

# Geostatistical Space–Time Models: A Review<sup>1</sup>

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*Geostatistical space–time models are used increasingly for addressing environmental problems, such as monitoring acid deposition or global warming, and forecasting precipitation or stream flow. Each discipline approaches the problem of joint space–time modeling from its own perspective, a fact leading to a significant amount of overlapping models and, possibly, confusion. This paper attempts an annotated survey of models proposed in the literature, stating contributions and pinpointing shortcomings. Stochastic models that extend spatial statistics (geostatistics) to include the additional time dimension are presented with a common notation to facilitate comparison. Two conceptual viewpoints are distinguished: (1) approaches involving a single spatiotemporal random function model, and (2) approaches involving vectors of space random functions or vectors of time series. Links between these two viewpoints are then revealed; advantages and shortcomings are highlighted. Inference from space–time data is revisited, and assessment of joint space–time uncertainty via stochastic imaging is suggested.*

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**KEY WORDS:** space–time models, geostatistics, time series, trend models, stochastic simulation.

## INTRODUCTION

The modeling of spatiotemporal distributions resulting from dynamic processes evolving in both space and time is critical in many scientific and engineering fields: environmental sciences, climate prediction and meteorology, hydrology and reservoir engineering, to name but a few. Geostatistical space–time models have been applied for modeling spatiotemporal distributions in several scientific disciplines. Examples of such applications include determination of space–time trends in the deposition of atmospheric pollutants (Eynon and Switzer, 1983; Bilonick, 1985; Rouhani and others, 1992; Oehlert, 1993; Vyas and Christakos, 1997), characterization

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of space–time variability of the Earth’s geophysical parameters (Haslett and Raftery, 1989; Séguret and Huchon, 1990; Handcock and Wallis, 1994; Bogaert and Christakos, 1997a), modeling of temporal evolution of spatial patterns in soil moisture content (Goovaerts and Sonnet, 1993; Papritz and Flühler, 1994; Heuvelink, Musters, and Pebesma, 1997), estimation of rainfall or piezometric head fields (Bras and Rodríguez-Iturbe, 1984; Rouhani and Wackernagel, 1990; Armstrong, Chetboun, and Hubert, 1993), modeling of spatiotemporal patterns of diseases and exposure to pollutants (Christakos and Lai, 1997; Carroll and others, 1997; Christakos and Hristopulos, 1998), characterization of population dynamics in ecology (Hohn, Leibhold, and Gribko, 1993), and design of sampling networks for monitoring spatiotemporal processes (Rodríguez-Iturbe and Mejía, 1974; Switzer, 1979; Guttorp, Sampson and Newman, 1992; Mardia and Goodall, 1993).

Geostatistical spatiotemporal models provide a probabilistic framework for data analysis and predictions that builds on the joint spatial and temporal dependence between observations. Most often, stochastic models cannot explain by themselves causal effects stemming from the physical processes generating the data, one exception being the kinetic-molecular movement within a gas. The physics of the phenomenon under study can be accounted for by deterministic models involving solution of the appropriate governing equations, e.g., the flow equation in the case of modeling piezometric head levels in an aquifer. Such deterministic models typically require a large number of input parameters that are difficult to determine due to limited and/or indirect (soft) sampling. Stochastic models, on the other hand, are based typically on a small number of parameters that can be inferred and modeled; they aim at building a process that only mimics some patterns of the observed spatiotemporal variability, without necessarily following the underlying governing equations. The model randomness may not originate from the actual physical process; it is most often a (model-dependent) measure of our ignorance (uncertainty) regarding the unique physical process, whose parameters are not completely known. Stochastic models are then considered as alternative approaches until more elaborate physically based models become available.

However, aspects of stochastic spatiotemporal models can be interpreted in the realm of physically based models (Christakos and Raghu, 1996; Jones and Zhang, 1997). Several researchers have suggested linking the trend component of stochastic models to deterministic models (Venkatram, 1988; Haslett, 1989; Pereira, Soares, and Branquinho, 1997; Haas, 1998), and they subsequently analyze the joint space–time distribution of the residual data (observed minus deterministically predicted values). In meteorological applications, for example, model predictions are refined via interpolation based on errors determined at “calibration” locations where both

predictions and observations are available. This refinement procedure, when performed by means of spatial statistics techniques, is called Optimal Statistical Objective Analysis (OSOA) (Gandin, 1963) and is mainly focused on the spatial aspect of the error field, as noted by Haslett (1989).

Space–time data are traditionally analyzed through models initially developed for spatial or temporal distributions. The joint space–time dependence is often not fully modeled nor exploited in estimation or forecasting of the unknown value at an unmonitored location.

Often, analysis may be focused on smooth interpolated attribute maps of the attribute of interest over specific time instants. Such maps are constructed using only contemporaneous data, possibly including covariates, and statistics inferred from them (Tabios and Salas, 1985; Hudson and Wackernagel, 1994). The objective might be to compare the various maps or detect persistence or changes in the spatial patterns over time; see, for example, Goovaerts and Chiang (1993) and Simard and Marcotte (1993) for soil science and ecological applications, respectively.

Alternatively, analysis may be focused on modeling time series of the attribute of interest. Multivariate time series (TS) models are then considered, generally referred to as spatial time series (Cliff and others, 1975; Bennett, 1979), where each spatial location is associated with a distinct time series. When the TS are spatially correlated, their parameters are made correlated in space, see, for example, Bras and Rodríguez-Iturbe (1984, chapter 3) for developments in a hydrologic context, and Haslett and Raftery (1989) for a meteorological application. Time series models typically assume a regular sampling over time, and a temporal lag operator is defined for modeling causality between current and previous observations along the time axis (Box, Jenkins, and Reinsel, 1994). Such a lag operator cannot be easily generalized to the spatial domain (where data are seldomly located on a regular grid) to include an instantaneous spatial dependence (Cressie, 1993, p. 450). Spatial time series models yield predictions only at those specific partially informed locations, thus further modeling is required for allowing the all important procedure of mapping in space.

Geostatistics provides tools for joint analysis of the space and time components, and builds on the extension of established spatial techniques developed independently in geology (Matheron, 1962; Journel and Huijbregts, 1978), forestry (Matérn, 1980), and meteorology (Gandin, 1963), to include time as an additional space dimension. Such extension does not require regularity of sampling either in space or in time. Simultaneity of data in space, a case not handled easily by spatial TS models because of lack of instantaneous spatial dependence, reduces here to a purely spatial problem. Because causation in space or time is not called for, spatial or temporal lag operators need not be defined.

Different processes act on different spatial and temporal scales; hence, any averaging procedure, either spatial or temporal, alters the original spatiotemporal correlation of the process under study. Certain problems relate to the characterization of aggregate variables, e.g., the temporal evolution of the temperature averaged over a geographic region. Inference in such cases should account for the increased spatial (or temporal) continuity (Bacchi and Kottegoda, 1995). Geostatistical space–time models have been also developed for addressing the difference between scales regarding the original and aggregate processes (Rodríguez-Iturbe and Mejía, 1974; Sølna and Switzer, 1996).

The review that follows is focused on stochastic models involving extension of spatial (geostatistical) analysis tools to include the additional time dimension. The objective is to build a thread linking the various stochastic models proposed, as well as to highlight their assumptions, advantages, and limitations.

## THE JOINT SPACE–TIME FRAMEWORK

Consider a finite domain  $D$  in space, and a finite domain  $T$  in time, with  $D \subseteq R^d$  and  $T \subseteq R^1$ . Without loss of generality, assume that  $d = 2$ ; hence  $R^2$  is the two-dimensional (horizontal) space. A spatiotemporal random variable (RV)  $Z(\mathbf{u}, t)$  is a variable that can take a series of outcome values (realizations) at any location in space  $\mathbf{u} \in D$  and instant in time  $t \in T$ , according to a probability distribution. The RV  $Z(\mathbf{u}, t)$  is fully characterized by its cumulative distribution function (cdf), which gives the probability that the variable  $Z$  at location  $\mathbf{u}$  in space and instant  $t$  in time is no greater than any given threshold  $z$ :

$$F(\mathbf{u}, t, z) = \text{Prob}\{Z(\mathbf{u}, t) \leq z\}, \quad \forall z, (\mathbf{u}, t) \in D \times T$$

A spatiotemporal random function (RF)  $\{Z(\mathbf{u}, t), (\mathbf{u}, t) \in D \times T\}$  is defined as a set of usually dependent RVs  $Z(\mathbf{u}, t)$ , one for each location in space  $\mathbf{u} \in D$  and instant in time  $t \in T$ . A realization of the RF  $Z(\mathbf{u}, t)$  is a collection of realizations of its component RVs.

Although observations are placed into this combined space–time  $D \times T$  framework, there are fundamental differences between the coordinate axes, i.e., between space and time (Weyl, 1952; Reichenbach, 1958). A clear ordering of temporal data in past, present, and future exists, while such ordering cannot be defined for spatial observations. In the time domain, measurements are most often taken on one side of the time axis (the past)—hence estimation is most often in extrapolation mode. Isotropy is well defined in space, while it has no meaning in a space–time context due

to the intrinsic ordering and nonreversibility of time. Scales and distance units are different between space and time and cannot be directly compared in a physical sense. The combined space–time domain  $D \times T$  acknowledges these differences, and should be regarded only as a coordinate system, where observations are tagged by a spatial coordinate vector  $\mathbf{u} = (x, y, z)$  and a temporal coordinate  $t$ .

Consider a discretization of the three-dimensional (3D) space–time domain  $D \times T$ , into a set of  $N \times T$  “points,” where  $N$  and  $T$  are the number of “points” in the spatial and temporal domains, respectively. To any set of  $NT$  points in  $D \times T$  corresponds a vector of  $NT$  RVs  $\{Z(\mathbf{u}_1, t_1), \dots, Z(\mathbf{u}_N, t_T)\}$ , which is characterized by the  $NT$ -variate or  $NT$ -point cdf:

$$F(\mathbf{u}_1, t_1, \dots, \mathbf{u}_N, t_T; z_{11}, \dots, z_{NT}) = \text{Prob}\{Z(\mathbf{u}_1, t_1) \leq z_{11}, \dots, Z(\mathbf{u}_N, t_T) \leq z_{NT}\}$$

This multivariate or multipoint cdf characterizes the joint uncertainty about the  $NT$  actual values  $\{z(\mathbf{u}_1, t_1), \dots, z(\mathbf{u}_N, t_T)\}$ . The set of all such  $NT$ -variate cdfs, for any positive integers  $N, T$  and for any choice of the space–time locations, constitutes the spatiotemporal law of the RF  $Z(\mathbf{u}, t)$ .

