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Uncertainty treatment in Monte Carlo simulation

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Abstract. Guidelines and hints are given on how to introduce an uncertainty treatment in conformity with recent international recommendations into the Monte Carlo simulation of, for instance, radiation particle transport processes in order to establish confidence in the results. The main problem is how to calculate sufficiently accurately, at a justifiable computational expense, the sensitivity coefficients of the quantities of interest with respect to numerous input quantities involved, data and uncertainties of which are given. This problem is solved using identical random-number sequences together with the input data slightly varied in the range determined by the associated uncertainties. Simple examples of application are treated in detail.

1. Introduction

The Monte Carlo (MC) method is a powerful tool used in computational physics. Physical processes, including measurements, and involved physical quantities which are of interest and mathematically represented, for instance, by complex multidimensional integrals, can often more easily and transparently be simulated, calculated, and investigated using the MC method instead of experimental, analytical, or other numerical methods. In particular, MC simulation is applied to particle transport processes, for instance, in radiation metrology, dosimetry, monitoring, and protection. Examples are the calculation of response functions of neutron sensors such as Bonner spheres or proportional counters, and spectrum unfolding in neutron spectrometry. The main shortcoming of the MC method is the large amount of computing time required since the results converge rather slowly. The MC uncertainty vanishes in most cases proportional to $N^{-1/2}$ only, where N is the number of samples drawn randomly. Therefore, an extensive uncertainty treatment, which should be highly obligatory to establish confidence in the results obtained and to ensure their quality, is usually not implemented in the MC codes at present available and often applied such as the Monte Carlo N-Particle Transport Code System (MCNP) [1] which is widely used to simulate radiation particle transport processes. The sensitivity analysis which has sometimes been carried out, and the variance analysis of statistical errors already included in MCNP can be regarded as preliminary attempts towards a comprehensive uncertainty treatment in MC simulation. In this respect, see also the supplement to the MCNP recently published [2].

A world-wide consensus on uncertainty treatment was recently achieved and has been laid down in the *Guide to the Expression of Uncertainty in Measurement* [3] of the International Organization for Standardization (ISO), serving now as a *de facto* standard. The guide is based on the recommendation INC-1 (1980) [3] of the Bureau International des

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Poids et Mesures (BIPM). The German standards DIN 1319-3 [4] and DIN 1319-4 [5] of the Deutsches Institut für Normung (DIN) conform with the guide and the recommendation. The first-named author himself was strongly involved in the ISO and DIN activities to establish the guide and the above-mentioned standards. Since sufficient computing capacity is now available, it is about time also to implement an uncertainty treatment into MC simulation codes. This should be done in conformity with the way chosen in measurement data evaluation since MC simulation is quite similar to measurement.

The papers [3–5] referred to above offer an uncertainty treatment in linear approximation only. Uncertainties may also be handled conformally and more generally by applying the *Bayesian Theory of Measurement Uncertainty* [6] on the basis of Bayesian statistics [7], but this will in most cases require much more computation. Therefore, in a first step towards introducing an uncertainty treatment into MC simulation at all, in this paper we restrict ourselves to a first-order handling of uncertainties, also because of the large computational expense necessary in MC simulation. The economy of computation will be one of the main aspects of this paper. Uncertainty components due to the MC process itself as well as those due to the uncertainties of the input quantities are taken into account.

2. Introductory, basic example

We first deal in detail with the following simple, but basic example since it already exhibits the most important characteristics and problems of uncertainty treatment in MC calculation. After that, no serious difficulty will remain in establishing generalizations to more complex cases.

Let a physical quantity Y of interest be given as a function $F(X)$ of an *input quantity* X in the form of the integral

$$Y = F(X) = \int_0^1 G(X, z)\,\mathrm{d}z. \tag{1}$$

With a given input datum x as an *estimate* of the input quantity X, and with N random numbers z_j independently drawn from a uniform probability density between $z = 0$ and $z = 1$, the arithmetic mean of the integrand values yields an estimate y of the *output quantity* Y:

$$y = \frac{1}{N}\sum_{j=1}^{N} G(x, z_j). \tag{2}$$

When this value y and the random numbers z_j are taken as random variables, that is, the mean y as an *estimator* of the physical quantity Y, the expectation value $\mathrm{E}y$ of this mean with respect to the z_j is the integral of equation (1) with x inserted for X, i.e. $\mathrm{E}y = F(x)$.

