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Improved metamodel-based importance sampling for the performance assessment of radioactive waste repositories

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ABSTRACT

In the context of a probabilistic performance assessment of a radioactive waste repository, the estimation of the probability of exceeding the dose threshold set by a regulatory body is a fundamental task. This may become difficult when the probabilities involved are very small, since the classically used sampling-based Monte Carlo methods may become computationally impractical. This issue is further complicated by the fact that the computer codes typically adopted in this context requires large computational efforts, both in terms of time and memory. This work proposes an original use of a Monte Carlo-based algorithm for (small) failure probability estimation in the context of the performance assessment of a near surface radioactive waste repository. The algorithm, developed within the context of structural reliability, makes use of an estimated optimal importance density and a surrogate, kriging-based metamodel approximating the system response. On the basis of an accurate analytic analysis of the algorithm, a modification is proposed which allows further reducing the computational efforts by a more effective training of the metamodel.

1. Introduction

The technical context of the work presented in this paper is that of the performance assessment of a radioactive waste repository. This involves the estimation of the expected dose to a properly defined individual, due to radionuclides release and migration back to the biosphere. In this paper, we adopt the reliability model presented in [1] for estimating the repository barriers failure time distributions and the corresponding dose to the critical individual. Input parameter uncertainties are accounted for in terms of probability density functions; then, the output of the reliability model (i.e. a radiological dose) is itself an uncertain variable characterized by a probability density function. We are interested in estimating the probability that the dose exceeds some defined regulatory threshold [2–6].

A typical approach to the estimation of the probability of a random variable exceeding a threshold is that of resorting to Monte Carlo (MC) simulation, which amounts to (i) sampling N values of the input parameters from their uncertainty distribution and (ii) running the model in correspondence of each of the N sets of input parameters in order to compute the corresponding output doses [3–6]. The failure probability, i.e. the probability of exceeding the threshold can then be estimated by dividing the number of "failure" scenarios in which the dose threshold is exceeded by the total number of scenarios simulated, N.

Repository barriers are designed to offer a high level of protection towards radionuclide release and migration, so that the event of the dose exceeding the regulatory threshold is rare. The estimation of the probability of such event requires a large number of simulations and, consequently, large computational times by standard MC simulation schemes. It is, thus, necessary to develop alternative simulation techniques, for performing the estimation with affordable computational costs.

The estimation problem can be framed as it is done in structural reliability, where the rare event of interest is the failure of the structure computed by complex finite elements models [7–9] . Exploiting this framework analogy, in this work, we propose to resort to the meta-IS algorithm introduced in [7] for estimating the probability that the radiological dose from the repository exceeds the regulatory threshold.

The general idea underlying the algorithm is that of combining the two main approaches usually proposed as alternative to brute force MC for improving the computational efficiency, i.e. the metamodel approximations and variance reduction techniques. The first approach consists in defining a surrogate model to provide a fast, approximated response and use it in the repeated runs of MC simulation. The main limit of this approach is in the difficulty of quantifying the approximation error [7]. The second approach aims at making MC sampling more efficient, so that less

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model runs are required to achieve a given accuracy of estimation. In order to efficiently combine these two approaches, several metamodels have been proposed in literature, such as quadratic response surfaces [10–12], polynomial chaos expansions [13], support vector machines [9,14–16], neural networks [17,18] and kriging [19–21]. The major drawback of the direct substitution of the original performance function with a surrogate model is that it is often impossible to keep the approximation error under control [7]. On the other hand, one of the most popular variance reduction techniques is that of Importance Sampling (IS), whereby a suitable importance density is chosen so as to favor the MC samples to be near the failure region, thus forcing the rare failure event to occur more often [7]. In this regard, it is possible to show that there exists an optimal importance density so that the variance of the MC estimator is zero [22]. Unfortunately, this pdf is not implementable in practice, since its analytical expression depends on the unknown failure probability p_f itself. On the other hand, several techniques in various fields of research have been proposed to reduce some distances between the instrumental pdf and the optimal one [7].

The meta-IS algorithm considered in this work addresses this issue by exploiting a kriging metamodel in order to define a quasi-optimal importance sampling density. The estimate of the failure probability is, then, obtained as the product between the estimate provided by the surrogate function and a correction factor computed by comparing the surrogate and the real function in the failure region [7].

Through a careful analysis of the results of the meta-IS algorithm for the repository performance assessment, we identify a further improvement of the algorithm in terms of calls to the original model, which aims at compensating an apparent unbalanced effort between the estimation of the correction factor and the refinement of the metamodel itself. On the basis of a theoretical discussion to provide a formal justification of the proposed improvement, the meta-IS algorithm is modified and applied to the reliability model of the repository for failure probability estimation.

The paper is organized as follows. Section 2 briefly recalls the reliability model of the radioactive waste repository, Section 3 describes the Meta-IS algorithm and presents the results of its application to the performance assessment problem. In Section 4, the proposed modification is introduced from the theoretical and the operative points of view, and the results obtained with the two methods are compared. Some conclusions are drawn in the last section.

