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A Numerical Comparison Between Quasi-Monte Carlo and Sparse Grid Stochastic Collocation Methods

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Abstract. Quasi-Monte Carlo methods and stochastic collocation methods based on sparse grids have become popular with solving stochastic partial differential equations. These methods use deterministic points for multi-dimensional integration or interpolation without suffering from the curse of dimensionality. It is not evident which method is best, specially on random models of physical phenomena. We numerically study the error of quasi-Monte Carlo and sparse grid methods in the context of groundwater flow in heterogeneous media. In particular, we consider the dependence of the variance error on the stochastic dimension and the number of samples/collocation points for steady flow problems in which the hydraulic conductivity is a lognormal process. The suitability of each technique is identified in terms of computational cost and error tolerance.

AMS subject classifications: 60H15, 65C05, 65C20, 65C20

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1 Introduction

The simulation of natural phenomena are susceptible to uncertainties that may be present on initial conditions, boundary conditions, or material properties. A representative example is flow through porous media, where medium properties, such as hydraulic conductivity and porosity, are not precisely known due to the scarcity or limited accuracy of measurements.

A computational technique widely used for this purpose is the Monte Carlo method (*MC*). It entails generation of a large number of random realizations of input variables,

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solving deterministic flow simulations for each realization. This method is robust and conceptually simple, but requires intensive computational effort since the number of realizations needed to achieve statistical convergence is very large in general. On the other hand, other techniques for solving these problems have gained great attention in recent years: quasi-Monte Carlo (*QMC*) methods [8, 19, 21] and Sparse Grid (SG) collocation methods based on Smolyak quadrature [2, 4, 10, 30].

Traditionally, *QMC* methods are based on deterministic numerical integration [19] in analogy to the technique of Monte Carlo simulation. In *QMC*, pseudo-random sequences are replaced by deterministic, low discrepancy sequences. For these sequences, Koksma-Hlawka inequality yields a rate of convergence $\mathcal{O}(N_r^{-1}\log(N_r)^M)$, where N_r is the number of realizations and M represents the stochastic dimension [29]. Such an order of convergence is an improvement over the Monte Carlo method, which is $\mathcal{O}(N_r^{-1/2})$ [26].

From another standpoint, *SG* methods arise from the study of multivariate polynomial interpolation [24] and achieves fast convergence to the solution when it has sufficient smoothness in random space, offering high-order accuracy with convergence rate depending weakly on dimensionality. Both *QMC* and *SG* methods do not suffer from the curse of dimensionality, i.e., the exponential growth of the computational cost with the problem dimension, which is typical of tensor-product, multi-dimensional quadrature rules [22, 27, 30].

The purpose of this paper is to contrast *QMC* and *SG* methods. Previous studies in this direction were done by Bungartz et al. [6], who studied the potential of adaptive sparse grids for multivariate numerical quadrature. Their numerical results showed that the adaptive sparse grid is superior to *QMC* when the integrand is smooth. An analogous procedure is also adopted in context of asset-liability management (ALM) simulations. Gerstner et al. [12] show with different parameter setups how the accuracy of *MC*, *QMC* and *SG* methods depend on the variance and the smoothness of the corresponding integration problem and concluded that *QMC* and *SG* based on Gauss-Hermite quadrature formulas are often faster and more accurate than Monte Carlo simulation even for complex ALM models with many time steps.

However, such an analysis has not yet been reported for physical models involving spatially-correlated random input data, and this is the main motivation of the present work. Sparse grid methods have been thoroughly studied in this context and theoretical error estimates are available [23]. Efficient *QMC* implementations for these models have been recently proposed [14], though the error analysis is in a preliminary level (see also [33]). We focus our study in an elliptic equation that describes the fluid flow on a saturated, randomly heterogeneous porous media in which the hydraulic conductivity is a lognormal random field represented on the Karhunen-Loève expansion.

The paper is organized as follows. The next section introduces the model problem. The variational formulation of the problem and spatial discretization are given in Section 3. The *MC* and *QMC* algorithms are presented in Section 4. The sparse grid method is described in Section 5. Numerical experiments are discussed in Section 6.