MICHAEL BERBLINGER
CHRISTOPH SCHLIER

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Originalbeitrag erschienen in:
Computer physics communications 66 (1991), S. 157-166

Computer Physics Communications 66 (1991) 157–166
North-Holland

Monte Carlo integration with quasi-random numbers: some experience

Michael Berblinger and Christoph Schlier
Fakultät für Physik, Universität Freiburg, W-7800 Freiburg, Germany

Received 11 December 1990; in revised form 15 March 1991

We report on our general experience and on some test calculations with quasi-random numbers of the Halton type applied to Monte Carlo integration in several (4–8) dimensions. Compared with the traditional use of (pseudo-)random numbers we find that, at a prescribed level of accuracy, at least one order of magnitude in computing time may be saved even for a step function integrand.

1. Introduction

The advent of fast, inexpensive workstations has turned multidimensional integration by the Monte Carlo technique into a feasible method even for more than trivial accuracies. In a typical case one would use a computer with 1 Mflops (million floating-point operations per second), need 1000 flops (floating-point operations) to decide whether a random point belongs to the integration volume, have a hit rate of 1 in 1000, and run until 10 000 hits have been reached. This would mean 3 hours of computation (which is acceptable), and common wisdom would expect an accuracy of the order of 1% for the result, if the integrand is neither oscillating nor too long-tailed. (The error formula can be found in eq. (2) below.)

However, this accuracy *can be obtained at least an order of magnitude faster*, alternatively, an accuracy at least three times better can be obtained in the same computing time, if one uses *quasi-random numbers* instead of the traditional pseudo-random ones. Both kinds of numbers, or better: multidimensional point sequences, are uniformly distributed in some domain, generally the unit hypercube. But, whereas the latter are, in addition, as uncorrelated as possible (true random numbers would have no correlation whatsoever), the former are quite correlated, and chosen in such a way that new numbers do also *uniformly fill the gaps* between the old ones. An exact measure for this property is the discrepancy of the point set (see e.g. ref. [1]), which should be as small as possible. This deficiency of pseudo-random numbers has nothing to do with a further disadvantage of pseudo-random generators of the linear congruential type: random vectors produced by them "fall mainly in the planes" [2], i.e. lie on certain, not so random, hyperplanes.

Quasi-random number sequences of several kinds are well known in mathematics since at least three decades, and have, e.g., been treated in the books by Stroud on Multiple Integrals of 1971 [3], and by Davis and Rabinowitz on Numerical Integration of 1975 [4]. Their merits are, despite ref. [5], not too well known in the physics community. We ran into them in 1987, when we had started a project in which accurate integrals of the classical phase-space volume of molecular motion were needed [6]. After finding out that one could *save one order of magnitude in computer time* by their use, we have used them routinely.

In this short paper, we want to report on our experience mostly with one kind of quasi-random numbers: the type proposed by Halton [7] ("Halton numbers" for short), and on some recent test

calculations. We consider the question, which type of quasi-random numbers is the best one, still as open, because the answer *in practice* depends on many parameters (dimension of the integral, function to be integrated, shape of the integration domain, intended accuracy, type of computer), and a thorough study exercising all these parameters was not our goal, and has still to be done. The order of the paper is as follows: in section 2 we describe our physical problem. In section 3 we discuss the generation of Halton numbers, and include the kernel of the FORTRAN program we use. Section 4 shows results for several examples. We conclude in section 5 with some general recommendations for this type of multidimensional integration. Other recent papers with similar topic are refs. [8–10]. The integration of molecular phase space with quasi-random numbers of the Korobov type has been tested in ref. [11]. Pseudo-random numbers have been reviewed in refs. [5,12].