Inference of this spatiotemporal law requires repetitive realizations of the component RVs at each space–time location  $(\mathbf{u}, t) \in D \times T$ , which are never available in practice. The classical inference paradigm consists of pooling together pairs of measurements separated by the same space–time vector  $(\mathbf{h}, \tau) \in D \times T$ , with  $\mathbf{h} = \mathbf{u} - \mathbf{u}'$  and  $\tau = t - t'$ , and use these pairs as a set of repetitions. This pooling corresponds to the model decision (not a hypothesis) of “two-point” space–time stationarity.

The RF  $Z(\mathbf{u}, t)$  is said to be strictly stationary within  $D \times T$  if its spatiotemporal law is invariant by translation  $(\mathbf{h}, \tau) \in D \times T$ , implying that any two vectors of RVs  $\{Z(\mathbf{u}_1, t_1), \dots, Z(\mathbf{u}_N, t_T)\}$  and  $\{Z(\mathbf{u}_1 + \mathbf{h}, t_1 + \tau), \dots, Z(\mathbf{u}_N + \mathbf{h}, t_T + \tau)\}$  have the same multivariate cdf, whatever the translated vector  $(\mathbf{h}, \tau) \in D \times T$ , i.e.,

$$\begin{aligned} F(\mathbf{u}_1, t_1, \dots, \mathbf{u}_N, t_T; z_{11}, \dots, z_{NT}) &= \\ F(\mathbf{u}_1 + \mathbf{h}, t_1 + \tau, \dots, \mathbf{u}_N + \mathbf{h}, t_T + \tau; z_{11}, \dots, z_{NT}) & \\ \forall \mathbf{u}_1, t_1, \dots, \mathbf{u}_N, t_T, \text{ and } (\mathbf{h}, \tau) \in (D \times T) & \end{aligned}$$

The less demanding model decision of second-order stationarity involves only the two first moments of the RF  $Z(\mathbf{u}, t)$ , whereby the mean function  $m(\mathbf{u}, t)$  is modeled as constant, i.e.,

$$E\{Z(\mathbf{u}, t)\} = m, \quad \forall (\mathbf{u}, t) \in D \times T$$

and the space–time covariance function  $C_Z(\mathbf{u}, t; \mathbf{u}', t')$  is assumed to depend only on the spatial and temporal lags  $\mathbf{h} = \mathbf{u} - \mathbf{u}'$  and  $\tau = t - t'$ , i.e.,

$$E\{[Z(\mathbf{u}, t) - m][Z(\mathbf{u}', t') - m]\} = C_Z(\mathbf{h}, \tau)$$

In many cases, however, natural processes acting over a large region and/or span of time are better represented by nonstationary spatiotemporal RF models. Nonstationarity is usually limited to the mean (trend) component  $m(\mathbf{u}, t)$ , which is made dependent on the space location  $\mathbf{u}$ , or the time instant  $t$ , or both.

Two major conceptual viewpoints exist for modeling of spatiotemporal distributions via spatial statistics tools extended to include the additional time dimension, and are reviewed hereafter:

- The first viewpoint calls for a single spatiotemporal RF model  $Z(\mathbf{u}, t)$ , typically decomposed into a trend component modeling some “average” smooth variability of the spatiotemporal process  $Z(\mathbf{u}, t)$ , and a stationary residual component modeling higher frequency fluctuations around that trend in both space and time.
- The second viewpoint considers multiple vectors of RFs or vectors of TS. Two model subclasses can then be defined. Models in the first subclass treat the spatiotemporal RF  $Z(\mathbf{u}, t)$  as a collection of a finite number  $T$  of temporally correlated space RFs  $\mathbf{Z}(\mathbf{u})$ , while models in the second subclass view the RF  $Z(\mathbf{u}, t)$  as a collection of a finite number  $N$  of spatially correlated TS  $\mathbf{Z}(t)$ .

## THE SPATIOTEMPORAL RF MODEL APPROACH

A single spatiotemporal RF model  $Z(\mathbf{u}, t)$  is considered, typically decomposed into a mean component  $m(\mathbf{u}, t)$  modeling the trend, that is some “average” variability of  $Z(\mathbf{u}, t)$ , and a residual component RF  $R(\mathbf{u}, t)$  modeling fluctuations around that trend in both space and time. Two classes of models can be defined depending on whether the mean component is viewed as deterministic or stochastic:

- In the case of a deterministic space–time mean function  $m(\mathbf{u}, t)$ , the decomposition of the spatiotemporal RF  $Z(\mathbf{u}, t)$  is written as

$$Z(\mathbf{u}, t) = m(\mathbf{u}, t) + R(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (1)$$

where  $m(\mathbf{u}, t)$  is a deterministic function of the space–time coordinates  $\mathbf{u}$  and  $t$ , and  $R(\mathbf{u}, t)$  is a zero mean stationary spatiotemporal RF modeling space–time fluctuations around  $m(\mathbf{u}, t)$ .

- In the case of a stochastic mean  $M(\mathbf{u}, t)$ , the decomposition of  $Z(\mathbf{u}, t)$  is written as

$$Z(\mathbf{u}, t) = M(\mathbf{u}, t) + R(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (2)$$

where  $M(\mathbf{u}, t)$  is a nonstationary spatiotemporal RF modeling the space–time distribution of the mean process, with  $E\{M(\mathbf{u}, t)\} = m(\mathbf{u}, t)$ , and  $R(\mathbf{u}, t)$  is a zero mean stationary spatiotemporal RF modeling space–time fluctuations around  $M(\mathbf{u}, t)$ . Typically  $R(\mathbf{u}, t)$  is modeled as independent of (or at least uncorrelated with)  $M(\mathbf{u}, t)$ ,  $\forall(\mathbf{u}, t) \in D \times T$ .

A further decomposition of the deterministic space–time mean function  $m(\mathbf{u}, t)$  is sometimes adopted:

$$m(\mathbf{u}, t) = m_1(\mathbf{u}) + m_2(t), \quad \text{or} \quad m(\mathbf{u}, t) = m_1(\mathbf{u})m_2(t), \quad \forall(\mathbf{u}, t) \in D \times T$$

where  $m_1(\mathbf{u})$ ,  $m_2(t)$  are functions of the single space and time coordinates, respectively.

A similar decomposition can be adopted for  $M(\mathbf{u}, t)$  and for the residual RF  $R(\mathbf{u}, t)$ . For example, the residual RF  $R(\mathbf{u}, t)$  can be decomposed as

$$R(\mathbf{u}, t) = R_1(\mathbf{u}) + R_2(t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (3)$$

or

$$R(\mathbf{u}, t) = R_1(\mathbf{u})R_2(t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (4)$$

where  $R_1(\mathbf{u})$  is a purely spatial zero mean residual RF, and  $R_2(t)$  is a purely temporal zero mean TS, typically modeled independent of  $R_2(t)$ .

Note that model decompositions might include only a spatial or only a temporal deterministic trend component [ $m_1(\mathbf{u})$  or  $m_2(t)$ ] and a spatiotemporal stochastic residual  $R(\mathbf{u}, t)$ , as

$$Z(\mathbf{u}, t) = m_1(\mathbf{u}) + R(\mathbf{u}, t), \quad \text{or} \quad Z(\mathbf{u}, t) = m_2(t) + R(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T$$

The previous decompositions are often convenient, but represent model (subjective) decisions, since only  $z$ -data  $\{z(\mathbf{u}_\alpha, t_i), \alpha = 1, \dots, n, i = 1, \dots, T\}$  are available in the case of  $n$  monitoring stations all informed at the same  $T$  time instants (isotopic or rectangular sampling). Distinct measurements related to  $M(\mathbf{u}, t)$ ,  $m(\mathbf{u}, t)$ ,  $m_1(\mathbf{u})$ ,  $m_2(t)$ ,  $R(\mathbf{u}, t)$ ,  $R_1(\mathbf{u})$ , or  $R_2(t)$  are usually not available. Therefore, any decomposition into trend and residual should be based on ancillary information other than  $z$ -data, such as a deterministic (physical) equation relating the trend to  $z$ -values.

### Deterministic Trend Models

The deterministic trend  $m(\mathbf{u}, t)$  component is often modeled as

$$m(\mathbf{u}, t) = \sum_{l=0}^L \sum_{k=0}^K b_{kl} f_{kl}(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (5)$$

where  $m(\mathbf{u}, t)$  is comprised of  $KL$  known basis functions  $f_{kl}(\mathbf{u}, t)$  chosen suitable for fitting the observed “mean” variation of the  $z$ -data, and  $b_{kl}$ ,  $k = 0, 1, \dots, K$ ,  $l = 0, \dots, L$  are unknown coefficients to be fitted. For example, periodic functions  $f_{kl}(\cdot, t)$  can be used to account for seasonal variations along the time axis, and polynomial or piecewise continuous functions  $f_{kl}(\mathbf{u}, \cdot)$  can be used to model smooth variations or discontinuities in space.

