Quasi-Monte Carlo based uncertainty analysis: sampling efficiency and error estimation in engineering applications

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Abstract

In this paper, the potential benefits of quasi-Monte Carlo (QMC) methods for uncertainty propagation are assessed via two applications: a numerical case study and a realistic and complex building physical case study. The sampling efficiency of four quasi-Monte Carlo sampling strategies — Optimized Latin hypercube, Sobol' sequence, Niederreiter–Xing sequence and lattice sequence — are quantified and the errors of these quasi-Monte Carlo methods are estimated. In addition, for getting a better understanding of the potential factors that may influence the performance of quasi-Monte Carlo methods, the effect of the different parameters and the smoothness of the target function for the building physical case study are investigated for two quantities of interest. A sensitivity analysis is performed in which first and total order Sobol' indices are calculated and a kernel smoother is used to show the effect on the quantity of interest for certain input parameters. The outcomes show that quasi-Monte Carlo methods perform at least as well as the Monte Carlo method and are capable of outperforming the standard Monte Carlo method if the target function is sufficiently smooth and mainly depends on a limited number of parameters.

Keywords: Quasi-Monte Carlo; Uncertainty propagation; Building performance; Sampling efficiency; Error estimation; Sensitivity analysis; Sobol' indices; Kernel smoother

1. Introduction

The use of numerical simulations for complex systems is common. However, significant uncertainties may exist for many of the involved variables, and in order to ensure the reliability of our simulation results and the safety of such complex systems, a stochastic approach providing statistics of the probability distribution of the results is of crucial importance. In other words, a stochastic approach is required for identifying, characterizing, quantifying and displaying the uncertainty in the outcomes of analyses for these complex systems [1]. So far, the necessity of (global) uncertainty analysis for reliability evaluation and safety assessment has been addressed in a multitude of disciplines, e.g., [2, 3, 4, 5, 6, 7, 8]. A detailed evaluation of different levels of uncertainty treatments in risk analysis has been presented by Paté-Cornell [2] over two decades ago, and many approaches to perform uncertainty analysis in different disciplines are in use. Ricotti and Zio [3] investigate the use of artificial neural networks for sensitivity and uncertainty analysis of steam generator transient simulation. Cheung et al. [4] apply Bayesian uncertainty quantification techniques to turbulence modeling. In [5], a simple stochastic model is developed and can be embedded in the Monte Carlo probabilistic framework for the assessment of flood risk. In [6], systems analysis and Bayesian probability based probabilistic risk analysis are applied as a decision support tool for assessing a set of government safety decisions. In [7], a general probabilistic risk analysis framework is presented to quantify the uncertainties inherent in predictions of subsurface flow and transport. In [8], a combination of polynomial chaos expansion and Monte Carlo based probabilistic analysis is proposed for evaluating the risk of CO_2 storage in geological formations. Also, in building

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Nomenclature

n	the number of samples	t	the time (s)
d	the number of parameters	p_c	the capillary pressure (Pa)
μ	mean of the target	λ	the thermal conductivity (W/mK)
σ	standard deviation of the target	g_l	vapor flow (kg/m ² s)
f	the calculation objective	g_v	liquid flow (kg/m ² s)
r	the number of replications	L_v	the heat of vaporization (3.13106J/kg)
θ	standard error	K_l	the liquid permeability (s)
c_0	specific heat capacity of the material	p_v	the vapor pressure (Pa)
c_l	specific heat capacity of the liquid (4180J/kgK)	δ_v	the water vapor permeability (s)
c_v	specific heat capacity of the vapor (1880J/kgK)	ρ_l	the vapor pressure (Pa)
c_d	a constant depends on the dimension d	R_v	the gas constant of water (461.89J/kg.K)
ρ_0	material density (kg/m ³)	QMC	quasi-Monte Carlo
w	moisture content (kg/m ³)	n_{QMC}	the number of samples of one QMC sequence
T	the temperature (K)	n_{MC}	the number of samples of one MC sequence
		$\overline{Q_{n,r}}(f)$	mean of r n -run QMC evaluations
		$Q_n(f)$	a single n -run QMC evaluation

physical engineering, numerous uncertainties and variabilities exist in the material properties, in the construction geometries, in the climatic loads etc. The appraisal of these uncertainties is naturally connected to the assessment of the occurrence of damage patterns such as frost damage, mould growth and wood decay. Therefore, in order to guarantee the durability of our buildings and the safety of their occupants, a probabilistic assessment of building performance is necessary.

A variety of probabilistic modelling approaches for uncertainty propagation have been developed over the last decades [9, 10, 11, 12, 13]. Among them, sampling-based uncertainty propagation through Monte Carlo approaches is the most versatile and widely used, because of its general applicability and typical robustness [14]. More specifically, for uncertainty analysis, Monte Carlo method is considered to be the most reliable technique when an accurate failure probability need to be calculated from exact probability density functions and limit state equations. Complementarily, for robustness assessment, Janssen [14] states that "at the highest level quantification of the spread on the performance of structures, systems or solutions is desired, Monte Carlo based uncertainty analysis forms a frequently employed procedure". The use of Monte Carlo method for assessing the system safety can be found in virtually all engineering fields, from the assessment of human actions reliability [15], over the appraisal of nuclear safety system [16, 17], to the design of LNG fuel gas supply system [18]. Also, in building physical engineering, the sampling-based Monte Carlo analysis has been used for hygrothermal probabilistic assessment since over a decade ago [19] to estimate the inside temperature distribution from a carefully selected sample of input distributions. Recently, it has become a powerful tool for e.g. the risk assessment of installing interior insulation for wall retrofitting, in order to exploit the capacity for energy savings offered by interior insulation while avoiding hygrothermal failure [20]. The essential idea of this method is to repeat the execution of a deterministic core simulation with randomly selected values of the input variables, in order to obtain the probability distribution of the targeted output values. However, in cases where that deterministic core simulation is (relatively) time consuming, the number of needed repetitions should be minimized. In that respect, three criteria are crucial:

1. efficiency of the sampling scheme,
2. reliable estimation of the error,
3. sequential sample addition.

