

## I. INTRODUCTION

The understanding and the preservation of water resources and the natural environment are an issue of primary importance for our society. From an economic viewpoint, past experience shows that measures taken to control water and air pollution have resulted in socio-economic benefits that far outweighed their cost, such as reduction of medical and remediation expenses and improved life conditions. In order to implement effective measures to protect our water resources and our environment, it is necessary to gain a good understanding of environmental processes using mathematical and numerical modelling tools. The development of predictive tools that model accurately the natural processes of environmental importance will lead to better-informed public policy decisions. Considering that large experimental laboratory and field studies are expensive and limited in their scope, environmental modeling is the most cost-effective method for the investigation of the physical properties of environmental processes.

One of the difficulties in modelling natural processes is that they often exhibit high variability in space and time over large scales. Consider for example the fluctuations of the water levels and water quality indicators for the High Plain aquifer along the Mississippi; the distribution of ozone in the atmosphere over the US; or the variation of ambient temperature over a state for several years. These environmental processes are monitored using sparse and often uncertain measurements; requiring that a stochastic approach be taken to account for the inherent variability of the processes and the uncertainty in the prediction. A stochastic approach is useful because it provides estimates of the natural variable as well as their associated uncertainty. From the stochastic estimates we may draw spatio-temporal maps, which are used in a variety of applications, for they provide a

realistic visual representation of the distribution of the natural process in the space/time domain, as well as a quantitative assessment of its uncertainty (e.g., Bilonick, 1985; Dimitrakopoulos and Luo, 1993; Koussoulakou, 1994; Vyas and Christakos, 1997). Stochastic models are also useful for the analysis of multiphase flow and transport in heterogeneous media (Miller *et al.*, 1998).

A sound logical framework and a rigorous incorporation of the physical knowledge available are important aspects of scientific mapping in space/time. When we talk about any sort of science we are talking about two components: (a) an organized body of physical knowledge (ontological component), and (b) a distinctive methodology for obtaining and processing knowledge of the subject matter of the science (epistemological component). It is by virtue of the latter epistemological component that we can say, e.g., that modern physics is importantly different from scholastic physics. The epistemic viewpoint a discipline adopts is a part of its very characterization of its scientific content. In the case of modern geostatistics (e.g., IAMG, 1998), this viewpoint has led to the development of a novel group of concepts and methods, which have considerable advantages over classical geostatistics (popular classical geostatistics references include Matheron, 1971, 1978; Journel and Huijbregts, 1978; Isaaks and Srivastava, 1989; Armstrong and Carignan, 1997; and Armstrong, 1998). Indeed, the methods of classical geostatistics (e.g., kriging estimators) were primarily designed to fit into a pure inductive framework and, thus, to use hard data (i.e., sets of measurements). As a consequence, these methods lack the theoretical underpinnings and practical flexibility to account for important sources of physical knowledge (including physical laws, empirical models, higher-order space/time moments, and uncertain information).

A powerful member of the modern geostatistics group is the Bayesian maximum entropy method (BME; Christakos, 1990; 1992), which is a much more powerful and

general method than any type of kriging. The double epistemological goal of BME is informativeness (prior information maximization given general knowledge) and cogency (posterior probability maximization given specificatory knowledge). BME provides a systematic and rigorous approach for incorporating various physical knowledge bases into spatiotemporal analysis and mapping, including statistical moments of any order, physical laws, scientific theories, and uncertain observations.

My goal in this work is to provide some theoretical and computational advances in spatio-temporal mapping of environmental processes, with a particular interest on applications related to water resources and ground water modelling. In this context I investigated the BME method for spatio-temporal mapping, and I also looked at a numerical method for modelling of ground-water flow called the Space Transformation (ST) method (Hristopulos et al.; 1999). I found that the BME method is a powerful method for spatiotemporal mapping that has the flexibility to incorporate a variety of knowledge bases that cannot otherwise be included in existing methods of geostatistics. In the following Chapters I will present efficient numerical implementations of the BME method corresponding to different knowledge bases of interest in spatiotemporal mapping. The formulation and numerical implementation presented are tested using numerous numerical comparisons with existing methods which show the superiority of computational BME. BME is shown to be more accurate than classical geostatistical methods when combinations of hard and soft data are involved (Serre et al., 1998; Serre and Christakos, 1999). Furthermore, while classical methods usually employ a simple measure of estimation uncertainty (such as the estimation error variance), BME offers a more complete uncertainty analysis in terms of confidence sets. Valuable insights are also gained from the several case studies they were conducted in the area of aquifer modelling and environmental health (Serre and Christakos, 1999; Christakos and Serre; 1999).