMENSIONAL SPACE

The generalization of the Markov property to the continuous 2-D and 3-D spaces is not a trivial matter. For a discrete multi-dimensional space, the independence property similar to that enunciated in Section 2.2 can be extended quite easily. However, in the continuous space, a more subtle definition is needed. See, for example, the definition of a pseudo-Markov random field in Adler (1981).

The probability of events $\{F(\underline{X}) = F_0(\underline{X})\}$ in the interior of a closed domain (the past) is independent of events $\{F(\underline{X}) = F_1(\underline{X})\}$ in its exterior (the future), given $F(\underline{X})$ in an open neighborhood surrounding the domain boundary (the present). By analogy with the 1-D spatial Gauss-Markov process analyzed above, it turns out that a stationary Gauss-Markov process in either 1-D, 2-D, or 3-D is obtained from the solution of the following PDE (Vanmarcke, 1988; Whittle, 1962):

$$\left(\nabla^2 - \alpha^2\right) F(\underline{X}) = \sigma_0\, U(\underline{X}) \tag{15}$$

The 1-D case has been analyzed above. In 2-D, the Green's function of (15) with a zero RHS (Klein-Gordon equation) involves Hankel functions. The covariance function of the resulting process involves a Bessel function (Vanmarcke, 1988). In 3-D, the Green's function takes a simpler form, when subject to the homogeneous deterministic BCs $F(\underline{X}) = 0$ as X_1, X_2, X_3 or $r = \sqrt{X_1^2 + X_2^2 + X_3^2}$ goes to infinity:

$$G\left(\underline{X}, \underline{X}'\right) = \frac{1}{4\pi} \frac{\exp\left(-\alpha|\underline{r} - \underline{r}'|\right)}{|\underline{r} - \underline{r}'|} \tag{16}$$

The resulting 3-D Gauss-Markov process $F(\underline{X})$ has a Green's function representation, called a fundamental solution to (15):

$$F(\underline{X}) = \frac{\sigma_0}{4\pi} \iiint_{-\infty}^{+\infty} \frac{\exp\left(-\alpha |\underline{r} - \underline{r}'|\right)}{|\underline{r} - \underline{r}'|} U(\underline{X}')\, d\underline{X}' \tag{17}$$

where

$$|\underline{r} - \underline{r}'| = \sqrt{(X_1 - X_1')^2 + (X_2 - X_2')^2 + (X_3 - X_3')^2} \tag{18}$$

and

$$d\underline{X}' = dx_1'\, dx_2'\, dx_3' \tag{19}$$

It is not difficult to check that $F(\underline{X})$, as given by (17) is indeed a zero-mean 3-D Gauss-Markov process having the following characteristics (Vanmarcke, 1988):

$$\begin{aligned} R_{FF}(\xi) &= \sigma_F^2 \exp(-\alpha|\xi|) \\ \sigma_F^2 &= \frac{\pi}{\alpha} \sigma_o^2 \\ \lambda^3 &= \frac{\pi}{\alpha^3} \end{aligned} \tag{20}$$

where λ is the correlation scale (one-sided) defined as:

$$\lambda^3 = \iiint_0^{+\infty} \rho_{FF}(\xi)\, d\xi = \frac{1}{2^3} \iiint_{-\infty}^{+\infty} \rho_{FF}(\xi)\, d\xi \tag{21}$$

Once again, it is important to keep in mind the dependence of the covariance model on the problem dimensionality. The discretization of the white noise field $U(\underline{X})$ into the white lattice process $\hat{U}$ was designed so that the variance σ_F^2 be preserved. However, the correlation structure of $F(\underline{X})$ will be preserved only if $\alpha \Delta = \frac{\Delta}{\lambda} << 1$, where Δ is the grid size. The effect of truncating the infinite sum at some value $|i,j,k| \leq n$ can be limited by ensuring that the relative error in the imposed variance, defined as:

$$\varepsilon^2 = \frac{\sigma_F^2 - \sigma_{F*}^2}{\sigma_F^2} \approx \frac{\pi \exp(-2m\alpha\Delta)}{(2\pi\alpha\Delta)^3} \tag{22}$$

is very small, (i.e., $\varepsilon^2 << 1$). Thus, the two requirements are:

Resolution: $\frac{\Delta}{\lambda} << 1$ for an adequate resolution (spatial integral discretization)

Accuracy: $\varepsilon^2 << 1 \;\Rightarrow\; n >> \left(\frac{\Delta}{\lambda}\right)^{-1}$ for an adequate accuracy (cut-off of infinite sum over space at distance equal to *n*, the lattice spacing).