2. Integration of the classical phase space

In molecular dynamics the classical phase-space volume for a motion of $s = \frac{1}{2}d$ degrees of freedom at some fixed energy E, and sometimes also fixed total angular momentum J is often needed. It provides, e.g., a semi-classical approximation of the number of quantum states, $N(E, J)$, of a system which is described by its classical Hamiltonian $H(\boldsymbol{p}, \boldsymbol{q})$. $N(E, J)$ is obtained by dividing the phase-space volume $\Gamma(E, J)$ by the size h^s of the quantum cell. The state density is $\rho(E, J) = \mathrm{d}N(E, J)/\mathrm{d}E$, a differentiation which can easily be done numerically by locally fitting a power law to $N(E, J)$. An application where values of $N(E, J)$ and $\rho(E, J)$ are needed is the computation of the unimolecular decay rate of an activated molecule. This is given by RRKM-theory [13] as $k(E, J) = N^{\ddagger}(E, J)/h\rho^{*}(E, J)$, where ‡ denotes properties of the so called "transition state", and * those of the "activated molecule". Another application, where uniformly distributed points in d-dimensional phase space are needed, are trajectory calculations which one wants to start with microcanonical initial conditions [14]. We will report on this elsewhere.

Our main object of calculation has been the highly excited molecule H_3^+, and its transition state for decay into $H^+ + H_2$. The potential-energy surface for this molecule, hence the Hamiltonian for its motion are well known. The integral needed is

$$\Gamma(E, J_0) = \int\int \ldots \int\int \Theta(E - H(\boldsymbol{p}, \boldsymbol{q})) \times \delta(J - J_0)\, \mathrm{d}p_1\, \mathrm{d}q_1 \ldots \mathrm{d}p_s\, \mathrm{d}q_s, \quad (1)$$

where $\Theta(\cdot)$ is the unit step function ($\Theta = 1$ if the argument is > 0, else $\Theta = 0$), and $H(\boldsymbol{p}, \boldsymbol{q})$ the Hamiltonian of the system. The δ-function fixes J to the given value J_0. In case of the transition state, $H(\boldsymbol{p}, \boldsymbol{q})$ must also be taken at fixed value $R^{\ddagger}$ of the reaction coordinate, while P_R must not be integrated. The dimension d of the original integral is thus 12 and 10 for activated molecule and transition state, respectively. Since Monte Carlo integration is very ineffective compared with analytical, or standard one-dimensional numerical integration, it is always advisable to reduce the dimension of the Monte Carlo step as much as possible. We did this by pre-integrating analytically four dimensions. For the activated molecule we further integrated the step function $\Theta(E - H)$ over P_R, which means we solved the equation $H(P_R, R, p_2, q_2, \ldots) = E$ for P_R, and used $P_R(R, p_2, q_2, \ldots)$ as the Monte Carlo integrand, with the additional benefit that the integrand is now a continuous function. Finally, we did all Monte Carlo integrals at fixed reaction coordinate R, and post-integrated over R numerically, except for the transition state, where R is constant anyhow. The Monte Carlo integral had thus $d = 6$ dimensions.

The accuracy of this Monte Carlo integration can, of course, not be assessed by comparison with exact values, since these are unknown. Therefore we divided the integration into groups of 10 partial computations and monitored their variance, σ^2. In each group the number of Monte Carlo hits, N_{hit}, was prescribed (not the number of trials, N_{trial}, which is, however, nearly proportional to N_{hit}). Variation of N_{hit} allows one to determine the law by which the standard deviation σ depends on N_{hit}, and to adapt the calculation to a prescribed level of accuracy. Had we used

pseudo-random numbers, then σ/Γ should be $c_1/\sqrt{N_{\text{hit}}}$, where for a step function integrand and large N_{hit}, c_1 is given by (e.g. ref. [4])

$$c_1 = (1 - N_{\text{hit}}/N_{\text{trial}})^{1/2}. \tag{2}$$

Since there is no proof that in the quasi-random case σ is an unbiased statistics, it is important to check the procedure by examples, whose results are also known analytically. Therefore we integrated also two model systems: a nonrotating, collinear, anharmonic triatomic "molecule" with $d = 4$, and the hypersphere with $d = 6$. The latter can be thought of as the phase-space volume of three uncoupled harmonic oscillators, and its volume is $\frac{1}{6}\pi^3$ for unit radius. For the former the Hamiltonian was