Firstly the sampling scheme should be as efficient as possible, which can be described as using as few samples as possible to obtain a targeted accuracy of the outcomes. When the quantity of interest is an expected value, the rate of convergence of the Monte Carlo method is $n^{-1/2}$, with n the number of function evaluations, if the target function is square integrable. This can be improved to n^{-1} by using a more uniform sampling scheme based on low-discrepancy points, albeit with some additional smoothness conditions on the target function. To be more precise the convergence contains a $(\log n)^d$ factor which will be discussed later. These are called quasi-Monte Carlo methods, see, e.g., [21, 22, 23]. This faster convergence rate therefore opens the possibility of a more efficient sampling scheme, provided the implied constant for the quasi-Monte Carlo method is not too big. Secondly, monitoring this sampling convergence should be possible, in other words, estimation of the accuracy of the outcomes should be feasible. Such error estimation allows terminating the computation when the targeted accuracy has been reached. Thirdly, sequential additions of samples should be possible. By doing so, a targeted accuracy can be reached without incurring the cost of restarting the whole computation for a larger number of samples.

Next to the plain Monte Carlo (MC) method of random sampling with rate $n^{-1/2}$, Janssen [14] assessed regular Latin hypercube sampling (LHS) as well as optimised Latin hypercube sampling (OLHS). LHS was first introduced by McKay et al. [24]. Stein [25] proved that LHS gives an estimator for a function mean that has lower variance than plain Monte Carlo for any function having finite second moment. Further, Owen [26] expanded Stein's work by proving a central limit theory for LHS. OLHS optimizes a LHS towards a uniformity criterion [27], which could achieve an n^{-1} rate, similar to regular quasi-Monte Carlo methods. However, in (O)LHS the sample points are not random, and therefore a variance estimation of its outputs (property two from above) does not exist. Moreover, the number of samples is fixed in advance and hence property three from above is not satisfied. To overcome the above limitations, several studies have been conducted before. A method of the extension of LHS with correlated variables has been proposed by Sallaberry et al. [28], in order to limit the number of needed model evaluations. In addition, for obtaining an error estimation of the outputs of LHS, Iman [29] makes use of replicated sampling to estimate the sampling variance in results obtained with LHS. In order to further reach the three criteria from above, Janssen [14] hence promoted another form of Latin hypercube sampling, namely "replicated optimized Latin hypercube sampling" (ROLHS), wherein smaller sub-designs are sequentially added to reach the desired number of samples n , instead of using a single n -sample optimized Latin hypercube design. Due to the faster convergence rate of optimized Latin hypercube (OLHS) sampling over standard Monte Carlo (MC) and Latin hypercube sampling (LHS), the sampling efficiency of the replicated optimized Latin hypercube sampling (ROLHS) has the improved rate of the OLHS for each sub-design [14]. Furthermore, by making use of a "sample splitting" bootstrap method, Janssen [14] introduces a seemingly viable error quantification method.

Unfortunately, the ROLHS approach is still not fully in line with the second and third demand. With respect to point three, blocks of samples, instead of single samples, are sequentially added. More critically, the main drawback of this method is that correlations may exist between the smaller sub-designs, given that each small sub-design is optimized via the same algorithm. These correlations may in turn lead to an overly positive bias for the error estimation. Finally, the central limit theorem states that, if the different sub-designs are truly independent, the convergence rate of ROLHS is only $n^{-1/2}$, the same as basic random sampling, implying that it is less efficient than a single n -sample OLHS.

Instead of the replicated optimized Latin hypercube sampling, quasi-Monte Carlo (QMC) methods, which are typically constructed based on low-discrepancy sequences, can also be used for efficient uncertainty propagation. They have recently been used in many applications such as uncertainty quantification for PDEs with random coefficients [30], high dimensional integration in generalized linear mixed models in statistics [31], and mathematical finance related applications [32]. In addition, QMC methods are becoming popular for performing sampling-based (global) sensitivity analysis in order to improve the efficiency and reduce the CPU cost and time of the target calculation [33, 34, 35, 36]. More particularly, low-discrepancy sequences can directly fulfill the third criterion, as the addition of a single sample, is a property of such sequences. Their convergence rate will still be n^{-1} in this case [37], under some smoothness conditions on the target function. Moreover, some QMC methods can also achieve even higher order n^{-a} , $a > 1$, under more demanding assumptions on the target function. However, when simply adding one sample at a time, a convergence of n^{-1} is best possible, [37]. With respect to the second point above, there are "randomization procedures" for QMC methods which can make r independent copies of the sequence, as such obtaining r independent and unbiased estimates.

It is then straightforward to obtain an estimate of the standard error for the mean of these r independent estimates. In this paper we will assess the sampling efficiency and error estimation of some QMC methods for uncertainty propagation, and evaluate their sampling efficiency and error estimation via numerical and building physical case studies.

This paper is built up as follows. First, the quasi-Monte Carlo sampling strategies and related randomization techniques are briefly put forward in §2, with attention for the potential problems that they may bring w.r.t. high number of parameters and the number of “influential” parameters of the target function. Subsequently, two case studies — a numerical and a building physical application — are respectively performed in §3 and §4, with focus on both sampling efficiency and error estimation for the different sampling methods. In particular, the purely numerical examples in §3 are meant to illustrate the potential problems of applying QMC to the building physical application in §4. In addition, for obtaining a rational explanation of the results shown in §3 and §4, the potential factors that may effect the sampling efficiency of quasi-Monte Carlo methods are investigated. Finally, synthesizing all the findings, conclusions on which conditions determine the superiority of quasi-Monte Carlo over standard Monte Carlo and applying quasi-Monte Carlo methods to such forward uncertainty quantification problems are formulated. We want to point out that, this paper purely focuses on the probabilistic treatment that can be used to treat epistemic and aleatory uncertainties characterized by probability distributions but not epistemic uncertainties characterized by non-probabilistic methods such as intervals or fuzzy sets.