Dimitrakopoulos and Luo (1997) provided several forms of permissible spatiotemporal trends in a space–time context. Such spatiotemporal trends must have component functions that are linearly independent over any set of data available, in order for the corresponding space–time kriging systems to have a unique solution (Journel and Huijbregts, 1978, p. 318). Moreover, these component trend functions must ensure tensorial invariance of the space–time kriging system, so that the kriging estimator and variance are invariant under changes of the origin and/or units of the coordinate system (Matheron, 1973). Three general types of trend forms are proposed by Dimitrakopoulos and Luo (1997): traditional polynomial functions, Fourier expressions, and combinations of the two, all of which meet the linear independence condition. The vector  $\mathbf{f}' = [f_{00}(\mathbf{u}, t), \dots, f_{KL}(\mathbf{u}, t)]$  of component functions is written in  $D \times T$ , with  $D \subset R^2$ :

- Polynomial form:

$$\mathbf{f}' = [1, x, y, t, \dots, x^K, y^K, t^L]$$

- Fourier form:

$$\mathbf{f}' = [1, \sin(\omega_x x) \sin(\omega_y y) \sin(\omega_t t), \sin(\omega_x x) \sin(\omega_y y) \cos(\omega_t t), \dots, \cos(\omega_x \nu x) \cos(\omega_y \nu y) \sin(\omega_t \nu t), \cos(\omega_x \nu x) \cos(\omega_y \nu y) \cos(\omega_t \nu t)]$$

- Mixed form:

$$\mathbf{f}' = [1, x, y, t, \sin(\omega_t t), \cos(\omega_t t), x \sin(\omega_t t), x \cos(\omega_t t), y \sin(\omega_t t), y \cos(\omega_t t), \dots]$$

$K$ ,  $L$  are the space and time orders,  $\omega_x$ ,  $\omega_y$ ,  $\omega_t$  are the frequencies in directions  $x$ ,  $y$ ,  $t$ , and  $\nu$  is the order of the Fourier series.

When the trend function is modeled as a polynomial of order  $K$  in the space coordinate vector  $\mathbf{u}$  and  $L$  in the time coordinate  $t$ , these orders, called space–time continuity orders (Christakos, 1992; Christakos and Raghu, 1996), provide a quantitative assessment of the average continuity. Positive differences  $K - L$  imply space-dominant processes, while negative differences  $K - L$  imply time-dominant processes.

Trend forms with mixed polynomial and Fourier terms do not necessarily meet the tensorial invariance requirement, and hence must be checked



in each particular case. Polynomial trend forms of order  $K$  in space and  $L$  in time meet the tensorial invariance requirement if and only if all lower order terms up to  $K - 1$  and  $L - 1$  are present. Fourier trend forms of order  $\nu$  are acceptable if and only if all terms up to order  $\nu$  are present; similar conditions must be satisfied for the mixed trend models. In practice, trend forms up to order two for polynomials and one for Fourier series are often sufficient to model the smoothly varying trend component of the  $z$ -variability in space and time.

Loader and Switzer (1992) considered a generalized additive model of the type

$$m(\mathbf{u}, t) = m + p(\mathbf{u}) + q(t), \quad \forall (\mathbf{u}, t) \in D \times T \quad (6)$$

where  $m$  is the space–time stationary mean, and  $p(\mathbf{u})$ ,  $q(t)$  are suitably smooth function of  $\mathbf{u}$  and  $t$  satisfying the following constraints over the  $n$  space locations and  $T$  time instants:

$$\sum_{\alpha=1}^n p(\mathbf{u}_{\alpha}) = 0 \quad \text{and} \quad \sum_{i=1}^T q(t_i) = 0$$

In the case of isotopic sampling, the functions  $p(\cdot)$  and  $q(\cdot)$  can be estimated via a smoother [e.g., the loess smoother (Cleveland and Devlin, 1988)] operating on  $z_{\cdot}(\mathbf{u}_{\alpha})$  and  $z_i(\cdot)$ , defined as

$$z_{\cdot}(\mathbf{u}_{\alpha}) = \frac{1}{T} \sum_{i=1}^T z_i(\mathbf{u}_{\alpha}) - m^* = p(\mathbf{u}_{\alpha}) + \frac{1}{T} \sum_{i=1}^T r(\mathbf{u}_{\alpha}, t_i) - m^*$$

$$z_i(\cdot) = \frac{1}{n} \sum_{\alpha=1}^n z_i(\mathbf{u}_{\alpha}) - m^* = q(t_i) + \frac{1}{n} \sum_{\alpha=1}^n r(\mathbf{u}_{\alpha}, t_i) - m^*$$

where  $m^*$  is an estimate of the space–time stationary mean  $m$ , defined as

$$m^* = \frac{1}{Tn} \sum_{i=1}^T \sum_{\alpha=1}^n z(\mathbf{u}_{\alpha}, t_i) = m + \frac{1}{Tn} \sum_{i=1}^T \sum_{\alpha=1}^n r(\mathbf{u}_{\alpha}, t_i)$$

with  $r(\mathbf{u}_{\alpha}, t_i) = z(\mathbf{u}_{\alpha}, t_i) - m(\mathbf{u}_{\alpha}, t_i)$  being the corresponding residual estimates.

The estimates  $p^*(\mathbf{u})$  and  $q^*(t)$  of  $p(\mathbf{u})$  and  $q(t)$  are expressed in terms of the loess smoother weights  $\lambda_{\alpha}(\mathbf{u})$  and  $\lambda'_i(t)$  as

$$p^*(\mathbf{u}) = \sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}) z_{\cdot}(\mathbf{u}_{\alpha}) \quad \text{and} \quad q^*(t) = \sum_{i=1}^T \lambda'_i(t) z_i(\cdot)$$

where  $\lambda_{\alpha}(\mathbf{u})$  and  $\lambda'_i(t)$  are smoothing weights satisfying the condition

$$\sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}) = \sum_{i=1}^T \lambda'_i(t) = 1, \quad \forall \mathbf{u} \in D, \forall t \in T$$

Note that the weights  $\lambda_\alpha(\mathbf{u})$  and  $\lambda'_i(t)$  that control the smoothness of the resulting trend field  $m(\mathbf{u}, t)$  are not unique; instead, they are subjectively determined by selecting a bandwidth for the loess smoother.

### Inference of Residual Covariance

In the general space–time nonstationary case, consideration of a trend model of type (5) renders inference of the residual covariance  $C_R(\mathbf{h}, \tau)$  problematic. No residual data  $r(\mathbf{u}_\alpha, t_i)$  are directly available, instead they are estimated as  $r^*(\mathbf{u}_\alpha, t_i) = z(\mathbf{u}_\alpha, t_i) - m^*(\mathbf{u}_\alpha, t_i)$ . Consequently, the residual covariance  $C_R(\mathbf{h}, \tau)$  is actually that of the residual estimator  $R^*(\mathbf{u}, t)$ , which depends on the filtering algorithm used to evaluate  $m^*(\mathbf{u}_\alpha, t_i)$ . It is commonly argued that bias can be introduced because

$$\text{Cov}\{Z(\mathbf{u}_\alpha, t_i) - m^*(\mathbf{u}_\alpha, t_i), Z(\mathbf{u}_\beta, t_j) - m^*(\mathbf{u}_\beta, t_j)\} \neq C_R(\mathbf{u}_\alpha - \mathbf{u}_\beta, t_i - t_j)$$

A possible solution is to consider only linear combinations of  $z$ -data that filter the trend  $m(\mathbf{u}, t)$ . The corresponding class of random functions originally proposed in a purely spatial context (Matheron, 1973) is called intrinsic random functions of order  $K$  (IRF- $K$ ), and was further developed by Delfiner (1976). The IRF- $K$  framework was modified to incorporate a temporal drift by Séguret (1989), and was later adopted in a space–time context (IRF- $KL$ ) by Rouhani and Hall (1989), and Christakos (1992). Differences of  $z$ -data of order  $K$  in space and  $L$  in time could filter any polynomial trend  $p_{KL}(\mathbf{u}, t)$  of order  $K - 1$  and  $L - 1$  in  $\mathbf{u}$  and  $t$ , respectively. The variance of these differences (called generalized covariance of order  $KL$ ) can then be identified to the residual covariance  $C_R(\mathbf{h}, \tau)$ . However, such high-order differences are not directly available when data are not gridded, and, in addition, the corresponding generalized covariance model is not unique. The concept of generalized covariances already suffers from many practical limitations in the space domain. These are (1) the use of a restricted family of polynomial generalized covariances, and (2) the iterative trial-and-error selection and fit of generalized covariance components, which tends to yield models with large nugget effect because of the sensitivity of the fitting algorithm to outlier data (Journel, 1989). An alternative solution is to base inference of  $C_R(\mathbf{h}, \tau)$  on data pairs that are not affected by the trend, clearly not an easy task in the presence of complex space–time interactions.

Restriction of the decision of stationarity to a local neighborhood  $W(\mathbf{u}, t)$  around the “point”  $(\mathbf{u}, t) \in D \times T$  where estimation is performed allows accounting for deviations from global space–time stationarity, provided the local stationary mean can be reestimated within each neighborhood

from the corresponding data. This local reestimation can be explicit, or implicit as in ordinary kriging (OK) within moving local neighborhoods; the residual covariance used is modeled as stationary and inferred from the  $z$ -data for within-neighborhood distances only. Journel and Rossi (1989) argue that, when estimation is performed in interpolation mode, the simpler ordinary kriging procedure, with the overall trend contribution implicitly reestimated within each estimation neighborhood, is as efficient as including an explicit trend model, as for example in Eynon (1988), or Haas (1995). However, an important challenge in stochastic modeling of space–time data is future prediction, i.e., estimation in extrapolation mode. In this case, the particular trend model adopted has a paramount effect on the predicted values.

Note that the dichotomous relation (1) is most often a subjective modeling decision: there is no “true” temporal trend component, since there are no trend data. All trend values are model-specific outcomes resulting from the particular algorithm used to determine them. Consequently, the corresponding residual model is a collective term for all components of variability not included in the trend model, and no elusive “true” residual covariance exists. Instead, one should acknowledge the modeling decision (1), and accept its consequences, i.e., the specific trend and residual estimates.

### Stochastic Trend Models

Trend models of the type (5) are considered random if the coefficients  $b_{kl}$  multiplying the deterministic functions  $f_{kl}(\mathbf{u}, t)$  are modeled as outcomes of random variables, i.e.,

$$M(\mathbf{u}, t) = \sum_{l=0}^L \sum_{k=0}^K B_{kl} f_{kl}(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (7)$$

with

$$E\{B_{kl}\} = b_{kl}, \quad k = 0, \dots, K, l = 0, \dots, L$$

where the expected value of the random coefficients  $B_{kl}$ , hence the expected value of the random trend  $M(\mathbf{u}, t)$ , can be estimated from the  $z$ -data via a generalized regression procedure, similar to kriging a deterministic trend—see, for example, Goovaerts (1997, p. 148).