The empirical variance $s^2(y)$ associated with the mean y is given by the well known statistical formula

$$s^2(y) = \frac{1}{N(N-1)}\sum_{j=1}^{N}(G(x, z_j) - y)^2. \tag{3}$$

The expectation value of this empirical variance, also taken as a random variable similar to y, is

$$\sigma^2(y) = \mathrm{E}s^2(y) = \frac{1}{N}\left(\int_0^1 G^2(x, z)\,\mathrm{d}z - F^2(x)\right). \tag{4}$$

The standard deviation $s(y)$ is used as the *standard uncertainty* [3] associated with the estimate y of the output quantity Y due to the MC process. The integral in equation (4) must exist. Otherwise, the uncertainty is infinite. This can be avoided by transforming the integral in equation (1) using a suitable substitution $z = h(z')$, also with $0 \leqslant z' \leqslant 1$. Such a transformation can also reduce the integral in equation (4) if this integral exists, and is therefore often called a *variance reduction*. Naturally, the variance can also be reduced by enlarging the sample number N. Obviously, $\sigma(y) \sim N^{-1/2}$.

There is another standard uncertainty component $u_0(y)$ associated with the estimate y of the output quantity Y. It is due to the standard uncertainty $u(x)$ associated with the given estimate x of the input quantity X. Let $u(x)$ be given by a preceding data evaluation according to [3–6]. Then, $u_0(y) = |F'(x)|u(x)$ where $F'(x)$ is the derivative of $F(X)$ with $X = x$ inserted. The two uncertainty components $u_0(y)$ and $s(y)$ are of quite different and independent origins. Therefore, they combine as variances of independent random variables to form the combined standard uncertainty $u(y)$ associated with the estimate y of Y:

$$u^2(y) = F'^2(x)u^2(x) + s^2(y). \tag{5}$$

Two significant digits of the standard uncertainty $u(y)$ should be determined.

The derivative $F'(x)$, called the *sensitivity coefficient*, is in many cases not directly available in the form of an analytical expression and must therefore also be calculated numerically, i.e. also by the MC method. To this end, we apply the second-order approximation

$$F'(x) = \frac{F^+ - F^-}{\Delta x} + \mathrm{O}(\Delta x^2) \qquad F^\pm = F(x \pm \tfrac{1}{2}\Delta x) \tag{6}$$

with an increment Δx chosen as a suitable, small multiple of $u(x)$, i.e. $\Delta x = \alpha u(x)$. In the following, the superscripts $^\pm$ always refer to the varied values $x^\pm = x \pm \frac{1}{2}\Delta x$ inserted for the input variable X. Equation (6) follows from a Taylor expansion of $F(X)$ at x. The remainder term in equation (6) depends on the third derivative of $F(X)$ in the neighbourhood of x. Then, with estimates $y^\pm$ of $F^\pm$, we have

$$u_0(y) = \frac{|y^+ - y^-|}{\alpha} + \mathrm{O}(\alpha^2) \qquad \mathrm{E}y^\pm = F(x \pm \tfrac{1}{2}\alpha u(x)). \tag{7}$$

The uncertainty treatment in linear approximation as applied in this paper already requires that $F(X)$ is sufficiently linear in the neighbourhood of x determined by $u(x)$. For α of unity order of magnitude, the remainder term of equation (7) may therefore be neglected. Difficulties in this respect can occur if $F'(x) = 0$ or α is too large in the case of a nonlinear $F(X)$. However, α should be as large as is reasonable since the difference $\Delta y = y^+ - y^-$ in equation (7) may otherwise be small and, thus, will show a large relative dispersion in a MC calculation. We assume the two values y^+ and y^- to be obtained in two different MC processes with the same number N_0 of samples, $\sigma(y^\pm) \approx \sigma(y)$ according to equation (4), and a correlation coefficient ϱ associated with y^+ and y^-. This leads to the approximation

$$\sigma^2(\Delta y) = 2\sigma^2(y)(1 - \varrho) \qquad \text{or} \qquad \sigma(\Delta y)/\alpha = \frac{\sqrt{2C(1-\varrho)}}{\alpha\sqrt{N_0}}. \tag{8}$$

C denotes the large bracket in equation (4) and does not depend on α, ϱ, and N_0. The correlation coefficient ϱ depends on the increment parameter α.