2. Quasi-Monte Carlo sampling strategies and respective randomizations

The standard Monte Carlo (MC) method uses an average of function values as a simple estimator of the expected value. The central limit theorem states that if the integrand function f is square-integrable, the error of standard MC sampling behaves like $\sigma^2(f) n^{-1/2}$, where $\sigma^2(f) < \infty$ is the variance of f . This error bound is stochastic, and allows to state with a certain confidence level (probability) that the error is smaller than a certain multiple. A quasi-Monte Carlo (QMC) method takes exactly the same form but replaces the random samples by deterministic well chosen points by means of low-discrepancy sequences or point sets. The typical classical error bound for QMC is of the form $V(f) c_d n^{-1} (\log n)^d$ and holds when $V(f) < \infty$, which is the variation of f in the sense of Hardy and Krause and $c_d n^{-1} (\log n)^d$ is the discrepancy bound to call a sequence or point set to have low-discrepancy [21]. It is important to notice that the QMC error bound is a deterministic worst-case error bound and can therefore not be directly compared to the MC error bound. But since the error estimator for the QMC method in this paper will be based on taking multiple independent randomizations of the same QMC point set, to be discussed below, the QMC error bound will also be stochastic. For the efficiency analysis it is sufficient to understand the deterministic error bound. Three different QMC sequences will be used in the numerical experiments in this paper: a Sobol’ sequence [38], a Niederreiter–Xing sequence [39] and a lattice sequence [40]. The first two are from the digital net/sequence family, while the last one is from the lattice rule/sequence family. A scatter-plot of three QMC sequences together with the standard Monte Carlo sequence are shown in Figure 1, all four sequences contain 64 points. For MC points we can see clusters and gaps while for the QMC pointsets this does not happen. The QMC point sets on the other hand do show some structures. The most obvious are the “lattice structure” (i.e. lines) for the lattice point set. In addition, the three criteria from the previous section are now discussed in more detail.

2.1. Efficiency

The efficiency of the QMC method depends on the behavior of the error bound that can be applied. In the classical analysis this bound has the form $V(f) c_d n^{-1} (\log n)^d$. The condition to have $V(f) < \infty$ for QMC delivers the improved rate of n^{-1} over the MC method, where $\sigma^2(f) < \infty$ is needed for the rate of $n^{-1/2}$. Much of the current literature, e.g., Dick et al. [22], typically uses a slightly stronger condition to have all first order mixed partial derivatives to be square-integrable. Further demanding higher-order mixed partial derivatives to be square-integrable then enables getting higher-order convergence (e.g., [30]). On the other hand, discontinuous functions in general do not have any smoothness or finite variation $V(f)$ and thus the error bound does not apply. However, functions with kink discontinuities parallel to the coordinate axes are fine and it is known that in such a case QMC can still perform quite well [41].

In applications it is therefore important to understand the smoothness properties of the integrand since limited smoothness commonly occurs in many engineering applications. For instance, in building physical simulations, discrete parameters such as different materials and climates are often involved, which may introduce jump discontinuities in the behavior of the core simulation. However, in our numerical experiments in §4, we actually found that even though discrete parameters are included in the experiments, quasi-Monte Carlo methods can still outperform the standard Monte Carlo method, as long as these discrete parameters do not dominantly impact the uncertainty analysis.

A second important consideration w.r.t. efficiency of QMC is the apparent $(\log n)^d$ factor in the error bound, which would imply the number of samples needs to be of order e^d before the bound actually decreases for increasing n . Luckily for many interesting applications this effect is not noticed, hence the popularity of QMC methods. One way to quantify the effect of the dimensionality is through what can be loosely called “effective dimension”. While the nominal dimension d of the problem might be quite high, it often happens that only very few of the parameters have major influence on the quantity of interest. Van Gelder [42] performed a sensitivity analysis and showed that in many (building physical) engineering problems, even though the number of the total input parameters may be large, the number of effective parameters is usually fairly small.

2.2. Error estimation

Randomization techniques can be applied to get multiple independent quasi-random sequences, and in this way confidence intervals for the results can be constructed based on the standard error. An overview of different randomization techniques for quasi-Monte Carlo integration can be found in L’Ecuyer and Lemieux [43].

A common technique is that of random shifting where each point of the sequence is moved by (the same) shift. For digital sequences this is called a digital shift. In this paper the Sobol’ sequence is randomized by applying a random linear scramble combined with a random digital shift [44], for the Niederreiter–Xing sequence a random digital shift is applied and for the lattice sequence a random shift is applied. The additional random linear scrambling on the Sobol’ sequence is more advanced than the random scrambling and also slightly improves the uniformity of the sample points. All these randomized sequences still pertain their QMC properties.

Figure 1: Sampling schemes standard Monte Carlo (top left), Sobol’ sequence (top right), Niederreiter–Xing sequence (bottom left), lattice sequence (bottom right).

Starting from a deterministic QMC sequence the chosen randomization procedure is performed r times to obtain r independent QMC sequences and thereby r independent estimates of the quantity of interest. The estimator using r randomizations of the same sequence using n points is the average of the estimators $Q_n^{(i)}(f)$, $i = 1, \dots, r$, of each randomized sequence

$$\bar{Q}_{n,r}(f) = \frac{1}{r} \sum_{i=1}^r Q_n^{(i)}(f), \quad (1)$$

and an estimator for the standard error on this result is

$$\text{stderr}(\bar{Q}_{n,r}) \approx \sqrt{\frac{1}{r(r-1)} \sum_{i=1}^r \left(Q_n^{(i)}(f) - \bar{Q}_{n,r}(f) \right)^2}. \quad (2)$$

If the convergence for each $Q_n^{(i)}(f)$ behaves like n^{-a} then it can be seen from the above expression that the convergence for $\bar{Q}_{n,r}$ behaves like $r^{-1/2} n^{-a}$. That is, we get the MC rate for the number of realizations r and the QMC rate for the number of samples from the QMC sequence. Therefore r is usually picked as a small constant, while n gets increased to improve accuracy. The number of realizations does however influence the accuracy (and thus reliability) of the error estimator. In the numerical applications in this paper we choose $r = 10$.