Models involving a stochastic mean component are typically expressed as

$$Z(\mathbf{u}, t) = M(\mathbf{u}, t) + R(\mathbf{u}, t) = M_{\mathbf{u}}(t) + R(\mathbf{u}, t), \quad \forall(\mathbf{u}, t) \in D \times T \quad (8)$$

A deterministic temporal trend  $m_{\alpha}(t)$  at location  $\mathbf{u}_{\alpha}$  is first fitted as a function

of  $t$  by a least squares procedure, independently from other locations, using linear or trigonometric basis functions of  $t$  as in Eq. (5). The fitted parameters—that is the estimators  $B_{kl}^*$ ,  $k = 0, \dots, K, l = 0, \dots, L$ —are then regionalized in space, allowing a reconstruction of the spatiotemporal RF  $M(\mathbf{u}, t)$  at unsampled space locations  $\mathbf{u}$  and time instants  $t$  (Oehlert, 1993). Note that these parameters are likely to be cross-correlated, since they are derived from the same  $z$ -data, and such cross-correlation should be taken into account when the temporal trend parameters are regionalized in space, see for example Kyriakidis (1998).

In all rigor, model (8) should be rewritten as

$$Z(\mathbf{u}, t) = M_{\mathbf{u}}^{\text{alg}}(t) + R^{\text{alg}}(\mathbf{u}, t), \quad \forall (\mathbf{u}, t) \in D \times T \tag{9}$$

where  $M_{\mathbf{u}}^{\text{alg}}(t)$  is the RV associated to the specific algorithm used for determining the local trend values  $m_{\mathbf{u}}^{\text{alg}}(t)$ . Note that, unless the data configurations used to “fit” the  $m_{\mathbf{u}}^{\text{alg}}(t)$  values at different space locations  $\mathbf{u}, \mathbf{u}'$  are similar, stationarity of the resulting RVs  $M_{\mathbf{u}}^{\text{alg}}(t)$ ,  $M_{\mathbf{u}'}^{\text{alg}}(t)$ , or  $B_{kl}^{\text{alg}}(t)$ ,  $B_{kl}^{\text{alg}}(\mathbf{u}', t)$  is questionable.

A similar approach was proposed by Journel and Huijbregts (1972) in a purely spatial context. In this case, a common vertical pattern (trend) of nickel grades in a lateritic deposit was parametrized by known functions of depth, whose coefficients (trend amplitudes) were estimated locally at each drill hole by means of kriging with a trend model (universal kriging). The resulting coefficients were then regionalized in space (not accounting for their cross-correlation), yielding a 3D estimation of the random trend. Modeling of the residual field was not attempted, since the actual determination of mineable reserves was based on whether the estimated trend values were greater than a given cutoff grade. More recently, Voltz and Goulard (1994) proposed a similar procedure for regionalizing in space soil moisture retention curves, while also accounting for cross-correlation between the fitted parameters.

An alternative approach involving a stochastic trend model was proposed by Høst, Omre, and Switzer (1995) in their attempt to improve estimation by including noncontemporaneous data in a space–time modeling procedure. The proposed spatiotemporal RF model  $Z(\mathbf{u}, t)$  is decomposed as

$$\begin{aligned} Z(\mathbf{u}, t) &= M_1(\mathbf{u}) + R_2(t) + S(\mathbf{u}, t)R(\mathbf{u}, t), \quad \forall (\mathbf{u}, t) \in D \times T \\ &= M_1(\mathbf{u}) + R_2(t) + S(\mathbf{u})S(t)R(\mathbf{u}, t) \end{aligned}$$

where  $M_1(\mathbf{u})$  is a purely spatial component modeling the spatial mean variation,  $R_2(t)$  is a zero mean TS component viewed as the temporal modulation (time correction) of  $M_1(\mathbf{u})$  at discrete times, and  $R(\mathbf{u}, t)$  is a

spatiotemporal residual RF with zero mean and unit variance. The standard deviation (scale) of the  $z$ -data is modeled by a spatiotemporal RF  $S(\mathbf{u}, t)$  itself decomposed in a purely spatial  $S(\mathbf{u})$  and a purely temporal  $S(t)$  component.

Estimates  $m_1^*(\mathbf{u}_\alpha)$  of the mean field  $M_1(\mathbf{u})$  at each monitoring station location  $\mathbf{u}_\alpha$  are obtained as

$$m_1^*(\mathbf{u}_\alpha) = \frac{1}{T} \sum_{i=1}^T z(\mathbf{u}_\alpha, t_i), \quad \alpha = 1, \dots, n$$

i.e.,  $m_1(\mathbf{u}_\alpha)$  “data” are estimated as averages of the actual data  $z(\mathbf{u}_\alpha, t_i)$  over the  $T$  years.

Estimates  $r_2^*(t_i)$  of the temporal modulation field  $R_2(t)$  at each time instant  $t_i$  are calculated by the weighted linear combination:

$$r_2^*(t_i) = \sum_{\alpha=1}^n \lambda(\mathbf{u}_\alpha) [z(\mathbf{u}_\alpha, t_i) - m_1^*(\mathbf{u}_\alpha)], \quad i = 1, \dots, T$$

where the weights  $\lambda(\mathbf{u}_\alpha)$ , independent of  $t_i$ , are obtained by kriging the global mean  $E\{M_1\} = m_1$  from  $m_1^*(\mathbf{u}_\alpha)$  “data.” This amounts to identifying the variogram of  $Z(\mathbf{u}, t) - M_1(\mathbf{u})$  to that of the  $m_1^*(\mathbf{u}_\alpha)$  “data,”  $\forall t_i$ .

Estimates of scale components  $S_1(\mathbf{u})$ ,  $S_2(t)$ , and of residual component  $R(\mathbf{u}, t)$  at monitoring stations  $\mathbf{u}_\alpha$ ,  $\alpha = 1, \dots, n$  are obtained as

$$[s_1^2(\mathbf{u}_\alpha)]^* = \frac{1}{T} \sum_{i=1}^T [z(\mathbf{u}_\alpha, t_i) - m_1^*(\mathbf{u}_\alpha) - r_2^*(t_i)]^2$$

$$[s_2^2(t_i)]^* = \frac{1}{[w^2]^*} \sum_{\alpha=1}^n \lambda(\mathbf{u}_\alpha) [z(\mathbf{u}_\alpha, t_i) - m_1^*(\mathbf{u}_\alpha) - r_2^*(t_i)]^2$$

and

$$r^*(\mathbf{u}_\alpha, t_i) = \frac{[z(\mathbf{u}_\alpha, t_i) - m_1^*(\mathbf{u}_\alpha) - r_2^*(t_i)]}{s_1^*(\mathbf{u}_\alpha) s_2^*(t_i)}$$

where  $[w^2]^* = \sum_{\alpha=1}^n \lambda(\mathbf{u}_\alpha) [s_1^2(\mathbf{u}_\alpha)]^*$ .

Interpolated  $z$ -values,  $z^*(\mathbf{u}, t_i)$ , at unmonitored locations  $\mathbf{u} \in D$  and monitored time instants  $t_i \in \{t_1, \dots, t_T\}$ , were obtained by adding interpolated values of the various component fields (thus, all modeled as independent of each other). Such a modeling assumption should be checked in practice (as it was done in this study), since all component estimates are derived from the same (common) data set, the only available  $z(\mathbf{u}_\alpha, t_i)$  values, and hence they are likely to be cross-correlated.

## Stochastic Residual Models

Under the model decision of a space–time stationary mean  $m$ , the covariance function  $C_R(\mathbf{h}, \tau)$  of the residual RF  $R(\mathbf{u}, t)$  can be identified to the stationary covariance function  $C(\mathbf{h}, \tau)$  of the RF  $Z(\mathbf{u}, t)$ :

$$\begin{aligned} C_R(\mathbf{h}, \tau) &= E\{R(\mathbf{u}, t) \cdot R(\mathbf{u} + \mathbf{h}, t + \tau)\} \\ &= E\{[Z(\mathbf{u}, t) - m] \cdot [Z(\mathbf{u} + \mathbf{h}, t + \tau) - m]\} = C(\mathbf{h}, \tau) \end{aligned}$$

If the variability of the covariance function is assumed to have the same parametric form in space and time (another model decision), a geometric anisotropy can be adopted, as for example in Armstrong, Chetboun, and Hubert (1993):

$$C(\mathbf{h}, \tau) = f(\sqrt{a_1 \|\mathbf{h}\|^2 + a_2 \tau^2}) \quad (10)$$

where  $a_1, a_2$  are the anisotropy factors between the space and time axes,  $f(\cdot)$  is a positive definite function, and  $\|\mathbf{h}\|$  is the Euclidean norm of vector  $\mathbf{h}$ . The argument of  $f(\cdot)$  is a distance (metric) defined across the time and space domains, i.e., is a metric in the higher dimensional space  $R^{d+1}$ . For example, a vector defined by a shift of  $x = 3$  meters in the easting direction,  $y = 4$  meters in the northing direction, and  $t = 1$  hour in time is represented as a generalized distance of  $|\mathbf{h}'| = \sqrt{x^2 + y^2 + t^2} = 5.1$  m-hr.

There are, however, fundamental differences between space and time phenomena, as noted by Journel (1986); Consequently, the spatiotemporal covariance  $C(\mathbf{h}, \tau)$  is most often decomposed into the sum of purely spatial and purely temporal components. In geostatistical jargon, this corresponds to a zonal anisotropy model, see for example Bilonick (1985). Alternatively, the covariance model is decomposed into a product of purely spatial and purely temporal components, corresponding to a separability hypothesis—see, for example, Rouhani and Myers (1990) or De Cesare, Myers, and Posa (1997). These two decompositions of the space–time covariance function  $C(\mathbf{h}, \tau)$  are written:

$$C(\mathbf{h}, \tau) = C_1(\mathbf{h}) + C_2(\tau) \quad (11)$$

or

$$C(\mathbf{h}, \tau) = C_1(\mathbf{h})C_2(\tau) \quad (12)$$

where  $C_1(\mathbf{h})$  is a purely spatial covariance function, and  $C_2(\tau)$  is a purely temporal covariance function. Note that the previous covariance models correspond to decompositions (3) and (4), respectively.