The expression $\sigma(\Delta y)/\alpha$ in equation (8) is the standard deviation which is used as a measure of the uncertainty due to the MC calculation of the leading term of $u_0(y)$ according to equation (7). It can be significantly reduced if $\varrho \approx 1$. This can be achieved using strongly, positively correlated MC processes for the calculation of $y^\pm$, such as those with

identical sequences of random numbers (for this *correlation sampling*, see, e.g., [8]). Then, a relatively small number N_0 of samples, compared with N in equation (2), will already be sufficient to calculate $u_0(y)$ if α, which can disturb the correlation, is not too large. For $\alpha = 0$, all the terms of y^+ and y^- according to equation (2) are identical and, thus, $\varrho = 1$. If α is replaced by $-\alpha$, then y^+ and y^- interchange their meaning only, and ϱ will therefore not change, that is, ϱ will be an even function of α. Accordingly, assuming that ϱ is continuous but not necessarily differentiable for $\alpha = 0$, we expect $\varrho = 1 - B|\alpha|^\kappa$ for small α with $\kappa > 0$ and a small (unknown) constant B, i.e. $B|\alpha|^\kappa \ll 1$ ($B > 0$ because of $|\varrho| \leqslant 1$). Then (assuming $\alpha > 0$ now), $\sigma(\Delta y)/\alpha = (2BC/N_0)^{1/2}\alpha^{\kappa/2-1}$ will possibly be much smaller than $\sigma(\Delta y)/\alpha = (2C/N_0)^{1/2}\alpha^{-1}$ for $\varrho = 0$, i.e. with uncorrelated random-number sequences used for the calculation of y^+ and y^-. For $\kappa \leqslant 1$, ϱ has a cusp maximum at $\alpha = 0$ which sometimes occurs. For $\kappa = 2$ in particular, ϱ is differentiable at $\alpha = 0$, and $\sigma(\Delta y)/\alpha = (2BC/N_0)^{1/2}$ in equation (8) turns out to be essentially independent of α. The result obtained in this paragraph is very important and essential for the practice and economy of MC calculations of uncertainties, especially when numerous input quantities are involved (section 4). An approximation like $F'(x) = (F^+ - F(x))/(\frac{1}{2}\Delta x) + \mathrm{O}(\Delta x)$ should not be used instead of equation (6) since it is of first order only, but y, as an estimate of $F(x)$ replacing y^-, must be calculated in the same way and at the same expense of computing as y^-. The estimate y already calculated with N samples according to equation (2) is not suitable because there is no correlation associated with y^+ and this y.

Using the Taylor expansion $\Delta y = \alpha u(x)F'(x) + \mathrm{O}(\alpha^3)$, we obtain a more precise approximation for $\sigma^2(\Delta y)/\alpha^2$ with $\varrho \approx 1$ by replacing y, N, $F(x)$, and $G(x, z)$ in equation (4) by Δy, N_0, $\alpha u(x)F'(x)$, and $\alpha u(x)G'(x, z)$, respectively, where $G'(x, z) = \partial G(X, z)/\partial X$ with $X = x$ inserted:

$$\sigma^2(\Delta y)/\alpha^2 = \frac{u^2(x)}{N_0}\left(\int_0^1 G'^2(x, z)\,\mathrm{d}z - F'^2(x)\right) + \mathrm{O}(\alpha^2) \qquad (\varrho \approx 1). \tag{9}$$

This expression can be applied if $G'(x, z)$ and $F'(x)$ are available. An exact expression follows from

$$\sigma^2(\Delta y) = \sigma^2(y^+) + \sigma^2(y^-) - 2\,\mathrm{Cov}(y^+, y^-) \tag{10}$$

with $\sigma(y^\pm)$ according to equation (4) and, similarly,

$$\mathrm{Cov}(y^+, y^-) = \frac{1}{N}\left(\int_0^1 G^+G^-\,\mathrm{d}z - F^+F^-\right). \tag{11}$$

The reader who is familiar with MC programming should try $G(x, z) = z^x$ as an exercise ($x > -1$). This example can also be treated analytically. We obtain $\mathrm{E}y = F(x) = 1/(x+1)$, $\sigma^2(y) = C/N = (1/(2x+1) - 1/(x+1)^2)/N$, $F'(x) = -1/(x+1)^2$, and $G'(x, z) = xz^{x-1}$. For $x \leqslant -\frac{1}{2}$, the integral in equation (4) does not exist. With the substitution $z = (z')^{1/(x+1)}$ transforming the integral in equation (1), the integral in equation (4) can be made existent and the variance $\sigma^2(y)$ even made to vanish. Equation (5) with $\sigma^2(y)$ inserted for $s^2(y)$ yields

$$u^2(y) = \frac{u^2(x)}{(x+1)^4} + \frac{x^2}{N(x+1)^2(2x+1)} \qquad (x > -\tfrac{1}{2}). \tag{12}$$