2.3. Adding samples

Low-discrepancy point sets can actually be categorized in two groups: “fixed point sets” with fixed number of points, and “sequences” which can be used for n going to infinity. In general, fixed point sets have slightly better asymptotic discrepancy than their sequence counter-parts. Historically “lattice rules” were fixed point sets, but construction methods have been extended to be able to use “lattice sequences” [40], and this is the technology which is used in this paper. Both other two QMC techniques used in this paper, Sobol’ and Niederreiter–Xing, are also sequences. Moreover, all three are “base 2” sequences, which means that for every full power of 2 we actually obtain a fixed point set which has the good properties of a QMC fixed point set. In Hickernell et al. [37] it is shown that if these fixed point sets achieve higher order for every power of 2, then adding more samples and just averaging will not achieve the higher order rate, but it will recover the n^{-1} rate. This will be visible in the numerical case study in §3. W.r.t. the third crucial property from before, it is highly advantageous to be able to add single samples when calculating with expensive engineering models (for instance a single simulation of our building physical case study takes about 3 minutes running on a computer with an Intel (R) Xeon (R) E5-2665 2.40GHz CPU and 32GB of RAM), or to be able to add as few samples as possible.

3. Numerical case study

Since in many engineering applications the computational cost of the deterministic simulation is relatively high, a calculation object which has low computational cost is investigated first to illustrate the different factors laid out in §2. The plain Monte Carlo (MC) method will be compared to the three quasi-Monte Carlo methods introduced before: the Sobol’ sequence (Sobol’), the Niederreiter–Xing sequence (NX) and the lattice sequence (LS). Given that this numerical case study involves rather high number of runs, for which generation of the optimized Latin Hypercube schemes is excessive in computation time [14], these are not included in this section.

3.1. Calculation object

The following two test functions will be used

$$f_1(x) = \prod_{j=1}^d \left(1 + \gamma_j \left(x_j^2 - x_j + \frac{1}{6} \right) \right), \quad (3)$$

$$f_2(x) = \prod_{j=1}^d \left(1 + \gamma_j \left(x_j^6 - 3x_j^5 + \frac{5}{2}x_j^4 - \frac{1}{2}x_j^3 + \frac{1}{42} \right) \right). \quad (4)$$

Both functions integrate to 1 over $[0, 1]^d$, and this integral is the targeted output of the MC and QMC, where to all the x_j are sampled from a uniform distribution on $[0, 1]$. Moreover, function $f_1(x)$ is a product of $1 + B_2$ while $f_2(x)$ is a product of $1 + B_6$, where B_2 and B_6 are degree 2 and 6 Bernoulli polynomials. Both test functions have absolutely converging Fourier series, where the Fourier series of f_2 converges faster than that of f_1 . Lattice rules (and base 2 lattice sequences at powers of 2) benefit from faster converging Fourier series and this will be reflected in their convergence order.

For investigating how the number of dimensions affects the convergence behavior, each function is considered in 5 and 15 dimensions and in both of the functions the γ_j weights control the importance the parameter x_j , with larger γ_j indicating a larger impact of x_j . Similarly the weight of any subset of coordinates is given by the product of the corresponding γ_j 's. In this case study, the sum of the weights of all the parameters is normalized to $\sum_{j=1}^d \gamma_j = 1$. In order to study the influence of the number of effective parameters on the convergence behavior, each function is considered with two scenarios. In the first scenario, the same weight is assigned to each parameter. In the second scenario, 60% of the weight is assigned to the first parameter, 30% of the weight is assigned to the second parameter and the remaining 10% is equally distributed over the rest of the parameters. Therefore, in comparison to the first scenario, the second scenario contains less influential parameters.

To study the effect of adding samples two situations are considered. In the first situation sample sizes which are powers of 2 are chosen since all three QMC sequences are base 2 sequences, while in the second situation the sample sizes are not powers of 2. The higher-order convergence of lattice rules will be apparent on the test functions for sample sizes which are powers of 2. The first test function should show n^{-2} while the second test function should show n^{-6} . These rates are asymptotic and depend on the other factors discussed in §2, most importantly the influence of the dimensionality. From the theory it is expected to see n^{-1} convergence for the non-powers of 2 for all QMC sequences.

3.2. Sampling efficiency

The sampling efficiency can be described as the number of repetitions of the core simulation required in order to reach a targeted accuracy: sampling strategies requiring less runs of simulations are termed “more efficient”. This section first assesses the sampling efficiency of the four sampling schemes by comparing their absolute errors, which are calculated by taking the difference between the exact answer and the approximation. Since in the next section the error estimation will be assessed, in this section also the estimator for the average over r shifts is used as the QMC estimator, cf. (1), and thus the total number of function evaluations for quasi-Monte Carlo is $r \times n_{\text{QMC}}$, with n_{QMC} the number of QMC points. We take $r = 10$ to get a relatively robust error estimation, and $n_{\text{QMC}} = 2^3, 2^4, \dots, 2^{14}$ to obtain a relatively large overview of the convergence behavior of different sampling schemes. In order to make a fair comparison with the standard Monte Carlo sampling, we should therefore take the number of samples in the standard Monte Carlo method $n_{\text{MC}} = r \times n_{\text{QMC}}$, and hence $n_{\text{MC}} = 10 \times 2^3, 10 \times 2^4, \dots, 10 \times 2^{14}$. For the situation with sample sizes different from powers of 2, numbers close to the prior powers of 2 are chosen, see Figure 2 (g) and (h) which should be compared to (c) and (f) respectively. Since we are using randomized QMC sequences the result will be different for each randomization. In order to obtain a robust conclusion of the convergence behavior of each sampling scheme, 100 independent realizations of the $r \times n_{\text{QMC}}$ and n_{MC} (quasi-) Monte Carlo evaluations are performed and the aggregated results from these 100 independent realizations are hence represented by boxplots and displayed in Figure 2.

Figure 2: Box plots for 100 realizations of the absolute error in terms of the number of samples for the randomized QMC sequences and the plain Monte Carlo method (MC = Monte Carlo, Sobol = Sobol' sequence, NX = Niederreiter–Xing sequence, LS = Lattice sequence). To obtain a clear comparison of all the schemes, the absolute error is always plotted in the range from 10^{-10} to 10^{-1} only, thus eliminating some data for high numbers of runs in (b) and (f) where the error for LS is smaller than 10^{-10} . The four reference lines are respectively aligned with convergence rates of $n^{-1/2}$, n^{-1} , n^{-2} and n^{-6} .