$$H = \tfrac{1}{2}(p_1^2 + p_2^2) - kp_1p_2 + (1 - e^{-q_1})^2 + (1 - e^{-q_2})^2, \tag{3}$$

which leads to a phase space volume of

$$\Gamma(E) = \tfrac{1}{2}\sqrt{\frac{1-k}{1+k}}\left[1 - (1-E)^{1/2} - \frac{2-E}{2} \times \arcsin\left(\frac{E}{2-E}\right)\right], \tag{4}$$

valid for $0 \le E \le 1$. In these examples we cannot only use the standard deviation from groups of computations, but also the true error to determine the accuracy and efficiency of the method.

3. Generation of Halton numbers

The nth point in a Halton sequence [7] is a vector, whose components are Halton numbers, $h_n(p)$, to different bases p. (The numbers themselves are originally due to Van der Corput [15]). The p's should be mutually prime, and as small as possible (especially for small N_{hit}). The ideal procedure to produce $h_n(p)$ is to write n as number to base p, i.e. as $p_1p_2p_3\ldots p_k.0$, and to invert this to the fraction $h_n = 0.p_kp_{k-1}\ldots p_2p_1$. On most computers this is hard to program even in assembler code. However, Halton gave the following short algorithm, which produces h_{n+1} from h_n:

```
      y: = 1/p
      x: = 1 − h_n
L1    If x ≤ y then   y: = y/p                    (5)
                      goto L1
      else h_{n+1}: = (p + 1)y − x.
```

We have originally implemented this algorithm with floating-point (REAL) numbers, and since our tests showed its superiority compared with a pseudo-random number generator of the congruential type, we have used it in all our calculations until recently. However, it is not without problems. On some computers for some bases p we got infinite loops, so we had to test for "good" bases. The source of such problems is the "$\le$" relation in line 3 of eq. (5). Since REAL numbers are approximations to the true, p-ary fractions, $x \le y$ is *not* evaluated correctly in the computer. It is easy to see how this comes about by following the algorithm on a pocket calculator. On a HP 11C, e.g., the Halton numbers to base 3 are not 0, 1/3, 2/3, 1/9, 4/9..., but (since $1.0 - 2.0*0.333\ldots > 0.333\ldots$) they are 0, 1/3, 2/3, ϵ, $1/3+\epsilon$, $2/3+\epsilon$, $1/9+\epsilon$, $4/9+\epsilon$,... with $\epsilon \approx 10^{-9}$. So, the Halton numbers appear, but with some near-repetitions before the error "heals out". Under unfortunate circumstances infinite loops can occur. Double precision does not improve this situation; on the contrary, since ϵ is now of order 10^{-16}, things become worse. In his published algorithm of 1964 [16], which we found only recently, Halton solves this problem by introducing a small "bandwidth" E, within which the inequality $x \le y$ in the above program has to be fulfilled, i.e. the if-clause becomes $x \le y + E$. If the mantissa length of the REAL numbers is known, a judicious choice of E (different for each p!) can produce correct sequences. The price paid is a nonportable generator.

It is, therefore, preferable, to produce a correct sequence of Halton numbers by programming rational numbers using a pair of INTEGERs. The following algorithm implements this (and it is

actually not much slower than the one using REALs on many computers):

```
      SUBROUTINE HALTON
      COMMON/N/ N1, NRA1, NRB1
      COMMON/R/ RS1
      NXA1 = NRB1 - NRA1
C     Special case:
      IF (NXA1 .EQ. 1) THEN
          NRA1 = 1
          NRB1 = NRB1 * N1
          GOTO 19
      END IF
C     General case:
      NXB1 = NRB1/N1
10    IF (NXA1 .LE. NXB1) THEN                    (6)
          NXB1 = NXB1/N1
          GOTO 10
      ELSE
          NRA1 = (1 + N1) * NXB1 - NXA1
      END IF
19    RS1 = REAL(NRA1)/REAL(NRB1)
      RETURN
      END
```