3. Consistent Discretization of the Klein-Gordon Equation

3.1. ONE-DIMENSIONAL CASE

We examine again the 1-D spatial Gauss-Markov process of equation (8) with the RHS given by (11). Discretization of this PDE leads to:

$$\begin{aligned} \frac{d^2F}{dx^2} &= \frac{F_{i+1} - 2F_i + F_{i-1}}{\Delta^2} + O(\Delta^2) \\ U(x) = \frac{dW}{dx} &= \frac{W_{i+1/2} - W_{i-1/2}}{\Delta} + O(\Delta^2) \\ &= \frac{1}{\Delta}\int_{x_{i-1/2}}^{x_{i+1/2}} U(x)\,dx + O(\Delta^2) \end{aligned} \tag{23}$$

which leads to the FD system:

$$\frac{F_{i+1} - 2F_i + F_{i-1}}{\Delta^2} - \alpha^2 F_i = \sigma_o \frac{1}{\Delta}\int_{x_{i-1/2}}^{x_{i+1/2}} U(x)\,dx + O(\Delta^2) \tag{24}$$

Observe that $\overline{U}(x_i) = \frac{1}{\Delta}\int_{x_{i-1/2}}^{x_{i+1/2}} U(x)\,dx$ is a white sequence with variance $\sigma_{\bar{u}}^2 = \frac{1}{\Delta}$. For convenience, we define $\hat{U}(x_i)$ the white sequence with unit variance, such that:

$$R_{\hat{u}\hat{u}}(i\Delta) = 0 \text{ for } i \neq 0 \tag{25}$$

$$R_{\hat{u}\hat{u}}(i\Delta) = 1 \text{ for } i = 0 \tag{26}$$

The FD system to be solved can be expressed, using $\overline{U}(x_i) \equiv \frac{1}{\Delta^{1/2}}\hat{U}(x_i)$, as:

$$F_i = a\,(F_{i+1} + F_{i-1}) + b\,\hat{U}(x_i) \tag{27}$$

with

$$\begin{aligned} a &= \frac{1}{2 + (\alpha\Delta)^2} \\ b &= \frac{\sigma_o\,\Delta^{3/2}}{2 + (\alpha\Delta)^2} = \frac{2(\alpha\Delta)^{3/2}\sigma_F}{2 + (\alpha\Delta)^2} \end{aligned} \tag{28}$$

where α and σ_o are known in terms of the *true* $F(\underline{X})$ process:

$$\alpha = \frac{2}{\lambda_F} \qquad \sigma_o^2 = 4\,\alpha^3\,\sigma_F^2 \tag{29}$$

Equation (27) constitutes a system of simultaneous algebraic equations, which is solved numerically for all F_i. The resolution requirement is that:

$$\frac{\Delta}{\lambda} = \frac{1}{2}\alpha\Delta << 1 \tag{30}$$

whence the constraint on the parameter a is $1/6 << a < 1/2$. Note that $a >> 1/6$ is an approximate constraint for accuracy, while $a < 1/2$ is a constraint imposed for physical realizability of stationary fields in the continuous space. Also, note that the main problem is that of BCs. In practice, we should solve (8) for BCs obeying (13) on a domain larger than the domain of interest by several correlation scales.