All the different properties of the test functions have been investigated, however for conciseness only eight figures are shown in Figure 2. In relation to the smoothness (left column: higher smoothness; right column: lower smoothness), it is clearly illustrated that the sampling efficiency of all sampling schemes decreases, as the order of the smoothness of their integrands reduces, and that particularly the sampling convergence of the lattice sequence and Niederreiter–Xing sequence is strongly influenced by this factor. Moreover, with respect to the number of dimensions (first versus second row), it is shown that the sampling efficiency of all sampling schemes decreases as the number of dimensions increases. Furthermore, regarding the influence of the different variables (second versus third row), it can be seen that the sampling schemes converge faster for functions having a smaller number of dominant parameters. Additionally comparing the first and third row, it is demonstrated that, with respect to the number of dimensions, the number of important parameters tends to be the real impact factor. Finally, concerning the sample sizes (third versus last row), it can be observed that the sampling efficiency of the lattice sequence and Niederreiter–Xing sequences with sample sizes in powers of 2 is higher than when their sample sizes deviate from powers of 2. However, this improvement becomes smaller for the integrands with equal weight parameters, but that result is not shown in Figure 2. This degradation is only visible for sampling schemes which show better than n^{-1} convergence in the top plots, therefore the Monte Carlo method and the Sobol’ sequence perform similar as before. Overall we see that the QMC schemes outperform the Monte Carlo method, as expected. For sample sizes equal to powers of 2, the lattice sequence is overall the best performer, with the Niederreiter–Xing sequence second and the Sobol’ sequence third, and these ranks become more pronounced for more smooth functions with fewer dominating parameters. For sample sizes different from powers of 2, on the other hand, the differences between the lattice sequence, the Niederreiter–Xing sequence and the Sobol’ sequence become smaller, certainly for less smooth functions. As expected, all these results behave to the theory from §2.

3.3. Error estimation

In this section, the absolute error is compared with the estimated error to assess the accuracy of the suggested error estimation method, cf. the standard error calculations on the estimator (1) given by (2) for the QMC methods and the normal standard error calculation for the MC method. As in §3.2 we only show the results for a limited selection of tests, given that these are a good illustration of the overall findings. Hence, in this section, the error estimation for standard Monte Carlo, the Sobol’ sequence, the Niederreiter–Xing sequence and the lattice sequence with sample sizes not in powers of 2 for f_1 with unequal weight in 15 dimensions are studied and compared. All the other scenarios are also investigated, but since the outcomes and conclusions are very similar, they are not shown explicitly in this paper.

In order to evaluate the reliability of the estimated standard error, their convergence behavior is compared to the convergence of the absolute errors and additionally the ratios of estimated over absolute errors are analysed, see Figure 3. As in §3.2 we report box plots of 100 realizations of the randomized QMC schemes as well as the Monte Carlo method.

Figure 3 illustrates that, the estimated standard errors are all very close to their absolute errors for all the sampling schemes. They moreover evolve similarly in relation to the numbers of runs. Hence, we can conclude that, the use of randomization techniques and standard errors for error estimation is sufficiently accurate for our numerical tests. Moreover, it is also shown that for all the QMC schemes, the ratios of the estimated versus the absolute errors are typically bigger than 1 and usually smaller than 10, i.e., one decimal digit of precision. This demonstrates that the error of the Monte Carlo and quasi-Monte Carlo methods can be robustly and conservatively quantified based on the standard error.

4. Building physical case study

In the previous section, we assessed the sampling efficiency and error estimation of different sampling schemes by performing a numerical case study. For further assessing the performance of these quasi-Monte Carlo sampling schemes in a real-world engineering application, a building physical case study is investigated in this section.

Figure 3: Graphs in the left column confront absolute and estimated standard errors, graphs in the right column present the ratio of estimated versus absolute error.

4.1. Calculation object

As mentioned in §1, Monte Carlo based probabilistic assessment of building performance is crucial, since for any thermal retrofit of building component, in order to evaluate the robustness of the impact of our action, the hygrothermal performances, such as heat loss and moist freeze-thaw cycles, before and after retrofit need to be investigated [20]. Therefore, in this section, the hygrothermal performance of a massive masonry wall is taken as an exemplary “calculation object”. More specifically, two hygrothermal performance indicators — the cumulated transmission heat loss in §4.2.1 and the number of moist freeze-thaw cycles in §4.2.2 — are considered. The heat loss is used to analyze the energy consumption and the freeze-thaw cycles is an important indicator for assessing moisture damage, such as frost damage which can induce cracks, stone splinters and swelling of the building component. In other words, in this uncertainty analysis, the mean and standard deviation of the distributions of both cumulated heat loss and the number of moist freeze-thaw cycles over one year will be taken as the target outputs. The simulation duration is taken to be 3 years. The cumulated heat loss is calculated by taking the sum of the heat fluxes through the wall over the third year. On the other hand, for evaluating the risk of frost damage, the number of moist freeze-thaw cycles during the last year at 0.5 cm from the exterior brick surface is taken as the risk indicator; for the detailed formulation, we refer the readers to Vereecken et al. [20]. In addition, besides the mean and standard deviation of the distributions of both cumulated heat loss and the number of moist freeze-thaw cycles, we also investigated the convergence behaviors of different percentiles. Since their results are very similar to the convergence behavior of the standard deviation, these results are not explicitly presented in the paper.

4.1.1. General information

In order to obtain these target outputs, simulations of the heat and moisture transfers in the wall need to be executed. In building physics, the heat and moisture transfer in building components can be assessed by using a mass and energy conservative model [45]:

$$(c_0\rho_0 + c_l w) \frac{\partial T}{\partial t} + (c_l T \frac{\partial w}{\partial p_c}) \frac{\partial p_c}{\partial t} = \nabla(\lambda \nabla T - c_l T g_l - (c_v T + L_v) g_v), \quad (5)$$

$$\frac{\partial w_k}{\partial t} = \nabla(K_l \nabla p_c) + \nabla(\frac{\delta_v p_v}{\rho_l R_v T} \nabla p_c + \frac{\delta_v p_v}{\rho_l R_v T^2} (\rho_l L_v - p_c) \nabla T). \quad (6)$$

All symbols appearing in equation 5 and equation 6 are clarified in the nomenclature section at the beginning of this paper. In this paper, the hygrothermal model based on equation 5 and equation 6 are solved by using Delphin [46] under the relevant interior and exterior boundary conditions. For the heat transfer, the exterior boundary conditions include convection, short and long wave radiation, precipitation and latent as well as vapour exchange; at the interior surface, combined convection and long wave radiation is imposed. With respect to the moisture balance, the exterior boundary condition is made up by precipitation and vapour exchange. The required exterior climatic conditions are delivered by the climate data of one of three German cities (see Table 1). At the interior surface, only vapour exchange between the interior surface and indoor environment is imposed. Indoor climate conditions corresponding the European Standard EN [47] are applied.