Following Rodríguez-Iturbe and Mejía (1974), various researchers, e.g., Haas (1995), considered separable covariance models of the type:

$$C(\mathbf{h}, \tau) = \sigma_Z^2 \rho_1(\mathbf{h}) \rho_2(\tau) \quad (13)$$

where  $\sigma_Z^2$  is the global variance of  $Z(\mathbf{u}, t)$ ,  $\rho_1(\mathbf{h})$  is a purely spatial correlation function, and  $\rho_2(\tau)$  is a purely temporal correlation function. Note that the separable covariance (13) does not correspond to model decomposition (4); instead, this version of separability applies to the standardized spatio-temporal residual. Note that similar separable models are also adopted for generalized covariance functions (Rouhani and Hall, 1989; Christakos and Bogaert, 1996), and do not imply separability of the original (not generalized) covariance models.

Space–time models involving a mixture of geometric and zonal anisotropy have been also proposed in the literature (Bilonick, 1985; Stein, 1986; Bilonick, 1988; Buxton and Plate, 1994; Bogaert and Christakos, 1997a; Heuvelink, Musters, and Pebesma, 1997). These mixture models amount to decomposing the spatiotemporal RF model  $Z(\mathbf{u}, t)$  into all or some of the following components:

$$Z(\mathbf{u}, t) = m(\mathbf{u}, t) + R_1(\mathbf{u}) + R_2(t) + R_3(\mathbf{u}, t), \quad \forall (\mathbf{u}, t) \in D \times T$$

where  $R_1(\mathbf{u})$  is a purely spatial component,  $R_2(t)$  is purely temporal component, and  $R_3(\mathbf{u}, t)$  is a spatiotemporal component, often modeled with a space–time separable covariance of type (12), or as a pure nugget effect component. These mixture models rely entirely on the subjective decomposition of the space–time covariance  $C(\mathbf{h}, \tau)$  into nested structures, since no data on  $R_1(\mathbf{u})$ ,  $R_2(t)$ , or  $R_3(\mathbf{u}, t)$  are available; such decomposition should be ideally guided by physical interpretation.

### Shortcomings of Separable Models

A zonal anisotropy model of type (11) implies that the spatial behavior of the RF  $Z(\mathbf{u}, t)$  is considered to be the same at all time instants. Similarly, no change of the temporal pattern of  $Z(\mathbf{u}, t)$  from locations to locations can be accommodated. Separable covariance functions, such as Equation (12), are mathematically congenial, but share similar limitations with the zonal anisotropy models, in that variability in space and time do not interact. Such models arise from two separate processes (one temporal and one spatial) that act independently one from each other (Jones and Zhang, 1997). In addition, no guideline exists for inferring (separating) the two component structures,  $C_1(\mathbf{h})$  and  $C_2(\tau)$ , from the experimentally available spatial  $C(\mathbf{h}, 0)$  and temporal  $C(\mathbf{0}, \tau)$  covariances. For example, an experimental spatial covariance  $C(\mathbf{h}, 0)$  calculated along the space axes is inevitably influenced by temporal variability stemming from using data pairs

$\{z(\mathbf{u}_\alpha, t_i), z(\mathbf{u}_\alpha + \mathbf{h}, t_i)\}$  and  $\{z(\mathbf{u}_\beta, t_j), z(\mathbf{u}_\beta + \mathbf{h}, t_j)\}$  taken at different time instants  $t_i, t_j$ , and thus cannot be identified straightforwardly to the model spatial covariance component  $C_1(\mathbf{h})$ . Note also that, when periodicities are included in the temporal model  $C_2(\tau)$  via hole effect models as in Bilonick (1985) or Buxton and Plate (1994), a loss of phase information occurs (Yao, 1996). Periodic behaviors may be better modeled via periodic trend models (Séguret, 1989), or by restoring the phase information (Yao, 1998).

Zonal anisotropy can lead to invalid kriging systems for certain data configurations, as noted by Myers and Journel (1990): covariance models built from a sum of one-dimensional (1D) structures may be only conditionally positive definite in higher dimensional spaces, when they should be strictly positive definite to ensure nonsingularity of the corresponding systems of normal (kriging) equations. Rouhani and Myers (1990) confirmed a number of problems associated with zonal anisotropy when performing kriging, an example being the singularity of the kriging system for a “rectangular” data configuration, e.g., when pressure heads are read at two different locations at the same time instants. Similar problems arose when data are taken at the same location at small time intervals. Dimitrakopoulos and Luo (1994) recast the findings of Myers and Journel (1990) in a space–time context, and highlighted the problematic case of rectangular data configurations: if kriging is performed using only positive semidefinite space–time covariance functions, the resulting data-to-data covariance matrix is singular, no matter the number of data involved. The problem is eliminated if the positive semidefinite covariance function is replaced by a strictly positive definite covariance function.

In certain cases, covariance functions are calculated and modeled locally within each moving window neighborhood using fully automatic fitting algorithms (Christakos, 1992; Haas, 1995). This procedure, although restricting the decision of stationarity regarding the mean and the covariance within local neighborhoods, is limited by data shortage, is sensitive to outliers, and often yields pure nugget effect models for the resulting spatiotemporal covariance.

### **Inference of Nonstationary Spatial Residual Covariance**

Often, the spatiotemporal residual RF  $R(\mathbf{u}, t)$  is viewed as a collection of  $T$  independent time replicates of a unique residual spatial RF  $R(\mathbf{u})$ . In such case, the sole spatial covariance  $C_R(\mathbf{h})$  characterizes the entire spatiotemporal residual correlation, since  $R(\mathbf{u}, t)$  is assumed to be indepen-



dent of the time instant  $t \in T$ . Note that adoption of a constant pattern of spatial residual correlation over time amounts to assuming that all significant temporal structure is incorporated in the previously fitted purely temporal trend  $m(t)$  or spatiotemporal trend  $m(\mathbf{u}, t)$ . Under such assumption, two realizations  $\{r_t^{(s)}(\mathbf{u}), \mathbf{u} \in D\}$  and  $\{r_{t'}^{(s')}(\mathbf{u}), \mathbf{u} \in D\}$  corresponding to two close time instants ( $t - t'$  small) can differ substantially, because they are independent, although their pattern of spatial correlation is the same. This may result in artifact temporal “discontinuities” in the global realization  $z^{(l)}(\mathbf{u}, t)$ , possibly severe if the variance of the residual component  $R(\mathbf{u}, t)$  is large. Alternatively, such discontinuities could represent the effect of measurement error, in which case, such effect could have been modeled in the nugget effect component, and filtered via factorial kriging; see, for example, Wackernagel (1995, p. 100).

Given the above model assumption, two main approaches exist for estimating the residual spatial covariance  $C_R(\mathbf{h})$ :

1. infer independently the  $T$  stationary spatial covariances  $C_R(\mathbf{h}, t_i)$  at each of the  $T$  time instants  $t_i$ ,  $i = 1, \dots, T$  from the residual “data”  $r(\mathbf{u}_\alpha, t_i) = z(\mathbf{u}_\alpha, t_i) - m(t_i)$ , then average over the  $T$  time instants available:

$$C_R(\mathbf{u} - \mathbf{u}') = \frac{1}{T} \sum_{i=1}^T C_R(\mathbf{u} - \mathbf{u}'; t_i) \quad (14)$$

2. use the  $T$  replicates  $\{r(\mathbf{u}_\alpha, t_i), i = 1, \dots, T\}$  of the spatial RF  $R(\mathbf{u})$  to estimate covariance values  $C_{\alpha\beta}^R = C_R(\mathbf{u}_\alpha, \mathbf{u}_\beta)$  specific to any two station locations  $\mathbf{u}_\alpha, \mathbf{u}_\beta$  as

$$C_{\alpha\beta}^R = C_R(\mathbf{u}_\alpha, \mathbf{u}_\beta) = \frac{1}{T} \sum_{i=1}^T r(\mathbf{u}_\alpha, t_i) r(\mathbf{u}_\beta, t_i) \quad (15)$$

Covariance estimates for specific pairs of stations via such averaging are routinely computed in meteorology (Gandin, 1963; Creutin and Obled, 1982; Haslett, 1989). The inference procedure (15) appears not to require any decision of stationarity in space; however, transformation of the discrete set or table of  $C_R(\mathbf{u}_\alpha, \mathbf{u}_\beta)$  values into a functional model  $C_R(\mathbf{h})$  inevitably requires interpolation in space, hence some additional decision of smooth variability of the spatial covariance. Attention should be also given to the positive definiteness of either the covariance table or covariance function finally retained.

In some cases, in addition to the averaging (15) over time, spatial replicates of data pairs separated by approximately the same vector  $\mathbf{h}$  are also averaged; this last averaging is needed to infer covariance values

$C_R(\mathbf{u}_\alpha, \mathbf{u})$  between the  $n$  data locations  $\mathbf{u}_\alpha, \alpha = 1, \dots, n$  and an uninformed location  $\mathbf{u} \in D$ . The final estimate of  $C_R(\mathbf{h})$  is thus computed as

$$C_R(\mathbf{h}) \simeq \frac{1}{Tn(\mathbf{h})} \sum_{i=1}^T \sum_{\alpha=1}^{n(\mathbf{h})} r(\mathbf{u}_\alpha, t_i) r(\mathbf{u}_\alpha + \mathbf{h}, t_i) \quad (16)$$

by averaging  $T$  replicates over the time span and, subsequently,  $n(\mathbf{h})$  spatial replicates over the spatial domain  $D$ . Note that expression (16) is an estimate of expression (14).