For $x = 1$ and $u(x) = 0.01$, we need $N = 10^6$ MC samples to verify $y = 0.5000$ with $\sigma(y) = 0.000\,29$, but only $N_0 = 10^4$ MC samples to verify the last digit of $u_0(y) = 0.0025$ if the features described in the two preceding paragraphs with $\alpha = 1$ are used. With

uncorrelated random-number sequences ($\varrho = 0$), the standard deviation due to the MC calculation of $u_0(y)$ is

$$\sigma(\Delta y)/\alpha = \frac{\sqrt{2/(2x+1) - 2/(x+1)^2}}{\alpha\sqrt{N_0}} \qquad (x > -\tfrac{1}{2}; \varrho = 0) \tag{13}$$

according to equation (8), whereas identical random-number sequences yield

$$\sigma(\Delta y)/\alpha = \frac{u(x)\sqrt{x^2/(2x-1) - 1/(x+1)^4}}{\sqrt{N_0}} \qquad (x > +\tfrac{1}{2}; \varrho \approx 1) \tag{14}$$

according to equation (9). With the mentioned data inserted for the quantities, the value $\sigma(\Delta y)/\alpha = 0.000\,10$ obtained from equation (14) turns out to be smaller by a factor of 42 than the value calculated from equation (13). For $x \leqslant \frac{1}{2}$, the integral in equation (9) does not exist. The integral in equation (1) must then be transformed applying again a suitable substitution of the integration variable.

3. Generalization to histories of indefinite length

We now replace the integration variable z in equation (1) by a whole sequence $\boldsymbol{z} = \{z_1, z_2, \ldots\}$ of integration variables z_i and call a particular sequence $\boldsymbol{z}_j$ of random numbers a *history* ($0 \leqslant z_i \leqslant 1$). The integral in equation (1) becomes a multiple integral of an infinite number of dimensions. For its existence and computability, we assume that for any history, that is, for any successive random choice of values of the integration variables, the integrand function $G(x, \boldsymbol{z})$ can be calculated completely already after a particular finite number ν of these random values has been chosen. Thus, in this sense, every history is assumed to have its own finite *length* ν. This does not mean that a finite upper bound of the lengths of all histories exists mathematically. (Strictly speaking, the bound does exist since indeed an extremely large, although only finite variety of possible histories can be drawn from a pseudo-random-number generator.) MC processes involving such histories of indefinite, but in fact finite lengths occur, for instance, when neutrons randomly entering a shielding set-up are multiply scattered and are finally either absorbed or leave the set-up.

All the formulae of section 2 remain valid if z is replaced by the sequence $\boldsymbol{z}$, and z_j by $\boldsymbol{z}_j$. To achieve a strong positive correlation of the MC processes of y^+ and y^-, the corresponding histories in the calculation of y^+ and y^- should follow identical random-number sequences [8] although these histories may have different lengths. This fact can also disturb the correlation significantly since the 'tail' of the longer history does not correlate with the shorter history. This effect will increase with an increasing α, since α also enlarges the difference between y^+ and y^-. But too small an α should not be used because of equation (8). How to 'synchronize' the corresponding histories is a matter of implementation (section 5). With very long histories, the correlation can also be disturbed in cases where even a very small data variation results in large changes of the integrand function or of the random path of a particle.

If random events are counted as in the following example, that is, if the integrand $G(x, \boldsymbol{z})$ assumes only the values 0 or 1, then, with a small α and a relatively small number N_0, we will obtain $|y^+ - y^-| = M/N_0$ for the standard uncertainty in equation (7), with a *natural* number M and thus relatively large increments $1/N_0$. Together with a small α, these can cause another difficulty. Since $G^2(x, \boldsymbol{z}) = G(x, \boldsymbol{z})$ in this case, equation (4) reads $\sigma^2(y) = F(x)(1 - F(x))/N$, and Ny, as a random sum of values 0 or 1, follows a binomial distribution with the probability $p = F(x) \leqslant 1$ of a value $G(x, \boldsymbol{z}) = 1$ occurring. Let $\mathcal{G}$ be the set of points $\boldsymbol{z}$ where $G(x, \boldsymbol{z}) = 1$. In the particular case $\mathcal{G}^- \subseteq \mathcal{G}^+$, we have

$G^+G^- = 1$ for $\boldsymbol{z} \in \mathcal{G}^-$ only, $F^- \leqslant F^+$, and $\mathrm{Cov}(y^+, y^-) = F^-(1 - F^+)/N$ according to equation (11). Then,

$$\sigma^2(\Delta y)/\alpha^2 = \frac{(F^+ - F^-)(1 - F^+ + F^-)}{N\alpha^2} \qquad \varrho = \sqrt{\frac{F^-(1 - F^+)}{F^+(1 - F^-)}}. \quad (15)$$

$N\Delta y$ also follows a binomial distribution.