The initialization is:

```
      NRA1 = 0
      NRB1 = 1
      N1 = p, the base one wishes to use.
```

This implementation is fully portable, and should produce identical results on any computer. It avoids early integer overflow, and works up to sequence lengths of at least $2^{31}/p_{\max}$ on a 32-bit computer, where $p_{\max}$ is the largest base employed. (In detail: it is the variable NRB1 which overflows first when reaching 2^{31}. NRB itself jumps from p^k to p^{k+1} when N_{trial} reaches p^k. Note, however, that the REAL numbers RS1 *do* repeat on most computers after $\sim 10^7$ trials, since there are generally only $2^{23} \approx 8 \times 10^6$ different mantissas available. This could easily be remedied by typing the variable RS1 in double precision.) So we feel that at the moment the algorithm shown above suffices for all practical problems. If still larger numbers of points were needed, a data type INTEGER*8 would be obligatory or must be simulated. The time for a single CALL to HALTON is 19 μs on a PC running at 20 MHz with processors 386/3167, 36 μs on an IBM RT, 4.2 μs on an IBM RISC Powerstation 320, and 3.6 μs on an IBM 3090–180. This is less than a CALL to RANECU (implemented according to ref. [12]), which is the pseudo-random number generator used for our comparisons.

4. Results

We present results for three sample calculations of increasing complexity: First, the integration of the 6-dimensional hypersphere, which one can think of as the phase-space volume of three uncoupled harmonic oscillators. Second, a computation of the phase-space volume of the nonrotating collinear "molecule" described by the Hamiltonian, eq. (3), and finally an example from our production runs, which compute the phase-space volume of the activated H_3^+-molecule.

The first example is the unit hypersphere in 6 dimensions, whose volume is $V_6 = \frac{1}{6}\pi^3$. The integration domain is the 6-dimensional hypercube with side length 2 and volume 64, so the probability of a hit is 8.075%. (Incidentally, the general volume ratio of d-dimensional hypersphere and enclosing hypercube is $(\frac{1}{4}\pi)^{d/2}/\Gamma(\frac{1}{2}d+1)$, which asymptotically behaves as $d^{-(d+1)/2}$. That shows that in high-dimensional Monte Carlo integrations the probability of a hit is expected to drop *more than exponentially* with increasing d.)

Two integration formulas were used, either

$$V_6 = \int\int\int\int\int\int \Theta\left(1 - r_1^2 - r_2^2 - r_3^2 - r_4^2 - r_5^2 - r_6^2\right) \mathrm{d}r_1\, \mathrm{d}r_2\, \mathrm{d}r_3\, \mathrm{d}r_4\, \mathrm{d}r_5\, \mathrm{d}r_6, \tag{7a}$$

where $\Theta(\cdot)$ is the unit step function, and the Monte Carlo integral has 6 dimensions, or

$$V_6 = \int\int\int\int\int \left(1 - r_1^2 - r_2^2 - r_3^2 - r_4^2 - r_5^2\right)^{1/2} \times \mathrm{d}r_1\, \mathrm{d}r_2\, \mathrm{d}r_3\, \mathrm{d}r_4\, \mathrm{d}r_5, \tag{7b}$$

where the step function has been pre-integrated over r_6, and a Monte Carlo integral in 5 dimensions with a continuous integrand is left over. Figure 1 and 2 show the results. In each case an integration with a prescribed number of hits, N_{hit},