3.2. MULTI-DIMENSIONAL CASE

In 3-D, we obtain after a similar discretization of the governing equation (15):

$$\imath\left(F_{i-1,j,k} + F_{i,j-1,k} + F_{i,j,k-1} + F_{i+1,j,k} + F_{i,j+1,k} + F_{i,j,k+1}\right) + \tag{31}$$

where $\hat{U}(i,j,k)$ is a white (uncorrelated) sequence on the lattice, with unit variance. The parameters a and b are now given by:

$$a = \frac{1}{6 + (\alpha\Delta)^2} \qquad b = \frac{\sigma_o\,\Delta^{1/2}}{6 + (\alpha\Delta)^2} \tag{32}$$

We have also shown that α and σ_o are related to the true (continuous) process $F(\underline{X})$ according to (20). Obviously we have $0 < a < 1/6$. However, the resolution requirement $\Delta/\lambda << a < 1/6$ yields $1/8 << a < 1/6$. It is worth noting how strict these constraints are, which is one of the major limitations of this method. On the other hand, however, one should also take note of the very close similarity of (31) to the structure of the system of algebraic equations appearing in any FD-based flow and/or transport problem. As such, the method discussed herein is an extremely efficient algorithmic platform to perform successive realization generation and flow and transport simulations in a Monte Carlo fashion.

4. Bayesian Conditioning of Multi-Dimensional Gauss-Markov Fields

In the probabilistic approach to subsurface flow and contaminant migration, the hydraulic properties of the (naturally heterogeneous) geologic medium are represented as spatially correlated random fields with known *prior* statistics (*posterior* statistics are discussed below). For gaussian fields, or their one-to-one transforms, the priors can be reduced to the first and second order moments: mean and 2-point covariance function. The covariance yields two kinds of information: the single-point variance, and the 2-point correlation function. In hydrogeology, the type of information used for determining these prior statistics may consist of sample statistics obtained directly from site-specific data, statistical information inferred from other geologic sites, and various qualitative or indirect information (geological facies, geophysical logs, etc).

In addition, once prior statistics have been identified, the random field may be further conditioned, that is constrained to match a given set of observations within the specific site at hand. Bayesian conditioning of a stationary prior field $Y(x)$ leads to a non-stationary posterior field, or conditional field, $Y^*(x)$. Denote Z the vector of observations and Y the state vector corresponding to field $Y(x_i)$ at a set of locations x_i. In the case of a gaussian prior, it can be shown that the conditional random field ì(x) is a linear combination of the random prior at point x, the random prior at all data points, and the data values themselves. The posterior mean, that is the mean of the conditional field, is denoted <ì> or $<Y|Z>$. It can be shown that the posterior mean is the best linear unbiased *estimator* of Y, in the Bayesian sense. Furthermore, in the case of a gaussian prior, it can be shown that <ì> is a linear combination of the prior mean vector $<Y>$ and the data vector Z. The resulting estimator <ì> is equivalent to the field produced by simple kriging. The reader is referred to Journel and Huijbregts (1978) and Delhomme (1979) for the geostatistical viewpoint on conditional estimation and to Ababou et al. (1994), and references therein, for the Bayesian estimation viewpoint. Both approaches can be viewed as statistical solutions to the problem of optimal spatial interpolation, or optimal estimation of spatial fields.

4.1. POINT CONDITIONING OF 1-D GAUSS-MARKOV FIELDS: ANALYTICAL METHOD AND VERIFICATION

We exploit here the special properties of Markov fields (more precisely, 2nd-order Markov fields) in 1-D space. Using the past-future analogy, this property can be simply stated as follows: the *future* depends only on the *present* and not on the *past*. In other words, if two point measurements are made, defining an interval, the random field values outside that interval depend only on the two point measurements, and not on the random field values inside that interval. The reverse holds true also. That is, the values inside and outside the domain — conditioned in the two point measurements — are mutually independent.

This property allows us to condition the PDE-driven Markov field by solving a 2-point boundary value problem. Moreover, any number of conditioning points may be included. Consider for instance the case of M conditioning points, which define a total of M + 1 intervals:

$$\begin{array}{ll} (1) & : [-\infty,\ x_1] \\ (2) & : [x_1,\ x_2] \\ . & \quad . \\ . & \quad . \\ . & \quad . \\ (M) & : [x_{M-1},\ x_M] \\ (M+1) & : [x_M,\ +\infty] \end{array} \tag{33}$$