As an example, we consider neutron reflection at a wall of reduced thickness X (thickness times density of scattering nuclei of the wall material times scattering cross section) with a given estimate x and an associated standard uncertainty $u(x)$ given as well. The quantity to be determined is the albedo $Y = \lim_{N\to\infty}(\mathrm{E}M/N)$, where $\mathrm{E}M$ is the expectation value of the random number M of reflected neutrons when N neutrons impinge on the wall from one side. Assuming multiple scattering inside the wall without energy loss and absorption, and considering a one-dimensional approximation in the direction perpendicular to the wall, we can solve the problem not only by the MC method, but also analytically: M follows a binomial distribution with the reflection probability $Y = F(X) = X/(X + 1)$. This model results from a neutron conservation and transport differential equation and is equivalent to the following MC model. The proof is omitted here. We obtain $y = M/N$, $\mathrm{E}y = F(x) = x/(x + 1)$, $\sigma(y) = (x/N)^{1/2}/(x + 1)$, $F'(x) = 1/(x + 1)^2$, $u_0(y) = u(x)/(x + 1)^2$, and

$$u^2(y) = \frac{u^2(x)}{(x + 1)^4} + \frac{x}{N(x + 1)^2}. \quad (16)$$

With the MC method, we assume that the position ξ_i of a neutron at the ith scattering (taken as a reversion of the flight direction; $\xi_0 = 0$) at a nucleus inside the wall changes by $\Delta\xi_i = \pm \ln z_i$ to the next scattering. $\Delta\xi_i$ is the random reduced free path of the neutron. With each of the scattering histories of the impinging neutrons, we have either $G(x, \boldsymbol{z}) = 1$ if the neutron leaves the wall on the side it has come from, i.e. its position becomes negative, or $G(x, \boldsymbol{z}) = 0$ if the neutron penetrates the wall, i.e. its position becomes greater than x. An analytical expression for $G(x, \boldsymbol{z})$ is not known. For $x = 1$ and $u(x) = 0.01$, we need $N = 10^6$ MC histories to verify $y = 0.5000$ with $\sigma(y) = 0.0005$, but $N_0 = 10^5$ MC histories to verify the last digit of $u_0(y) = 0.0025$. The enlarged value $\alpha = 4$ has been used because of the effect described in the preceding paragraph. The standard uncertainty

$$u_0(y) = \frac{u(x)}{(x + 1)^2 - (\frac{1}{2}\alpha u(x))^2} \quad (17)$$

according to the leading term of equation (7), and $u_0(y) + \sigma(\Delta y)/\alpha$ are shown as functions of α in figure 1 (the latter also for $\varrho = 0$). The standard deviation $\sigma(\Delta y)/\alpha$ associated with $u_0(y)$ has been calculated using equation (15) since every history belonging to a wall of particular thickness also belongs to a wall of larger thickness, thus, $\mathcal{G}^- \subseteq \mathcal{G}^+$. $u_0(y)$ and $\sigma(\Delta y)/\alpha$ have also been estimated by arithmetic means and standard deviations, respectively, of $u_0(y)$ values obtained from MC runs repeated 20 times. Moreover, $\varrho = (x^-/x^+)^{1/2} = 1 - \alpha u(x)/(2x)$ according to equation (15) for small α, thus, $\kappa = 1$ (section 2). Figure 1 illustrates for the example considered that identical random-number sequences and values α between 1 and 10 should be preferred when y^+ and y^- are calculated.

4. Generalization to numerous quantities involved

Let $\boldsymbol{X} = (X_1 \ldots X_m)^\top$ ($^\top$ means transposition) be the set of m *input quantities* involved, represented as a column vector, estimates $\boldsymbol{x}$ of which are taken from the pool of input