The resulting covariance model (16), being stationary in space, lacks specificity as noted by Switzer (1989), in that it does not differentiate two locations  $\mathbf{u}, \mathbf{u}'$  informed by different neighboring time series. Various models have been proposed for obtaining nonstationary  $C_R(\mathbf{u}_\alpha, \mathbf{u})$  values from the experimentally available  $C_{\alpha\beta}^R$  values. These include Empirical Orthogonal Functions analysis (Creutin and Obled, 1982; Obled and Creutin, 1986; Rao and Hsieh, 1991), modulation of the stationary covariance model (16) by simple kriging weights to yield location-specific kriging variances (Switzer, 1989), approaches based on deformations of the geographical space (Sampson and Guttorp, 1992; Mardia and Goodall, 1993; Meiring, and others, 1997), Bayesian estimators (Loader and Switzer, 1992; Brown, Le and Zidek, 1994), and kernel-type estimators (Egbert and Lettenmaier, 1986; Oehlert, 1993). A detailed discussion regarding these models can be found in Guttorp and Sampson (1994). Alternatively, covariance values between any two pairs of locations can be expressed as a function of other covariates, such as the difference in elevation values (Switzer, 1979), or in addition, the difference in slope and aspect values (Carroll and Cressie, 1997) between the two locations. Note that the resulting covariance values for all pairs of locations should be checked to be jointly permissible, i.e., positive definite. Application of recently developed algorithms for automatic covariance or cross-covariance modeling under positive definiteness constraints (Rehman, 1995; Yao and Journal, 1998) to the problem of computing nonstationary spatial covariance functions warrants further investigation.

## THE MULTIPLE RF/TS MODELS APPROACH

This class of spatiotemporal models views the spatiotemporal process  $Z(\mathbf{u}, t)$  as a set of temporally correlated RFs, or a set of spatially correlated TS, depending on which domain (space or time) is more densely informed.

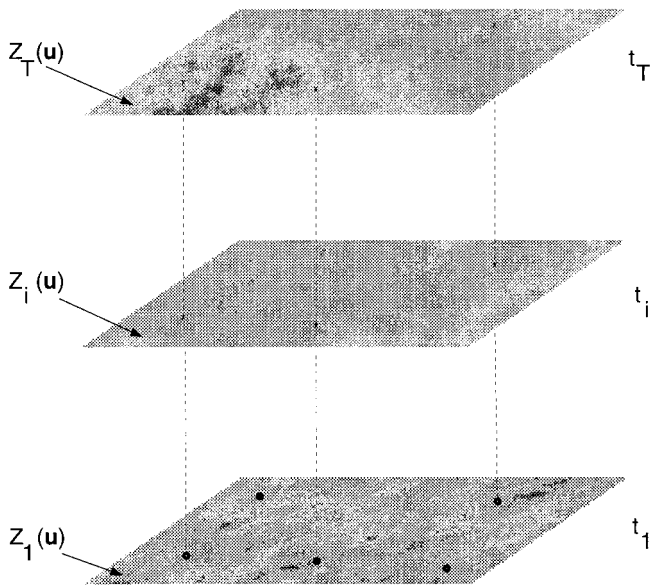
Vectors of RFs

The spatiotemporal RF  $\{Z(\mathbf{u}, t), \mathbf{u}, t \in D \times T\}$  is modeled as a collection of a finite number  $T$  of temporally correlated space RFs (Egbert and Lettenmaier, 1986; Goovaerts and Sonnet, 1993; Papritz and Flühler, 1994; Bogaert and Christakos, 1997b). The following representation is adopted for the spatiotemporal process  $Z(\mathbf{u}, t)$  (Fig. 1):

$$\begin{aligned} Z(\mathbf{u}, t) = \mathbf{Z}(\mathbf{u}) &= [Z_t(\mathbf{u})] = [Z_{t_1}(\mathbf{u}), \dots, Z_{t_T}(\mathbf{u})]' \\ &= [Z_1(\mathbf{u}), \dots, Z_T(\mathbf{u})]' \end{aligned} \tag{17}$$

i.e.,  $T$  RFs are considered, one at each time instant  $t_i, i = 1, \dots, T$ . Spatial maps of the attribute distribution can be constructed only for the  $T$  time instants  $\{t_1, \dots, t_i, \dots, t_T\}$ , and no time interpolation is possible without some additional modeling.

Assuming stationarity, the matrix of covariance values  $\mathbf{C}(\mathbf{h})$  between



**Figure 1.** Conceptual model for vectors of random functions (RFs)  $Z_i(\mathbf{u}), i = 1, \dots, T$ .

data at any two time instants separated by the same spatial lag  $\mathbf{h}$  is written:

$$\mathbf{C}(\mathbf{h}) = \begin{bmatrix} C_{11}(\mathbf{h}) & \cdots & C_{1j}(\mathbf{h}) & \cdots & C_{1T}(\mathbf{h}) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ C_{i1}(\mathbf{h}) & \cdots & C_{ii}(\mathbf{h}) & \cdots & C_{iT}(\mathbf{h}) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ C_{T1}(\mathbf{h}) & \cdots & C_{Tj}(\mathbf{h}) & \cdots & C_{TT}(\mathbf{h}) \end{bmatrix} \quad (18)$$

where

$$\mathbf{C}_{ij}(\mathbf{h}) = \text{Cov}\{Z_i(\mathbf{u}), Z_j(\mathbf{u} + \mathbf{h})\} \simeq \frac{1}{n} \sum_{\alpha=1}^n [z(\mathbf{u}_\alpha, t_i) - m_{\cdot i}][z(\mathbf{u}_\alpha + \mathbf{h}, t_j) - m_{\cdot j}]$$

is the cross-covariance between data at time instants  $t_i$  and  $t_j$ , with  $m_{\cdot i} = (1/n) \sum_{\alpha=1}^n z(\mathbf{u}_\alpha, t_i)$  being an estimate of the mean of the RF  $Z_i(\mathbf{u})$  at time instant  $t_i$ . For  $\mathbf{h} = \mathbf{0}$ , matrix  $\mathbf{C}(\mathbf{0})$  is the stationary variance–covariance matrix of the  $T$  sets of data, one per time instant  $t_i$ .

The number  $T$  and the corresponding instants in time are frozen, hence no time interpolation between these  $T$  instants is possible without further modeling. For example, in the case of pollution monitoring, only  $T$  maps of the contaminant spatial distribution can be generated at the given time instants  $\{t_1, \dots, t_i, \dots, t_T\}$ , i.e., only  $T$  time “snapshots” of the process  $Z(\mathbf{u}, t)$  can be obtained.

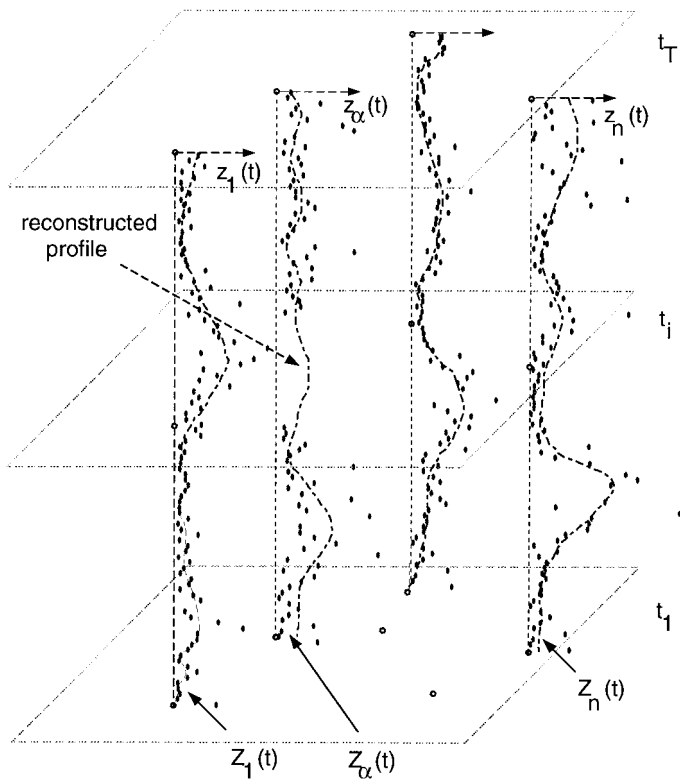
### Vectors of TS

The spatiotemporal RF  $Z(\mathbf{u}, t)$  is now modeled as a finite number  $n$  of spatially correlated TS (Fig. 2) with the following representation:

$$\mathbf{Z}(\mathbf{u}, t) = \mathbf{Z}(t) = [\mathbf{Z}_u(t)] = [\mathbf{Z}_{u_1}(t), \dots, \mathbf{Z}_{u_n}(t)]' = [\mathbf{Z}_1(t), \dots, \mathbf{Z}_n(t)]' \quad (19)$$

i.e.,  $n$  time series are considered, one at each location  $\mathbf{u}_\alpha$ . TS reconstruction is possible only at the  $n$  locations  $\{\mathbf{u}_1, \dots, \mathbf{u}_\alpha, \dots, \mathbf{u}_n\}$ .

Assuming stationarity, the matrix of covariance values  $\mathbf{C}(\tau)$  between data at any two station locations separated by the same temporal lag  $\tau$  is written:



**Figure 2.** Conceptual model for vectors of time series (TS)  $Z_{\alpha}(t), \alpha = 1, \dots, n$ .

$$\mathbf{C}(\tau) = \begin{bmatrix} C_{11}(\tau) & \cdots & C_{1\beta}(\tau) & \cdots & C_{1n}(\tau) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ C_{\alpha 1}(\tau) & \cdots & C_{\alpha\alpha}(\tau) & \cdots & C_{\alpha n}(\tau) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ C_{n1}(\tau) & \cdots & C_{n\beta}(\tau) & \cdots & C_{nn}(\tau) \end{bmatrix} \tag{20}$$

where

$$C_{\alpha\beta}(\tau) = Cov\{Z_{\alpha}(t), Z_{\beta}(t + \tau)\} \approx \frac{1}{T} \sum_{i=1}^T [z(\mathbf{u}_{\alpha}, t_i) - m_{\alpha}][z(\mathbf{u}_{\beta}, t_i + \tau) - m_{\beta}]$$

is the cross-covariance value between data at station locations  $\mathbf{u}_{\alpha}$  and  $\mathbf{u}_{\beta}$

for the temporal lag  $\tau$ , with  $m_{\alpha} = (1/T) \sum_{i=1}^T z(\mathbf{u}_{\alpha}, t_i)$  being an estimate of the mean of the time series  $Z_{\alpha}(t)$  at location  $\mathbf{u}_{\alpha}$ . For  $\tau = 0$ , matrix  $\mathbf{C}(0)$  is the stationary variance–covariance matrix between the  $n$  time series.