The conditional Markov field can be generated on $[-\infty, +\infty]$ by solving (independently) the 2-point, white noise-driven, boundary value problems:

$$\begin{gathered} \frac{d^2Y}{dx^2} - \alpha^2\, Y = f(x) \\ Y(x_i) = Y_i \;;\; Y(x_{i+1}) = Y_{i+1} \end{gathered} \tag{34}$$

on each interval $[x_i,\ x_{i+1}]$. The boundary conditions at $x_o = -\infty$ and $x_{M+1} = +\infty$ must be zero in order to ensure convergence of the conditional statistics to the unconditional ones at infinite distances from the conditioning points. Thus, we can use $Y_o = 0,\ Y_{M+1} = 0$ for external, far field, BCs. On the other hand, the values $\{Y_1, Y_2, \ldots.. Y_M\}$ represent the M measurements (*internal* BCs). The solution of the above 2-point boundary value problem can be obtained by the Green's function approach. The full Green's function for the 1-D operator is developed on a finite interval [-R,+R], with *homogeneous* Dirichlet conditions $Y(+R) = Y(-R) = 0$. We denote this Green's function by $G_R(x,y)$. The final result is:

$$G_R(x,y) = -\frac{1}{2\alpha}\,\frac{ch[\alpha(2R - |x-y|)] - ch[\alpha|x+y|]}{sh(2\alpha R)} \tag{35}$$

Incidentally, as $R \to \infty$, we recover the infinite domain (free space) Green's function:

$$G(x,y) = -\frac{1}{2\alpha}\exp(-\alpha|x-y|) \tag{36}$$

which corresponds to the unconditional field.

For each interval $[x_i,\ x_{i+1}]$ equating $x_{i+1} = 2R_i$ and using a simple transformation of coordinates, the Green's function is found to be:

$$G_{Ri}(x,y) = -\frac{1}{2\alpha}\,\frac{ch[\alpha(x_{i+1} - x_i - |x-y|)] - ch[\alpha(x + y - x_i - x_{i+1})]}{sh[\alpha(x_{i+1} - x_i)]} \tag{37}$$

where x and y are both in $[x_i,\ x_{i+1}]$. Therefore, the solution $Y_A(x)$ satisfying the *homogeneous* conditions $Y_A(x_i) = 0$ and $Y_A(x_{i+1}) = 0$ is given by:

$$Y_A(x) = \int_{x_i}^{x_{i+1}} G_{Ri}(x,y)\ f(y)\ dy, \qquad x_i \le x \le x_{i+1} \tag{38}$$

This solution needs to be modified in order to obtain the correct BCs, which are usually non-zero. Thus, let:

$$Y(x) = Y_A(x) + Y_B(x) \tag{39}$$

where: (i) Y satisfies the original PDE, which is inhomogeneous and has *inhomogeneous* BCs; (ii) Y_A satisfies the same inhomogeneous equation, but with *homogeneous* conditions $Y_A = 0$; and (iii) Y_B satisfies the homogeneous equations with zero RHS, but with the correct *inhomogeneous* conditions $Y_B(x_i) = Y_i$, $Y_B(x_{i+1}) = Y_{i+1}$. It is easily seen that $Y = Y_A + Y_B$ is indeed the solution of (34) as stated above. To obtain Y_B, we solve:

$$\begin{gathered}\frac{d^2 Y_B}{dx^2} - \alpha^2 Y_B = 0 \\ Y_B(x_i) = Y_i\ ;\ Y_B(x_{i+1}) = Y_{i+1}\end{gathered} \tag{40}$$

This yields a solution of the form:

$$Y_B(x) = a_i \exp(\alpha x) + b_i \exp(-\alpha x) \qquad (x_i \le x \le x_{i+1}) \tag{41}$$

where the coefficients (a_i, b_i) are obtained by substituting the above BCs. This gives:

$$\begin{aligned} a_i &= \frac{Y_{i+1} \exp(-\alpha x_i) - Y_i \exp(-\alpha x_{i+1})}{2\, sh(\alpha (x_{i+1} - x_i))} \\ b_i &= \frac{-Y_{i+1} \exp(\alpha x_i) + Y_i \exp(\alpha x_{i+1})}{2\, sh(\alpha (x_{i+1} - x_i))} \end{aligned} \tag{42}$$