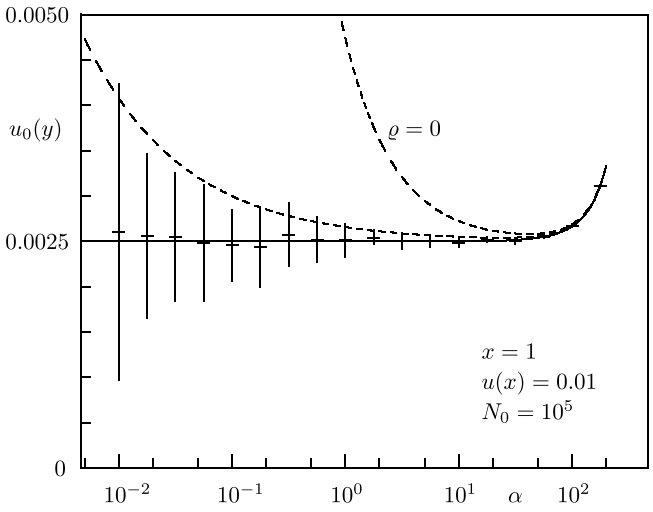

Figure 1. Standard uncertainty $u_0(y)$ associated with the estimate y of the output quantity and due to the uncertainty of the input quantity. It is calculated for the example and data considered in section 3 from equation (17) as a function of the increment parameter α (full curve). It is also given as mean values (crosses) of $u_0(y)$ values obtained from 20 repeated MC runs, where the vertical cross bars show the corresponding standard deviation $\sigma(\Delta y)/\alpha$ estimated accordingly and associated with $u_0(y)$ due to the MC calculation. The broken curves show $u_0(y)+\sigma(\Delta y)/\alpha$ calculated according to equation (15), the upper curve for $\varrho = 0$. Values α between 1 and 10 should be preferred, values of $\alpha \geqslant 200$ are unsuitable.

data available. The input quantities comprise directly measured quantities, influence and correction quantities, output quantities of preceding evaluations, and quantities the data of which are obtained from literature. Furthermore, let the *uncertainty matrix* $\boldsymbol{U}_{\boldsymbol{x}} = (u(x_k, x_l))$ of $\boldsymbol{X}$ also be given, which is associated with the input data $\boldsymbol{x}$ and possibly obtained from a preceding measurement data evaluation according to [3–6]. $u(x_k, x_k) \equiv u^2(x_k)$ is the squared standard uncertainty of X_k associated with x_k, and $u(x_k, x_l)$ is the joint uncertainty component of the pair X_k and X_l $(k \neq l)$, measured by a covariance. Similarly, let $\boldsymbol{Y} = (Y_1 \ldots Y_n)^\top$ be the column vector of the n *output quantities* Y_k, the quantities or parameter of interest, estimated values $\boldsymbol{y}$ of which are to be calculated by MC simulation together with the uncertainty matrix $\boldsymbol{U}_{\boldsymbol{y}}$ of $\boldsymbol{Y}$ associated with $\boldsymbol{y}$. If input or output functions are involved, then a quantity X_k or Y_k of its own must be assigned to every ordinate, abscissa, or parameter of interest, e.g. to every channel or bin. The MC random variables z_i with values $0 \leqslant z_i \leqslant 1$ used in succession during a particular MC history are also composed to form the column vector $\boldsymbol{z}$ as in section 3. Taking $\boldsymbol{z}$ as a random variable, it is assumed to be uniformly distributed in the unit cube $\mathcal{C} = \{\boldsymbol{z} | 0 \leqslant z_i \leqslant 1; i = 1, 2, \ldots\}$. The dimensions of the vectors introduced may be very large.

A functional relationship between $\boldsymbol{X}$ and $\boldsymbol{Y}$, called the *model* and represented in the general form $\boldsymbol{Y} = \boldsymbol{F}(\boldsymbol{X})$, must be available so that $\boldsymbol{y}$ can be uniquely calculated from the given data $\boldsymbol{x}$, that is, $\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{x})$. The functions F_i forming the column matrix $\boldsymbol{F}$ need not necessarily be given explicitly as analytical expressions, they may consist in an algorithm, only implicitly available in the form of a given computer code such as MCNP [1], or they may represent the whole solution procedure of an inverse problem. They may also depend on the uncertainty $\boldsymbol{U}_{\boldsymbol{x}}$ of the input quantities, for instance, in an adjustment procedure such

as the least-squares method. We introduce the MC model

$$\boldsymbol{Y} = \boldsymbol{F}(\boldsymbol{X}) = \int_{\mathcal{C}} \boldsymbol{G}(\boldsymbol{X}, \boldsymbol{z})\,\mathrm{d}\boldsymbol{z}. \tag{18}$$

Because of constraints involved due, for instance, to geometry or particle interaction kinematics, the integrand vector function $\boldsymbol{G}(\boldsymbol{X}, \boldsymbol{z})$ may vanish in subregions of the unit cube $\mathcal{C}$.