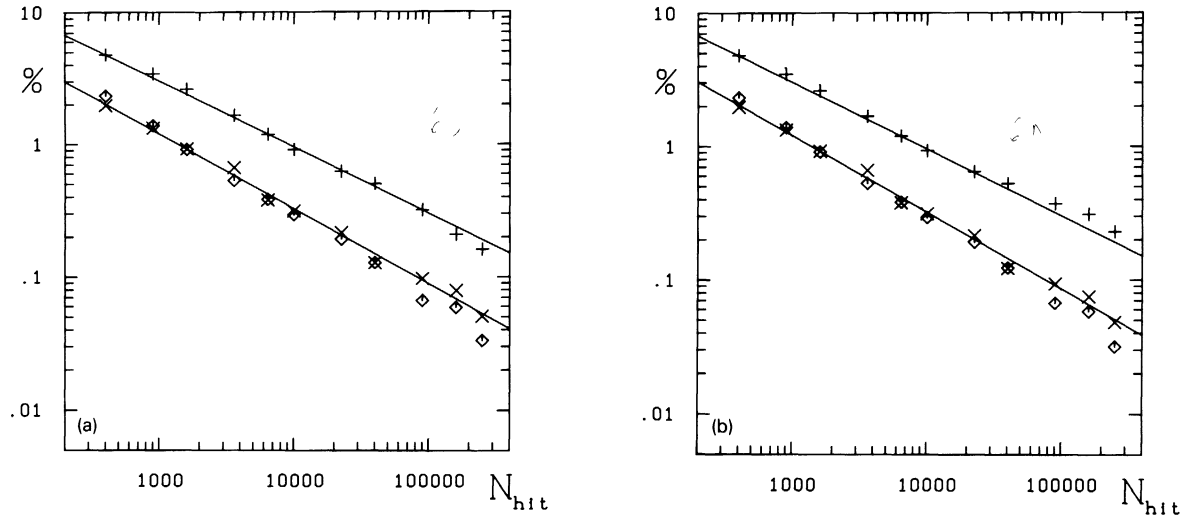

Fig. 1. Monte Carlo integration of the six-dimensional hypersphere with a step function integrand (eq. (7a)): Each integration with a given number of hits, N_{hit}, is repeated 100 times (for $N_{\text{hit}} \leq 22\,500$) or 10 times (for $N_{\text{hit}} > 22\,500$). (a) The averaged relative standard deviation (in %) from these sets is plotted against N_{hit}: + = pseudo-random, × = quasi-random (Halton), ◇ = quasi-random (Sobol). The upper straight line is the result *expected* for the pseudo-random case from eq. (2), viz. $0.959\ N_{\text{hit}}^{-0.500}$, it coincides practically with a straight line fitted to the crosses, which has exponent $a_2 = -0.527$. The lower line is a fit to the results with Halton points, the exponent is $a_2 = -0.565$. The Sobol fit (not shown) has $a_2 = -0.637$. (b) Same as above, except that the rms-average of the true relative errors of the integration has been plotted. The fitted exponents are: −0.474 (pseudo-random), −0.574 (Halton), and −0.642 (Sobol). The similarity between figs. (a) and (b) is expected, since the standard deviation is a consistent estimate for the error.