Equations (37) to (42) give a complete characterization of the conditional random field $Y(x)$. The random part $Y_A(x)$ is a zero-mean stochastic integral of white noise, while the remaining part $Y_B(x)$ is deterministic and depends on the measurements. It follows that $Y_B(x)$ represents the posterior mean of the conditional random field $Y(x)$. Thus, we have:

$$< Y(x) > = Y_B(x) \tag{43}$$

or:

$$< Y(x) > = \frac{Y_{i+1}\, sh(\alpha (x - x_i)) - Y_i\, sh(\alpha (x - x_{i+1}))}{sh(\alpha (x_{i+1} - x_i))} \tag{44}$$

within each measurement interval $[x_i,\ x_{i+1}]$. Note that (44) gives the kriged Markov field in closed form, that is kriging can be performed analytically in this case. The posterior variance, or estimation variance, can also be developed analytically as follows. We have by construction:

$$Var[Y(x)] = Var[Y_A(x)] \tag{45}$$

Upon substituting the stochastic white noise integral for Y_A, we obtain for $x_i \le x \le x_{i+1}$

$$Var[Y(x)] = \sigma_F^2 \int_{x_i}^{x_{i+1}} G_{Ri}(x,y)^2\, dy \tag{46}$$

Substituting the previous expression for G_{Ri}, and integrating, yields:

$$Var[Y(x)] = \frac{1}{4\alpha^3} \frac{2\alpha (x_{i+1} - x_i) + sh(2\alpha (x_{i+1} - x_i)) - sh(2\alpha (x - x_i)) - sh(2\alpha (x_{i+1} - x))}{2\, sh^2(\alpha (x_{i+1} - x_i))} \tag{47}$$

This expression gives the posterior variance, or kriging estimation variance, for each conditioning interval $x \in [x_i,\ x_{i+1}]$. As a matter of verification, note that we recover the correct prior variance:

$$\sigma_Y^2 = \frac{1}{4\alpha^3} \tag{48}$$

by letting x_i 6 & 4 and $x_{i\%1}$ 6 % 4. This expression coincides with that obtained directly from the Green's function representation of the unconditional Markov field.

4.2. RESULTS AND DISCUSSION

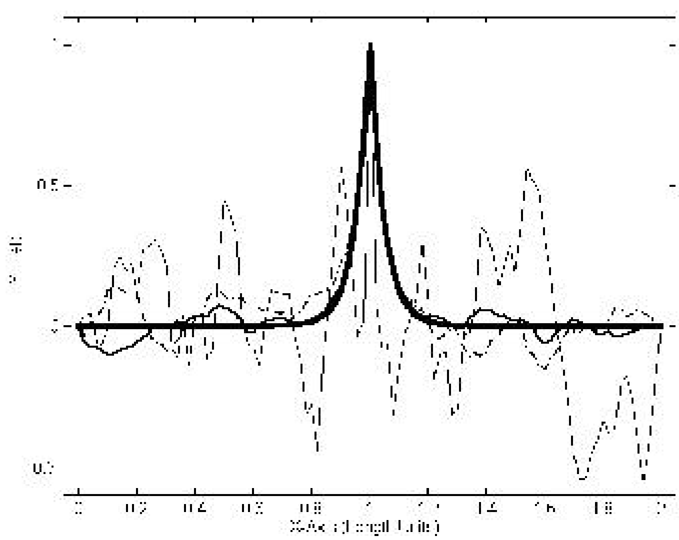

Figure 1. Comparison of a realization (fine solid) and the mean of 200 (thin dash-dot) and 1000 (thin solid) B-NNM realizations to equation (44) (thick solid).

An application and verification of the B-NNM algorithm is presented, together with analytical results, in Figure 1. The 1-D field has a ë = 0.1 (corresponding to five grid points) and is conditioned by imposing $Y(x=1) = 1.0$ for each of the Monte Carlo realizations. The substantial variability inherent in any particular realization is apparent. One should also note the relatively slow rate of convergence of the mean of the conditional realizations towards the *true* mean given by (44). A detailed analysis of convergence, depicted in Figure 2, indicated that the root mean square error (RMSE) for the mean of the conditional realizations approaches the *true* mean according to $(nmc)^{-1/2}$, where *nmc* is the number of Monte Carlo realizations involved.