4.1.2. Input parameters

The analysis of the hygrothermal model involves a number of parameters, related to the component geometries, material properties, climate locations as well as surface characteristics. In order to perform an uncertainty analysis, the parameters which are expected to have an influence on the hygrothermal risks are considered probabilistic. On the other hand, the parameters with small variations or having less effect for the building physical case study are assigned fixed values. An overview of these deterministic and probabilistic parameters is given in Table 1. The basics characteristics of the material properties of three brick types used can be found in Table 2 [20]. It should be mentioned that in this case study, 7 probabilistic parameters (meteorological climate data, wall orientation, convective heat transfer coefficient, solar absorption coefficient, exposure factor WDR, brick thickness and material of the brick) are included in the analysis. In addition, 2 out of these 7 probabilistic parameters (meteorological climate data and material of the brick) belong to discrete distributions. Both discrete distributions contain 3 values, and to sample them, we first uniformly partition the interval $[0, 1]$ into three sub-intervals: $[0, \frac{1}{3}]$, $[\frac{1}{3}, \frac{2}{3}]$, $[\frac{2}{3}, 1]$. Next, we check which sub-interval the sample point falls into and pick the correspond value from its input distribution. Moreover, it should be noticed that

the convective heat transfer coefficient is conditional on the climate type and the brick material instantiates several more variables. It should also be added that while the parameters in Table 1 and Table 2 may not all explicitly be represented in equation 5 and equation 6, they all do affect the driving forces for the heat and moisture transfers in building components. For the detailed formulations, we refer the readers to Janssen et al. [45].

4.2. Sampling efficiency and error estimation

In this building physical case study, we assess the sampling efficiency and the accuracy of the suggested error estimation of five different sampling schemes: standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol', Niederreiter–Xing and lattice sequence. However, since the calculation time for the building physical case studies is much longer than the numerical case study in §3, in this section, we limit $n_{\text{QMC}} \in [2^3, \dots, 2^7]$ while maintaining $r = 10$. We consider the optimized Latin Hypercube sampling as a QMC method. Likewise we use $r = 10$ different seeded designs which are then optimized, resulting in r different Latin Hypercube sampling schemes for each n , and then calculate the standard error over these r realizations as for QMC. In addition $R = 10$ independent replications of the $r \times n_{\text{QMC}}$ quasi-Monte Carlo evaluations are made at each of these five sample sizes to obtain a robust conclusion of the convergence behavior of each sampling scheme. This means there are R dots for each number of samples on the x -axis for each of the five methods (which are marked in different colors) in the following figures. It should also be mentioned that in order to distinguish the performance of different sampling schemes, instead of presenting the results of all the sampling schemes all together in one column exactly above the sample size involved, the results from different sampling schemes have been spread out slightly in Figures 4 and 5. In order to evaluate the error estimation, the standard errors and their ratios to the absolute errors with respect to the reference solution are also shown.

4.2.1. Heat loss

A reference solution was calculated using $r = 10$ replications of a 2^{12} -run randomized lattice sequence from [40] different from the lattice sequence we use in the actual tests (a 600-dimensional base-2 generating vector for order-2 weights up to $2^{13} = 8192$ points). The computational expense for this reference solution is approximately 2 weeks (calculated by a 16 core Intel (R) Xeon (R) CPU E5-2665 2.40GHz computer with 32GB of RAM). The reference solutions for the mean and standard deviation of the resulting heat loss distribution are 206.78 kWh 46.43 kWh with standard errors of 0.0062 and 0.0387 respectively. The absolute error with respect to the reference solution of standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol', Niederreiter–Xing and lattice sequence, are shown in Figure 4 (a) and (b). Moreover, the estimated errors, as well as their ratios with the absolute errors, are shown in Figure 4 (c), (d), (e) and (f).

In Figure 4 it can be seen that for the sampling efficiency of the mean in (a) and the convergence behavior of estimated standard errors in (c), all the quasi-Monte Carlo sampling strategies outperform the standard Monte Carlo. However, for the standard deviation which is shown in (b) and (d), the enhanced performance of quasi-Monte Carlo methods becomes less obvious. A possible explanation for that is the limited accuracy of the reference solution, as the standard error of that reference is still 0.0387, which may lead to a bias in the absolute error calculations. Therefore, we focus the analysis on the estimated standard errors in (c) and (d) instead. From the graphs we observe that, with the exception of the lattice sequence for estimating the standard deviation of the heat loss in (d), the quasi-Monte Carlo methods all show the expected n^{-1} convergence.

Furthermore, graphs (e) and (f) demonstrate that, for standard Monte Carlo, Sobol', Niederreiter–Xing and lattice sequence, the ratios of their estimated standard errors to the absolute errors with respect to the reference solution are typically bigger than 1 and often smaller than 10. Hence, the errors of these four (quasi-) Monte Carlo methods can be quantified robustly and conservatively based on the suggested error estimation method. On the other hand, OLHS appears to be the most efficient in graphs (c) and (d), but caution is required, as the estimated standard errors may be too small, given that the ratios in graphs (e) and (f) are often smaller than 1. This confirms the earlier suspicion about the correlations of the r different OLHS designs which are constructed starting from different sets of random points, but all use the same optimization algorithm.