In many cases, quantities such as some Q are estimated with N histories (or samples) of arbitrary lengths and weights w_j according to

$$q = \frac{p}{p'} = \frac{\sum_{j=1}^{N} Q_j w_j}{\sum_{j=1}^{N} w_j}. \tag{19}$$

Considering all MC histories possibly involved, the nominator p and the denominator p' according to equation (19) can also be taken as estimators

$$p = \frac{1}{N}\sum_{j=1}^{N} Q_j w_j \qquad p' = \frac{1}{N}\sum_{j=1}^{N} w_j \tag{20}$$

the expectation values of which are the multi-dimensional integrals

$$\mathrm{E}p = \int_{\mathcal{C}} Q(\boldsymbol{x}, \boldsymbol{z}) w(\boldsymbol{x}, \boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \qquad \mathrm{E}p' = \int_{\mathcal{C}} w(\boldsymbol{x}, \boldsymbol{z})\,\mathrm{d}\boldsymbol{z}. \tag{21}$$

Both these integrals are of the form according to equation (18) and can thus also be taken as components of $\boldsymbol{Y}$ with $\boldsymbol{X} = \boldsymbol{x}$ inserted, and the MC calculated data of p and p' can be taken as components of $\boldsymbol{y}$. If an MC history terminates after a particular random number z_i has been drawn, then $w(\boldsymbol{x}, \boldsymbol{z})$ can be taken as independent of the following random numbers. If a history is excluded because of constraints, then $w(\boldsymbol{x}, \boldsymbol{z}) = 0$ for this history. If $\boldsymbol{z}$ is to be drawn from a probability distribution different from the uniform distribution in $\mathcal{C}$, the integral to be calculated can always be transformed into the standard form according to equation (18), whereby the probability distribution is included into $w(\boldsymbol{x}, \boldsymbol{z})$.

The following equations are generalizations of equations (1)–(5). With the number N of MC samples or histories, the estimate of $\boldsymbol{Y}$ is the arithmetic mean

$$\boldsymbol{y} = \frac{1}{N}\sum_{j=1}^{N} \boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z}_j). \tag{22}$$

This mean $\boldsymbol{y}$, taken as a random variable, i.e. as an estimator of $\boldsymbol{Y}$ similar to y in equation (2), has the expectation value

$$\mathrm{E}\boldsymbol{y} = \int_{\mathcal{C}} \boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z})\,\mathrm{d}\boldsymbol{z} \tag{23}$$

as desired according to equation (18). The empirical covariance matrix of the mean is

$$\boldsymbol{S}_{\boldsymbol{y}} = \frac{1}{N(N-1)}\sum_{j=1}^{N} (\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z}_j) - \boldsymbol{y})(\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z}_j) - \boldsymbol{y})^{\top}. \tag{24}$$

When $\boldsymbol{S}_{\boldsymbol{y}}$ is also taken as a random variable similar to $\boldsymbol{y}$, its expectation value matrix is

$$\mathrm{E}\boldsymbol{S}_{\boldsymbol{y}} = \frac{1}{N}\left(\int_{\mathcal{C}} \boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z})\boldsymbol{G}^{\top}(\boldsymbol{x}, \boldsymbol{z})\,\mathrm{d}\boldsymbol{z} - \mathrm{E}\boldsymbol{y}\mathrm{E}\boldsymbol{y}^{\top} \right) \tag{25}$$

which converges to zero for large N. The integral in equation (25) must exist. Every functional value $\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{z}_j)$ is assumed to be computable by an algorithm with a history of a

finite length according to section 3, although it need not be explicitly given in the form of analytical expressions.

We now introduce the *sensitivity matrix* $\boldsymbol{F_x} = (\partial F_i/\partial X_k)$, with $\boldsymbol{X} = \boldsymbol{x}$ inserted. It consists of all the partial derivatives of the output quantities with respect to all input quantities $\boldsymbol{X}$, with the given input data $\boldsymbol{x}$ inserted for $\boldsymbol{X}$. In most cases of MC calculations, these derivatives, too, which are the sensitivity coefficients and form $\boldsymbol{F_x}$, are not explicitly available in the form of analytical expressions. Therefore, each of them must be calculated numerically. This can be done as described in sections 2 and 3, similar to equation (6), using increments $\Delta x_k = \alpha_k u(x_k)$ of x_k:

$$\left.\frac{\partial F_i}{\partial X_k}\right|_{\boldsymbol{X}=\boldsymbol{x}} = \frac{F_{ik}^{+} - F_{ik}^{-}}{\Delta x_k} \qquad F_{ik}^{\pm} = F_i(\ldots, x_k \pm \tfrac{1}{2}\Delta x_k, \ldots). \tag{26}$$