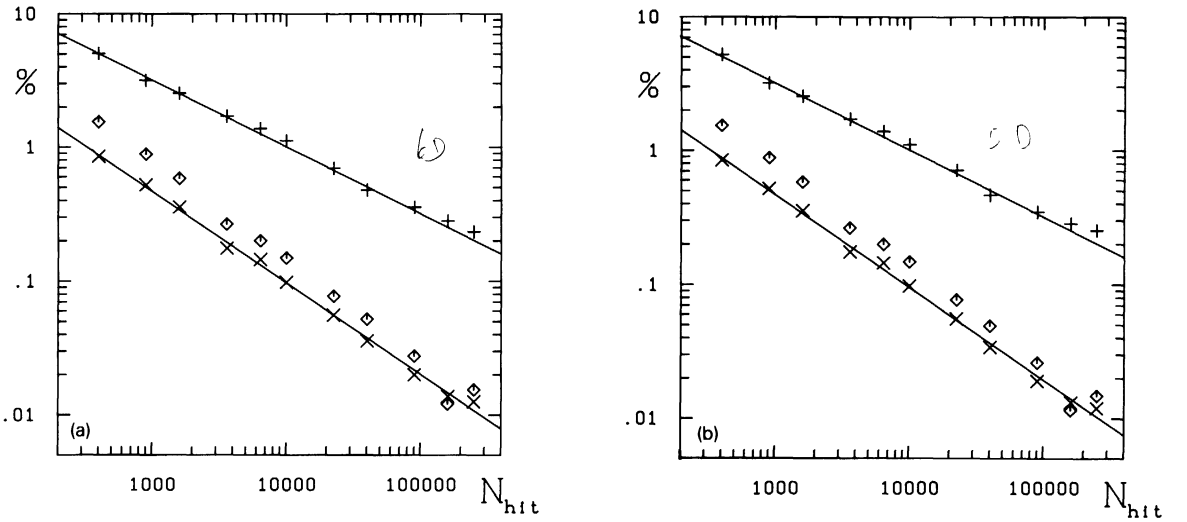

Fig. 2. Monte Carlo integration of the six-dimensional hypersphere after one pre-integration, which makes the Monte Carlo integral five-dimensional and the integrand continuous (eq. (7b)): As in fig. 1 except for the upper straight line, which is now (from an equation analogous to eq. (2)) $1.011\ N_{\text{hit}}^{-0.500}$, and the fitted exponents, whose values are: (a) −0.481, −0.682, −0.755, and (b) −0.480, −0.690, and −0.764.

was repeated with new random numbers, 100 times for N_{hit} between 400 and 22 500, and 10 times for the larger values of N_{hit}. The relative standard deviation of the ensemble, σ/Γ, and the rms-averages of the true errors δ/Γ are plotted in figs. 1a and 1b, and 2a and 2b, respectively. The random numbers were drawn from the pseudo-random number generator RANECU [12,17], the Halton generator described in section 3 above, and in this example also from the Sobol-type quasi-random number generator described in ref. [10]. We also tried Richtmyer sequences (not plotted), but notwithstanding their theoretical merits [1,4] they were little better than pseudo-random numbers under our conditions. A cursory test with the Korobov numbers from ref. [3] was also disappointing.

In all three cases integrated according to eq. (7a), the dependence of the deviations on N_{hit} fits very well to a power law. Exponents are given in the figure captions. For the integration with pseudo-random numbers, the observed exponent -0.527 fits well to the expected one, -0.500. However, also the quasi-random method does not show a too different power law. This seems to be due to the fact that we integrate a *step function*. We think one can prove (along the lines indicated also in ref. [10]), that any Monte Carlo method used to integrate a step function should show an error proportional to $N^{1/2-1/2d}$ (i.e. $N^{-0.583}$ for $d=6$). We do, however, not know of a formal proof in the literature. This power law is virtually indistinguishable from $N^{-1/2}$ for $d \gtrsim 6$. Only if one integrates *smooth* integrands one would expect the quasi-random method to have a different functional dependence on N_{hit}, which the literature [1] gives as $(\ln N_{trial})^d/N_{trial}$. A glimpse of this improvement can perhaps be seen in figs. 2a and 2b, which give the same results as above integrated according to eq. (7b), i.e. with a continuous (but still not smooth) integrand. But even here a power law seems to do well in the three decades of N_{hit} we have used. An unambiguous decision between the dependencies $(\ln N_{trial})^d/N_{trial}$ and $N_{hit}^{1/2}$ becomes difficult by the fact that both functions are parallel just in the region where we observe our data.

Very obvious is the increase in accuracy by the use of quasi-random numbers, which is about 3 for the integration according to eq. (7a) and about 10 for eq. (7b), both for an accuracy of about 1%. At higher levels of accuracy these factors tend to be even greater. It is also obvious, that there is no significant difference between the results with Sobol or Halton sequences.