The total number  $n$  and the corresponding spatial locations are frozen—hence no space interpolation or extrapolation between these  $n$  locations is possible without some additional modeling. For example, in the case of stream flow readings or acid deposition measurements, only  $n$  stream flow records or deposition profiles can be reconstructed at  $n$  given station locations  $\mathbf{u}_{\alpha}$ ,  $\alpha = 1, \dots, n$  (Solow and Gorelick, 1986; Rouhani and Wackernagel, 1990; Rouhani and others, 1992).

A formulation using vectors of time series in a continuous spatial domain is also possible—see, for example, Kyriakidis (1999). In this case, temporal covariance models  $C(\tau; \mathbf{q}(\mathbf{u}_{\alpha}))$  are first determined at each station location  $\mathbf{u}_{\alpha}$ , independently from one location to another. Here  $\mathbf{q}(\mathbf{u}_{\alpha})$  denotes a vector of parameters specific to station location  $\mathbf{u}_{\alpha}$ , e.g., the sills and ranges of the components of the temporal covariance model at station location  $\mathbf{u}_{\alpha}$ . These station specific parameters  $\mathbf{q}(\mathbf{u}_{\alpha})$  are then (co)regionalized in space for determining location-specific temporal covariance models  $C(\tau; \mathbf{q}(\mathbf{u}))$ . Simulation of the unknown time series  $\{Z_{\alpha}(t), t \in T\}$  at any location  $\mathbf{u} \in D$  can be then performed independently from other locations, using the location-specific covariance model  $C(\tau; \mathbf{q}(\mathbf{u}))$ . Spatial correlation is induced in the simulated series through the spatial correlation of the parameters  $\mathbf{q}(\mathbf{u})$ , and by sampling the local conditional distributions at each time instant by a realization of a spatially correlated probability field (Srivastava, 1992). Alternative approaches for generalizing the framework of spatial time series to a continuous spatial domain have been proposed by Wikle, Berliner, and Cressie (1998), who used a hierarchical Bayesian methodology, and Wikle and Cressie (1997), and Meiring, Guttorp, and Sampson (1998), who adopted a space–time Kalman filtering procedure.

Within the vector (multivariate) interpretation (17) or (19), each element RF  $Z(\mathbf{u}, t)$  can be itself decomposed into a trend plus a residual component as in relations (1) or (2). For example, Egbert and Lettenmaier (1986) decomposed each year into  $L$  seasons, over which conditions were assumed to be stationary. The spatial variation of the  $l$ th season was modeled separately by decomposing the corresponding spatiotemporal RF  $Z^l(\mathbf{u}, t)$  into a sum of a spatial mean RF  $M_1^l(\mathbf{u})$  and two residual spatiotemporal RFs modeling yearly and weekly variations around  $M_1^l(\mathbf{u})$ , respectively, all correlated across seasons. In their study, however, space–time data were used only to infer the correlation structure for each season and

no estimation was performed. First, spatial covariance values specific to each station pair were calculated by averaging spatial replicates over time as in Equation (15). Then, a kernel estimator was used to infer covariance values between station locations and unmonitored locations.

Models of type (17) are relevant to cases with sparse sampling in time and dense sampling in space, e.g., water pollution investigations where samples are collected at numerous locations but on few occasions. Models of type (19) are suitable for cases in which data are dense in time and sparse in space, e.g., data taken at few piezometric or rain gages at many time instants. In both cases, inference, i.e. computations and modeling of the  $T(T + 1)/2$  or  $n(n + 1)/2$  direct and cross-variograms/covariances, becomes tedious as  $T$  or  $n$  becomes larger. Note that it is also possible to extend the time series formulation to a continuous spatiotemporal domain, by regionalizing station-specific time series parameters, which are modeled independently at each station location—see, for example, Kyriakidis (1998); in this latter case, inference of  $n(n + 1)/2$  direct and cross-variograms/covariances is circumvented.

## COMMON LINKS

There exist interesting links between the approach considering a single spatiotemporal RF and the approach considering multiple vectors of RFs or TS. These links have been investigated partially by Bogaert (1996) for the case of separable space–time covariance models of type (13), and are generalized hereafter.

Consider, for example,  $T$  space RFs  $\{Z_i(\mathbf{u}), i = 1, \dots, T\}$  correlated across time. In the nonisotropic case, i.e., attribute levels are measured at  $T$  time instants  $\{t_1, \dots, t_T\}$  at different  $n_i \neq n$  spatial locations  $\mathbf{u}_{\alpha_i}$ ,  $\alpha_i = 1, \dots, n_i$ , the simple cokriging (SCK) estimator  $Z_k^*(\mathbf{u})$  for the unknown  $z(\mathbf{u}, t_k)$  at location  $\mathbf{u} \in D$  and time instant  $t_k$  is written as

$$Z_k^*(\mathbf{u}) - m_k = \sum_{i=1}^T \sum_{\alpha_i=1}^{n_i} \lambda_{\alpha_i}(\mathbf{u}, t_k) [Z_i(\mathbf{u}_{\alpha_i}) - m_i] \quad (21)$$

where  $m_i$  is the space stationary mean of the RF  $Z_i(\mathbf{u})$  defined at time instant  $t_i$ . Typically, only data closest to the “point”  $(\mathbf{u}, t_k) \in D \times T$  being estimated are considered, in which case  $n_i$  is replaced by  $n_i(\mathbf{u}, t)$  with  $n_i(\mathbf{u}, t) < n_i$ . The number of data retained and the size of the search neighborhood need not be the same for all time instants  $t_i, i = 1, \dots, T$ .

The SCK weights  $\lambda_{\alpha_i}(\mathbf{u}, t_k)$  are obtained from the SCK system:

$$\sum_{j=1}^T \sum_{\beta_j=1}^{n_j} \lambda_{\beta_j}(\mathbf{u}, t_k) C_{ij}(\mathbf{u}_{\alpha_i} - \mathbf{u}_{\beta_j}) = C_{ik}(\mathbf{u}_{\alpha_i} - \mathbf{u})$$

$$\alpha_i = 1, \dots, n_i, i = 1, \dots, T \quad (22)$$

By denoting the vector of SCK weights for the  $n_i$  data at the  $t_i$ th time instant as  $\Lambda_i(\mathbf{u}, t_k)$ , the vectorial representation of the above SCK estimator is

$$Z_k^*(\mathbf{u}) = \sum_{i=1}^T [\Lambda_i(\mathbf{u}, t_k)]' [\mathbf{Z}_i(\mathbf{u}) - \mathbf{m}_i] + m_k \quad (23)$$

where

- $\Lambda_i(\mathbf{u}, t_k) = [\lambda_{1_i}, \dots, \lambda_{n_i}]'$  is the  $n_i \times 1$  vector of cokriging weights assigned to the  $z_i$  data at locations  $\mathbf{u}_{\alpha_i}$ ,  $\alpha_i = 1, \dots, n_i$ ,
- $\mathbf{Z}_i(\mathbf{u}) = [Z_i(\mathbf{u}_1), \dots, Z_i(\mathbf{u}_{n_i})]'$ , and
- $\mathbf{m}_i$  is the  $n_i \times 1$  vector of stationary (constant) means  $m_i$  of the  $T$  spatial RFs  $Z_i(\mathbf{u})$ ,  $i = 1, \dots, T$ .

The  $T$  vectors of cokriging weights  $\Lambda_i(\mathbf{u}, t_k)$  are obtained from the solution of the single SCK system (22), expressed in matrix form as

$$\begin{bmatrix} \mathbf{K}_{11} & \cdots & \mathbf{K}_{1T} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{T1} & \cdots & \mathbf{K}_{TT} \end{bmatrix} \times \begin{bmatrix} \Lambda_1(\mathbf{u}, t_k) \\ \vdots \\ \Lambda_T(\mathbf{u}, t_k) \end{bmatrix} = \begin{bmatrix} \mathbf{k}_{1k} \\ \vdots \\ \mathbf{k}_{Tk} \end{bmatrix} \quad (24)$$

where

- $\mathbf{K}_{ij} = [C_{ij}(\mathbf{u}_{\alpha_i} - \mathbf{u}_{\beta_j})]$  is the  $n_i \times n_j$  matrix of auto- and cross-covariances between the  $n_i$  and  $n_j$  data  $z_i(\mathbf{u}_{\alpha_i})$ ,  $\alpha_i = 1, \dots, n_i$  and  $z_j(\mathbf{u}_{\beta_j})$ ,  $\beta_j = 1, \dots, n_j$  at time instants  $t_i$  and  $t_j$ , respectively, and
- $\mathbf{k}_{ik} = [C_{ik}(\mathbf{u}_1 - \mathbf{u}), \dots, C_{ik}(\mathbf{u}_{n_i} - \mathbf{u})]'$  is the  $n_i \times 1$  vector of data-to-unknown auto and cross-covariances.

Under the model decision of second-order space–time stationarity, the cross-covariance  $\mathbf{K}_{ij}$  between measurements at any pair of time instants  $t_i$  and  $t_j$  does not depend on these specific instants but only on the temporal lag  $\tau = t_i - t_j$  separating them. Hence, the following relation holds true:

$$\mathbf{K}_{ij} = \mathbf{K}_{\tau_{ij}} = [C(\mathbf{h}_{\alpha\beta}, \tau_{ij})], \quad \forall \mathbf{h}_{\alpha\beta} \in D, \forall \tau_{ij} = t_i - t_j \in T$$

where  $[C(\mathbf{h}_{\alpha\beta}, \tau_{ij})]$  is the matrix of data-to-data space–time covariances.