The sensitivity matrix $\boldsymbol{F_x}$ determines the propagation of the uncertainties expressed by the uncertainty matrix $\boldsymbol{U_x}$ of the input quantities $\boldsymbol{X}$. Accordingly, in linear approximation, the contribution of $\boldsymbol{U_x}$ to the uncertainty matrix $\boldsymbol{U_y}$ of the output quantities $\boldsymbol{Y}$ is $\boldsymbol{U'_y} = \boldsymbol{F_x U_x F_x^{\top}}$ [3–6]. This uncertainty matrix $\boldsymbol{U'_y}$ due to $\boldsymbol{U_x}$, and the MC uncertainty matrix $\boldsymbol{S_y}$ are of different and independent origins. Thus, they combine as covariance matrices of independent random variables to form the combined uncertainty matrix $\boldsymbol{U_y}$ associated with the estimate $\boldsymbol{y}$ of $\boldsymbol{Y}$:

$$\boldsymbol{U_y} = \boldsymbol{F_x U_x F_x^{\top}} + \boldsymbol{S_y}. \tag{27}$$

After p and p' defined in equation (19) as components of $\boldsymbol{y}$, and the uncertainty components $u^2(p)$, $u^2(p')$, and $u(p, p')$ associated with them as components of the uncertainty matrix $\boldsymbol{U_y}$ have been calculated, the standard uncertainty $u(q)$ or the relative standard uncertainty $u(q)/|q|$ associated with the estimate $q = p/p'$ of the quantity Q according to equation (19) follows from

$$\frac{u^2(q)}{q^2} = \frac{u^2(p)}{p^2} - \frac{2u(p, p')}{pp'} + \frac{u^2(p')}{p'^2} \tag{28}$$

obtained by applying the uncertainty propagation procedure again.

Constraints involved in $\boldsymbol{X}$, given in the form $\boldsymbol{X} = \boldsymbol{H}(\boldsymbol{W})$ with r unconstrained parameters $\boldsymbol{W}$ ($r < m$), do not affect the MC calculations since $\boldsymbol{F_w} = \boldsymbol{F_x H_w}$ (with $\boldsymbol{H_w}$ defined similarly to $\boldsymbol{F_x}$) and $\boldsymbol{U_x} = \boldsymbol{H_w U_w H_w^{\top}}$ and $\boldsymbol{U'_y} = \boldsymbol{F_x U_x F_x^{\top}} = \boldsymbol{F_x}(\boldsymbol{H_w U_w H_w^{\top}})\boldsymbol{F_x^{\top}} = (\boldsymbol{F_x H_w})\boldsymbol{U_w}(\boldsymbol{F_x H_w})^{\top} = \boldsymbol{F_w U_w F_w^{\top}}$. Thus, $\boldsymbol{U_x}$ can be determined from the uncertainty matrix $\boldsymbol{U_w}$ of $\boldsymbol{W}$ before the MC calculations are carried out. $\boldsymbol{U_x}$ turns out to be singular, i.e. $\operatorname{rank}\boldsymbol{U_x} \leqslant \operatorname{rank}\boldsymbol{U_w}$, but this fact does not matter. If the constraints are given in the form of m' equations $\boldsymbol{J}(\boldsymbol{X}) = \boldsymbol{O}$ ($m' < m$; $\boldsymbol{O}$ is the zero column matrix), choose $r = m - m'$ suitable components of $\boldsymbol{X}$ to form $\boldsymbol{W}$ and solve the system of equations for the remaining m' components of $\boldsymbol{X}$. In this way, $\boldsymbol{X} = \boldsymbol{H}(\boldsymbol{W})$ is obtained again. r of these m equations are identities. Constraints given as inequalities cannot be taken into account within the framework of the first-order approximation of introducing uncertainty treatment into MC simulation as described in this paper. In such cases, the more general, higher-order Bayesian uncertainty theory [6] should be applied.

5. Implementation

As examples of application in practice, we tried to implement an uncertainty treatment into simple MC codes and into the very large and complex MCNP [1]. A detailed description of the code implementations and of the experience gained could not be included in this

theoretical paper although the material will be useful in practice. This material has therefore been laid down in a separate document which is available from the first-named author on request. This document also comprises hints for implementing the history synchronization—MCNP already works with a history synchronization called 'correlated sampling' [1, pp 2–140]—and generally applicable, short FORTRAN code segments for controlling the history synchronization, the sensitivity analysis according to equation (26), and the uncertainty propagation according to equation (27).

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