Table 1: Probabilistic and deterministic input parameters and distributions

Input parameter	Input distribution
<i>Climatic conditions</i>	
Meteorological climate data	$D(\text{Essen, Bremerhaven, Munich})$
<i>Wall conditions</i>	
Wall orientation [degree from north]	$U(0, 360)$
Convective heat transfer coefficient [$W/m^2 K$]	Essen $N(7.34, 2.11)$ Bremerhaven $N(11.67, 3.17)$ Munich $N(7.22, 1.77)$
Moisture transfer coefficient [s/m]	$7.7 \times 10^{-9} h_{conv}$
Solar absorption coefficient	$U(0.4, 0.8)$
Exposure factor WDR	$U(0, 1.5)$
Long wave emissivity	0.9
<i>Brick layer</i>	
Thickness [m]	$U(0.15, 0.5)$
Material	$D(\text{Brick 1, Brick 2, Brick 3})$
<i>Interior surface</i>	
Interior relative humidity	EN 15026, RH curve A
Total heat transfer coefficient [$W/m^2 K$]	8
Moisture transfer coefficient [s/m]	3×10^{-8}

$U(a, b)$: uniform distribution between a and b ; $D(a, b)$: discrete uniform distribution with options a and b ; $N(\mu, \theta)$: normal distribution with mean value μ and standard deviation θ

Table 2: Brick type properties

Material property	Brick 1	Brick 2	Brick 3
Capillary absorption coeff. [$kg/m^2 s^{0.5}$]	0.125	0.46	0.04
Bulk density [kg/m^3]	2087	1786	1080
Thermal capacity [$J/kg K$]	870	1000	834
Dry thermal conductivity λ_{dry} [$W/m K$]*	0.9	1.08	0.996
Dry vapour resistance factor [-]	24.8	14.3	45.1
Capillary moisture content [kg/m^3]	130	206.7	101
Saturation moisture content [kg/m^3]	209	323	253

Moisture dependent thermal conductivity: $\lambda(w) = \lambda_{dry} + 0.56 \cdot w$ with w the moisture content in m^3/m^3

Figure 4: (a)–(b): sampling efficiency of different sampling schemes, (c)–(d): convergence behavior of the estimated standard errors of different sampling schemes, (e)–(f): ratio of the estimated standard errors of each sampling schemes to their absolute errors. The reference lines in (c)–(d) show $n^{-1/2}$ and n^{-1} convergence.

4.2.2. Freeze-thaw cycles

A reference solution was calculated using $r = 10$ replications of the same 2^{12} -run randomized lattice sequence as in §4.2.1. The reference solutions for the mean and standard deviation of the number of moist freeze-thaw cycles are 1.324 and 2.46 with standard errors of 0.0053 and 0.0153 respectively. Figure 5 is similar to Figure 4, but now for the number of moist freeze-thaw cycles.

In (a)–(b) and (c)–(d) of Figure 5, it is illustrated that, in contrast to the findings for the cumulated heat loss, there is no significant superiority of quasi-Monte Carlo sampling strategies over the standard Monte Carlo method with respect to quantifying the mean and standard deviation of the distribution of the number of moist freeze-thaw cycles. The reason for this degrading performance of quasi-Monte Carlo methods will be investigated in the following section. Moreover, it is shown in (e) and (f) of Figure 5 that, the error estimation allows a robust and conservative quantification of the error for Sobol', Niederreiter–Xing and lattice sequence, while an underestimation is again found for the OLHS.

Figure 5: (a)–(b): sampling efficiency of different sampling schemes, (c)–(d): convergence behavior of the estimated standard errors of different sampling schemes, (e)–(f): ratio of the estimated standard errors of each sampling schemes to their absolute errors. The reference lines in (c)–(d) show $n^{-1/2}$ and n^{-1} convergence.

4.3. Dominance and smoothness of parameters in the hygrothermal model

We recall the quasi-Monte Carlo error bound of the form $V(f) c_d n^{-1} (\log n)^d$ from §2. This bound implies that for large dimension d the number of samples n needs to be huge. However, in many high-dimensional problems, quasi-Monte Carlo methods have been shown to be superior to standard Monte Carlo, a contradiction that can be explained by the concept of effective dimension [41]. Even though a lot of parameters may be involved in our hygrothermal model the quantity of interest might be influenced by only a small number of dominant parameters. In such a case we can still expect the superiority of quasi-Monte Carlo over standard Monte Carlo. For many (building physical) engineering applications, Van Gelder [42] has shown that, even though the total number of input parameters may be large, the number of effective parameters is usually fairly small.

A requirement to obtain the QMC convergence rate is that the function needs to be sufficiently smooth. In building physical applications, discrete parameters such as different material properties and climate locations are often involved in the analysis, and these discrete parameters may bring discontinuity to the target function. In the next two sections we will analyze the influence of all continuous and discrete parameters, and the smoothness of our quantity of interest with respect to each of the parameters.

4.3.1. Analysis of dominance of the model parameters

A number of reviews about sensitivity analysis can be found in [48, 49, 50]. In this section the dominance of the input parameters is analyzed by using a variance-based global sensitivity analysis. In order to reduce the computational time when calculating the “Sobol’ sensitivity indices”, as suggested by Saltelli et al. [51], a Sobol’ sequence instead of the random sequence has been applied. More specifically their respective first and total order “Sobol’ indices” are calculated based on a Sobol’ sequence with 2048 points, bringing the total number of evaluations for this sensitivity analysis to $n(d + 2)$. Here, n is the base number of samples and d is the number of parameters in the building physical case study, thus n is 2048 and d is 7. Therefore, the total number of evaluations is $2048 \times (7 + 2) = 18432$.

To study the effect of the model parameters, Figure 6 shows the first order and total order Sobol’ sensitivity indices of the parameters for the heat loss and the number of freeze-thaw cycles objectives. From Figure 6 we see that the thickness of the wall is the most influential parameter in determining the output variance in calculation of the heat loss, with respect to both the first and the total order index. The rest of the parameters have relatively low first and total order index and thus tend to be less dominant. On the other hand, for the number of freeze-thaw cycles, Figure 6 presents a different scenario, as most of the 7 parameters have significant influence on the output variance, among which also the discrete parameters of climate location and brick properties.