The previous SCK system is the same as the SK system generalized to a space–time context, which can be written as



$$\begin{aligned}
& \begin{bmatrix} [C(\mathbf{u}_\alpha - \mathbf{u}_\beta, t_1 - t_1)] & \cdots & [C(\mathbf{u}_\alpha - \mathbf{u}_\beta, t_1 - t_T)] \\ \vdots & \ddots & \vdots \\ [C(\mathbf{u}_\alpha - \mathbf{u}_\beta, t_T - t_1)] & \cdots & [C(\mathbf{u}_\alpha - \mathbf{u}_\beta, t_T - t_T)] \end{bmatrix} \begin{bmatrix} [\lambda_{\alpha 1}(\mathbf{u}, t_k)] \\ \vdots \\ [\lambda_{\alpha T}(\mathbf{u}, t_k)] \end{bmatrix} \\
& = \begin{bmatrix} [C(\mathbf{u}_\alpha - \mathbf{u}, t_1 - t_k)] \\ \vdots \\ [C(\mathbf{u}_\alpha - \mathbf{u}, t_T - t_k)] \end{bmatrix} \quad (25)
\end{aligned}$$

Hence, under second-order space–time stationarity, systems (24) and (25) are equivalent, and the estimator (21) reverts to the SK estimator in a space-time context, i.e.,

$$Z_k^*(\mathbf{u}) - m_k = \sum_{i=1}^T \sum_{\alpha_i=1}^{n_i} \lambda_{\alpha_i}(\mathbf{u}, t_k) [Z_i(\mathbf{u}_{\alpha_i}) - m_k] \quad (26)$$

Note that, per symmetry, similar conclusions can be drawn for the case of  $n$  spatially correlated TS  $Z_\alpha(\mathbf{u})$ ,  $\alpha = 1, \dots, n$  defined at locations  $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ .

Links between multivariate autoregressive models and geostatistical space–time models have been investigated by several researchers. Bras and Colón (1978) showed that the geostatistical space–time model of Rodríguez-Iturbe and Mejía (1974), who considered separable spatiotemporal covariance functions, can be expressed in terms of a vector autoregressive process. This is also true for the multivariate contemporaneous autoregressive models—see, for example, Salas (1993) and the references therein. Boulanger (1989) showed the equivalence between autoregressive processes and geostatistical procedures, while Jones and Vecchia (1993) fitted a continuous Auto Regressive Moving Average (ARMA) model to unequally spaced data, and arrived to similar results as universal kriging.

Journal (1993) noted that sequential simulation using a random path for visiting the simulation grid nodes, and simple kriging involving conditioning to previously simulated data, can be regarded as a realization of an autoregressive process. The difference is that there is no notion of spatial ordering since the visiting path is random, and the parameters of the process, simple kriging mean and variance, are determined anew at each node  $\mathbf{u}$ . Note that the sequential simulation procedure does not require that the local conditional distributions be of any particular parametric type, not even of the same type from one node to another. As long as the local conditional distributions have mean and variance equal to the local simple kriging mean and variance, the covariance model is reproduced, and this

formulation is termed direct sequential simulation (Xu and Journel, 1994). Finally, note that kriging with a trend model (universal kriging) and Kalman filtering in a steady-state mode, i.e., no dynamic evolution, were shown to be equivalent in 1D (Chirlin and Wood, 1982).

### Pros and Cons

When a single spatiotemporal RF model  $Z(\mathbf{u}, t)$  is considered, spatiotemporal continuity is modeled by a joint space–time covariance function, whereas under the multiple RF models approach, spatiotemporal continuity is modeled via the Linear Model of Coregionalization (LMC) (Journel and Huijbregts, 1978, p. 171). A joint space–time covariance function allows estimation (through kriging in a space–time context) at any location  $\mathbf{u}$  in space and any instant  $t$  in time. Under the LMC, estimation (through cokriging) is possible only at “points”  $(\mathbf{u}, t)$ ,  $t \in \{t_1, \dots, t_T\}$  in the case of  $T$  temporally correlated RFs, and only at “points”  $(\mathbf{u}, t)$ ,  $\mathbf{u} \in \{\mathbf{u}_1, \dots, \mathbf{u}_n\}$  in the case of  $n$  spatially correlated TS. Inference of a joint space–time covariance is not possible when only few data are available at the same space location or same time instant, whereas this is not a limitation for the LMC. Conversely, as measurements either in the spatial or temporal domain become more abundant, the multivariate approach becomes less appealing because  $T(T + 1)/2$  or  $n(n + 1)/2$  auto- and cross-covariances have to be computed and modeled. In the case of  $T$  cross-correlated spatial RFs, typically a Markovian temporal evolution for the process of interest is assumed, so that the number of RFs involved in the LMC is kept small. This is a sound practice, since for a time-stationary process the temporal screening effect is very pronounced, i.e., data two or three time instants in the past have a very small influence on the value at the current time instant. In the case of  $n$  spatially correlated TS, the modeling procedure proposed by Kyriakidis (1998) allows a practical extension of the vectorial TS formulation to a continuous spatial domain. Note that recently developed algorithms for iterative fitting of a permissible LMC (Goulard and Voltz, 1992) or automatic modeling of positive definite covariance and cross-covariance tables via fast Fourier transform (Yao and Journel, 1998) could be considered for alleviating the inference burden. Finally, note that inference under the LMC does not require stationary in time in the case of  $T$  temporally correlated RFs, or stationary in space in the case of  $n$  spatially correlated TS.

A major difference between the vectorial time series approach and the single spatiotemporal RF approach is that in the latter framework only data from previous time instants are considered in the estimation procedure.

Such a framework is suitable for real-time estimation and forecasting, whereby data are only available in the past and the present, not in the future. When analysis is performed in a “batch” mode, i.e., data for many time instants and spatial locations are modeled after they have been acquired, and the goal is interpolation in space and time (also called smoothing in the time series jargon), both a forward and a backward filtering step should be performed (Gelb, 1974). In this batch mode case, the single random function approach is more appealing, and Solow (1984) argued that, for the 1D case, time series and geostatistical methods are isomorphic. In the real-time forecasting case, cokriging the unknown value  $z(\mathbf{u}, t_i)$  using contemporaneous data  $z(\mathbf{u}_\alpha, t_i)$  and data from one or two previous time instants  $z(\mathbf{u}_\alpha, t_{i-1})$ ,  $z(\mathbf{u}_\alpha, t_{i-2})$  appears a suitable approach. Modeling of the auto- and cross-covariances involved could be alleviated via collocated cokriging under a Markov model of the type proposed by Almeida and Journel (1994), which is very similar to adopting a separable space–time covariance function.

## DISCUSSION AND FUTURE DIRECTIONS

A review attempting to organize the numerous existing geostatistical space–time models is presented. Two major conceptual viewpoints are distinguished, one calling for a single spatiotemporal random function model, and the other calling for vectors of space random functions or vectors of time series. Links between these two viewpoints are investigated, and advantages and shortcomings are highlighted.

The present practice of stochastic modeling of spatiotemporal distributions is typically case specific: models are developed for each particular data set and each particular study goal. This could be regarded as a drawback, yet we see it as a blessing because modeling remains in the hands of practitioners, who select and tune the model to fit best the particular problem at hand.

It appears that theory, as indicated by the number of existing models, has somewhat outrun data availability. There exists a need for abundant, error-free measurements representative of the scale at which the phenomenon is modeled. Such data would allow validating otherwise subjective modeling decompositions. Ideally, a model decomposition in a spatiotemporal trend plus a residual should have a physical justification and interpretation. Any model component, whether trend or residual, that cannot be validated from actual data is but a model and should be clearly stated as such.

Benchmark case studies comparing the performance of the various

models proposed in the literature are also needed. Such comparative studies would allow a close look at the advantages and disadvantages of each model, and would enable validation of critical decisions involved in the modeling process. It would be also useful to test the performance of the various algorithms against a single or a few exhaustively known spatiotemporal fields. Such reference spatiotemporal fields should not be mere realizations of a Gaussian random function with a congenial separable space-time covariance; instead, it should correspond to an outcome of a complex transfer function based on a realistic input parameter field. For example, a pressure field derived from simulating flow in a highly structured (low entropy), non-Gaussian permeability field could be used as reference, against which the predictive ability of different space-time stochastic models could be evaluated. It would be also interesting to compare in practice batch algorithms (using all available data), such as kriging or cokriging in a space-time context, with the recursive Kalman filter algorithm.

Assessment of the joint space-time uncertainty, e.g., the probability that several attribute values at any set of "points" in  $D \times T$  be jointly no greater than a given threshold, is given scant attention. Within current models, the joint space-time uncertainty assessment is typically addressed by first obtaining a "best" estimate, in a least square sense, for the unknown value  $z(\mathbf{u}, t)$  at  $(\mathbf{u}, t) \in D \times T$ , and then attaching some Gaussian-related confidence intervals to the resulting kriging variances. A notable exception to this practice is the work of Bilonick (1988), who applied indicator kriging to determine non-Gaussian probability distributions for the unknowns.

Modeling of spatial uncertainty is routinely addressed in a purely spatial context through the use of conditional stochastic simulation (Deutsch and Journel, 1998). Similarly, uncertainty associated to reconstruction of temporal attribute profiles or prediction of future behavior at monitoring locations is addressed via simulation of the time series at these locations, either through spatial time series models (Bras and Rodrigues-Iturbe, 1984) or more recently via sequential cosimulation (Soares, Patinha, and Pereira, 1996). The challenge lies in extending the concept of conditional simulation to joint space-time distributions, as noted also by Haas (1998).

Remotely sensed soft information, which consists of nearly exhaustive observations indirectly linked to the attribute of interest, should be accounted for in the modeling procedure. Data-constrained, or parameter-rich, algorithms should be developed and tested; the objective being to incorporate as much information as possible into the modeling of joint space-time uncertainty, yet accounting for the relevance of each piece of information to the unknown. Various techniques already exist and have been applied in a purely spatial context for such integration purpose. An

additional challenge lies into exporting and assessing the applicability of these techniques in a space-time setting.

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