Finally, Figure 3 depicts a comparison of the B-NNM results in terms of the kriging estimation variance, or standard deviation (STD), against the closed form solution given by (47). One should note that the kriging estimation variance converges towards the *true* variance at the same rate as the mean far from the conditioning points. The rate of convergence, however, is significantly lower near the conditioning points, possibly because of boundary effects.

5. Conclusions

In this paper, a specialized method for generating conditional random fields has been presented and tested

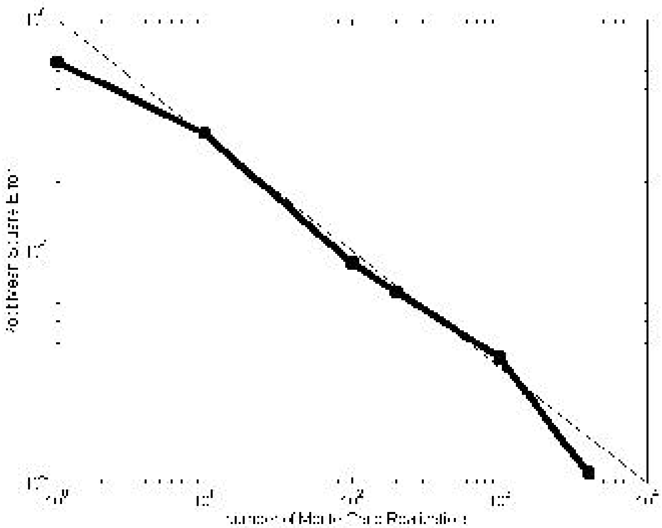

Figure 2. RMSE for the mean of conditional realizations, as a function of *nmc*. Fine solid line is the $(nmc)^{-1/2}$ behavior.

for a 1-D problem against closed form solutions. The method presented here requires very strict resolution and accuracy constraints that need to be imposed for the generated fields to honor the desired covariance structures, which depend on the dimensionality of the problem. On the other hand, the method leads to solution of systems of algebraic equations that are very similar to those appearing in any FD-based flow and/or transport problem. As such, the method presented here is a promising algorithmic platform for conducting environmental assessments in a Monte Carlo fashion and deserves further study.

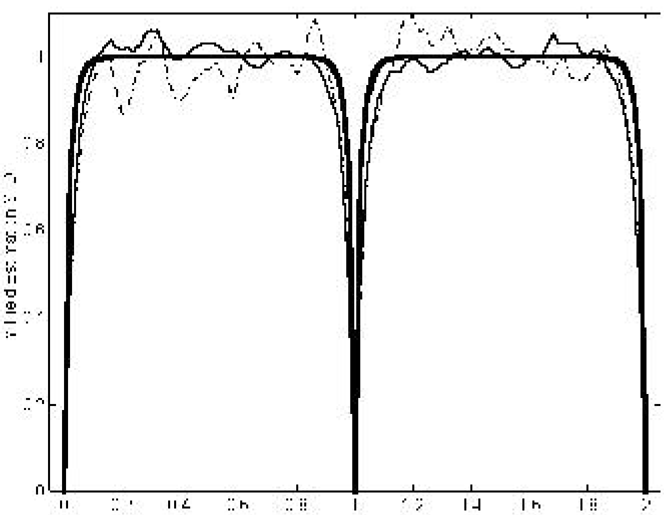

Figure 3. Comparison of kriging estimation STD, as obtained by B-NNM for 200 (thin dash-dot) and 1000 (thin solid) realizations, to equation (47) (thick solid).

6. Acknowledgements

This paper was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the Nuclear Regulatory Commission (NRC) under Contract No. NRC-02-93-005. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management, and the NRC Office of Nuclear Regulatory Research, Division of Regulatory Applications. The paper is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC. Comments by two anonymous reviewers and the Editor's office helped improve the quality of this paper.

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