It should be mentioned that, each of the two discrete parameters (climate type and brick type) is a combination of several factors: the climate type involves all the factors that relate to the exterior environment and the brick type instantiates 7 parameters as shown in Table 2. Thus, their influence could be larger than simply one discrete parameter. Moreover, the two discrete parameters could have a detrimental effect on the QMC convergence, since they (might) destroy the smoothness w.r.t. our quantity of interest. As can be seen in §4.2.1, for the calculations of the heat loss they do not have any negative effect and the convergence rate is $O(n^{-1})$ as wished for. For the calculation of the number of freeze-thaw cycles on the other hand, the convergence appears to be only that of the Monte Carlo method. In Figure 6, it can be seen that the climate type and the brick type do not have significant influence for the heat loss calculation while they do have a more substantial influence for the number of freeze-thaw cycles calculation. To further illustrate the effect of the two discrete parameters on these calculations, Figure 7 and Figure 8 contain box plots with respect to the climate type and brick type. The observations are from the 12800-run standard Monte Carlo analysis, as presented in §4.2.

Figures 7 and 8 confirm these observations. Figure 7 illustrates that the results of the heat losses are fairly close for all climate locations and brick properties. This indicates that these discrete parameters are not influential parameters for the heat losses. Figure 8 presents a different scenario: a significantly larger number of moist freeze-thaw cycles is obtained for the Munich climate relative to Bremerhaven and Essen. Similarly, a significantly smaller number of moist freeze-thaw cycles is observed when using brick type 2 versus brick types 1 and 3. Therefore, contrary to the situation for the heat losses, both discrete parameters are effective parameters with a dominant influence on the number of moist freeze-thaw cycles.

4.3.2. Analysis of smoothness of the model parameters

We analyze the smoothness with respect to the continuous parameters using a kernel smoother technique. A detailed introduction of this method can be found in Friedman et al. [52]. Briefly speaking, a kernel smoother is a statistical regression technique for fitting the real-valued function $f(x)$ by making use of its noisy observations. More specifically, in this study, a Gaussian kernel with bandwidth λ is used. A review of different bandwidth selection methods has been put forward in Turlach et al. [53]. In our analysis, we take $\lambda = 0.9 A n^{-0.2}$, where $A = \min(\sigma, \text{IQR}/1.34)$. Here, IQR is the interquartile difference, the difference between the 75th and the 25th percentile, and σ is the standard deviation of the observations. More details with respect to this bandwidth selection can be found in Silverman [54] and Härdle [55].

Figure 6: Sensitivity indices of heat loss (top) and number of freeze-thaw cycles (bottom): the darker shaded bars represent the first-order Sobol' indices, while the full height of the bar represents total-order indices of the target outputs.

Figure 7: Boxplot of the total heat loss as a function of each different climate and each different brick type

Figure 8: Boxplot of the number of freeze-thaw cycle as a function of each different climate and each different brick type.

Figure 9: Gaussian kernel smoother analysis of the total heat loss as a function of each continuous parameter.

Figure 10: Gaussian kernel smoother analysis of the number of moist freeze-thaw cycles as a function of each continuous parameter.

The results of the Gaussian kernel smoother analysis for the hygrothermal case study are presented in Figures 9 and 10, with respect to the heat losses and the number of freeze-thaw cycles respectively. For this analysis, we reuse the result of the 12800-run standard Monte Carlo analysis, as presented in §4.2. Figures 9 and 10 illustrate that, except for the convective heat transfer coefficient in Figure 10, the simulated functions are relatively smooth with respect to the continuous input parameters. On the other hand, oscillatory behaviors are found at the end of the approximating curve for the convective heat transfer coefficient in Figure 10. But since there are only 86 out of 12800 observations for the convective heat transfer coefficient larger than 18, these oscillatory behaviors may be due to the limited number of observations.

4.4. Discussion

We conclude that our hygrothermal model with respect to the heat loss and number of moist freeze-thaw cycles is relatively smooth with respect to the continuous parameters. Furthermore, compared with the result of the number of freeze-thaw cycles, the function of heat losses contains less effective parameters and the influence of the discrete parameters is relatively small. This explains why the numerical results in §4.2.1 for the heat loss show the nice $O(n^{-1})$ convergence expected of the quasi-Monte Carlo methods.

On the other hand, the function of freeze-thaw cycles contains more effective parameters which include the discrete parameters, as illustrated in Figures 6 (bottom) and 8. As a consequence, the numerical results in §4.2.2 illustrate that for quantifying the distribution of the number of freeze-thaw cycles the convergence rate of the quasi-Monte Carlo methods tends to be very similar to the standard Monte Carlo method.

5. Conclusions

Monte Carlo analysis has been established as a universal method for uncertainty propagation in the assessment of complex systems, see e.g. [56, 57, 58, 59]. If the deterministic core simulator is time consuming though, the amount of required repetitions should be kept low. In that respect three criteria are crucial:

1. the sampling approach should be as efficient as possible;
2. the sampling approach should allow a reliable estimation of the accuracy;
3. the sampling approach should facilitate sequential addition of samples until a satisfactory accuracy is met;

This journal has long-standing history with respect to optimising Monte Carlo sampling approaches [12, 14, 28, 50, 60, 61, 62]. In [12, 50, 62] the efficiency of Latin hypercube versus random sampling is evaluated, with respect to criterion 1. In [28, 61] the extension and replication of Latin hypercube sampling schemes is put forward, respectively addressing criteria 2 and 3. Janssen [14] focused on the sampling efficiency and convergence of (replicated) optimised Latin hypercubes, aiming at criteria 1, 2 and 3. This paper targets the continuation of this research line within this journal, through assessment of various quasi-Monte Carlo sampling schemes.

In the numerical case study we demonstrated and explained which factors can influence the convergence of the QMC methods and when they can outperform the standard Monte Carlo method. It was established that larger smoothness and lower (effective) dimensionality both contributed positively to the improved efficiency of QMC methods over random sampling. We further demonstrated the behavior and robustness of the standard error estimators for the (quasi-) Monte Carlo methods. In the building physical case study, we demonstrated that the sampling efficiency of the QMC methods are either higher or as good as those from the standard Monte Carlo method. However, it was illustrated again that the superiority of QMC over standard Monte Carlo may degrade if the target function depends on a larger number of dominant parameters or is lacking smoothness. Given the parallel observations in both the mathematical and building physical case study, our findings on the impact of smoothness and (effective) dimensionality are most plausibly equally valid for other engineering applications.

Acknowledgments

This work has been supported by the H2020 RIBuild project. RIBuild has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 637268.

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