2. Radioactive waste repository model

We consider a near surface disposal facility for low-intermediate level radioactive wastes [1,3]. We briefly recall the main assumptions in the model for the estimation of the expected dose; the interested reader can refer to [1,3] for further details.

The repository is described as a series system made up of 6 barriers, which are represented as binary components characterized by two states, working or failed, depending on whether or not the barriers are capable of performing their protection function with respect to the flow of water. The failure time of each barrier is assumed to be a random variable distributed according to an exponential probability density function $\lambda_l \exp(-\lambda_l t)$, where λ_l, $l = a, \ldots, f$ is the parameter of the pdf related to barrier l and the initial time corresponds to $t = 0$. The probability density function of the disposal system failure time, $f_s(t)$, can be analytically computed as

$$f_s(t) = \left(\prod_{l=a,\ldots,f} \lambda_l \right) \left(\sum_{l=a,\ldots,f} \frac{e^{-\lambda_l t}}{\prod_{k \neq l} (\lambda_k - \lambda_l)} \right), \tag{1}$$

Table 1
Quantiles of parameters λ_i [3].

Barrier	Parameter	5th Percentile	95th Percentile
Top cover	$\lambda_a(1/y)$	1/50	1/10
Waste container	$\lambda_b(1/y)$	1/25	1/5
Waste form	$\lambda_c(1/y)$	1/4000	1/300
Backfill	$\lambda_d(1/y)$	1/55	1/12
Bottom cover	$\lambda_e(1/y)$	1/26	1/6
Unsaturated zone	$\lambda_f(1/y)$	$8.64 \cdot 10^{-5}$	$6.09 \cdot 10^{-4}$

Note that, within this probabilistic modeling of the repository evolution, the "failure" of the last barrier, i.e. the unsaturated zone (UZ) (see Table 1), occurs when the radionuclides cross it and reach the aquifer: as proposed in [1], the corresponding "failure" rate is assumed to be $\lambda_f = 1/(R \times T)$, where R is the UZ retardation factor, $T = z/U_z$ is the average radionuclide travel time in the UZ, z is the UZ thickness and U_z is the infiltrating water velocity in the UZ.

For simplicity, in what follows we refer to a single species of radionuclide and neglect the contributions provided by the radionuclides generated by the decay chains of different species of radionuclides contained in the repository. Denoting by T(y) the time at which the waste placement activities end and assuming a constant waste placement rate, the expected value of the number of radionuclides released into the groundwater per unit time can be written as [1,3]

$$R_d(t) = S_d(t) f_s(t), \tag{2}$$

$$R_p(t) = S_p(t) f_s(t+T), \tag{3}$$

where the d and p indices indicate the "disposal" and "post-closure" periods, respectively, and $S_d(t)$(Bq[1] = 1/s) and $S_p(t)$(Bq) are the associated inventories of a specific radionuclide at time t [3].

In the hypotheses that (i) the groundwater flow and transport phenomena can be represented in one dimension and (ii) the repository release is dimensionless, then the time dependent expected radionuclide concentrations (Bq/m^3) in the groundwater before and after the closure of the repository can be evaluated by the following convolution integrals [1,3]

$$C_d(x,t) = \int_0^t R_d(t-\tau) C_g(x,\tau) d\tau, \tag{4}$$

$$C_p(x,t) = \int_0^T R_d(T-\tau) C_g(x,t+\tau) d\tau + \int_0^t R_p(t-\tau) C_g(x,\tau) d\tau, \tag{5}$$

where x(m) is the longitudinal distance in the flow direction, t is the time elapsed since the beginning of disposal operations both in Eqs. (4) and (2) and since the end of disposal operations both in (5) and (3), and $C_g(x,t)$(Bq/m^3) is the Green's function of the one-dimensional advection–dispersion equation [1,23]

$$C_g(x,t) = \frac{e^{-\nu_r t} e^{-(x - U_x^1 \cdot t)^2 / 4D_x^1 \cdot t}}{2\pi A R \theta \sqrt{D_x^1 t}}, \tag{6}$$

where ν_r is the radioactive decay constant of the considered radionuclide, $U_x^1 = U_x/R$(m/y) is the retarded groundwater velocity, $D_x^1 = D_x/R$(m^2/y) is the retarded longitudinal dispersion coefficient, A(m^2) is the aquifer cross-sectional area, $R = 1 + K_d \cdot \rho_b/\theta$ is the retardation factor, K_d(ml/g) is the distribution coefficient, ρ_b(g/m^3) is the bulk density and θ is the effective porosity.

The expected dose rate in x at time t is, then

$$D(x,t) = C_{d,p}(x,t) \gamma \delta, \tag{7}$$

[1] 1 Bq = 1 nucleus disintegration per second.