Our next example, the anharmonic collinear molecular model of eq. (3), has still the virtue that the result is known analytically, see eq. (4). So, we can again use the standard deviation *and* the true error to judge accuracy and efficiency of the integration. We have done two independent calculations at $E=0.3$ and 0.9, both with pseudo-random numbers and with Halton numbers. Again, groups of 10 integrations with the same N_{hit} were performed, the results are shown in tables 1 and 2. The relative standard deviation, σ/Γ, and the relative error, $\delta=(\Gamma-\Gamma_{true})/\Gamma_{true}$, as functions of N_{hit} are listed. From these data, to be more specific, we computed with $x=\sigma_R$, $|\delta_R|$, σ_H, or $|\delta_H|$:

(a) a one-parameter fit of $x\sqrt{N}_{hit}$ to a constant c_1, thus *assuming* that σ and $|\delta|$ are proportional to $\sqrt{N}_{hit}$, and

(b) a two-parameter fit of $\log x$ to $\log c_2 + a_2 \log N_{hit}$, assuming only some *power law* for $x(N_{hit})$. The result is again that *both* integration methods give a good fit to a square-root law. For the pseudo-random case that is the expected result, i.e. we expect from eq. (2) $c_1=0.853$ (for $E=0.3$) or $c_1=0.933$ (for $E=0.9$), and $a_2=-0.5$; so we feel that the observed agreement is good. For the quasi-random case the c_1-coefficient is unknown, and the expected power according to the arguments put forth above is -0.625.

The gain of using quasi-random numbers can best be measured by the ratio c_{1_R}/c_{1_H}, which lies between 3.7 and 4.9 for σ and between 17 and 88 for the true error δ.

Table 3 shows results at constant $N_{hit}=2000$ averaged over nine different energies. Again, the pseudo-random integration is similar to expectation, and the Halton method improves that by a factor of about 3 for the standard deviation, and about 15 for the true error. The consistent finding that the improvement through quasi-random numbers is much greater for the true errors than for

Table 1
Results from the collinear anharmonic molecular model (eq. (3), with $k = 0$) at $E = 0.3$ computed with pseudo-random and quasi-random (Halton) numbers. N_{hit} is the number of hits in each single integration (the number of trials is about 3.68 N_{hit}). vol is the average phase-space volume from 10 integrations (the exact value is 2.510062×10^{-2}). std-dev is the relative standard deviation within the groups of 10 integrations. err is the relative error of the mean of 10 integrations, i.e. the error of an integration with 10 N_{hit} hits. c_1 is the column average of $x\sqrt{N}_{hit}$ (where x = std-dev or |err|), i.e. the constant c_1 in a fit of $x(N_{hit})$ to $c_1/\sqrt{N}_{hit}$. a_2 is the exponent in a fit to a power law $x = \text{constant} \times N_{hit}^{a_2}$ (where x = std-dev or |err|)

N_{hit}	Pseudo-random			Quasi-random		
	vol (10^{-2})	std-dev (%)	err (%)	vol (10^{-2})	std-dev (%)	err (%)
100	2.539	7.85	1.14	2.523	3.03	0.536
200	2.579	5.41	2.74	2.513	2.11	0.139
400	2.530	2.76	0.79	2.517	1.16	0.289
1000	2.563	2.89	2.11	2.510	0.627	1.06E-2
2000	2.544	2.35	1.34	2.5113	0.389	4.87E-2
4000	2.524	1.26	0.555	2.5112	0.271	4.47E-2
10000	2.5170	0.939	0.279	2.5100	0.188	−3.09E-3
20000	2.5178	0.649	0.307	2.5102	0.122	4.67E-3
40000	2.5139	0.400	0.152	2.5094	8.93E-2	−2.41E-2
100000	2.5115	0.228	5.95E-2	2.50989	7.17E-2	−6.16E-3
200000	2.5100	0.222	3.89E-3	2.50992	2.45E-2	−5.08E-3
400000	2.5122	0.158	8.44E-2	2.51011	1.31E-2	2.67E-3
1E6	2.51117	8.73E-2	4.49E-2	2.51015	9.86E-3	4.20E-3
2E6	2.51056	6.68E-2	2.02E-2	2.51017	7.90E-3	5.05E-3
4E6	2.51032	4.39E-2	1.07E-2	2.51012	3.71E-3	3.05E-3
c_1 (%)		86	33		17.5	1.93
a_2		−0.480	−0.523		−0.613	−0.429

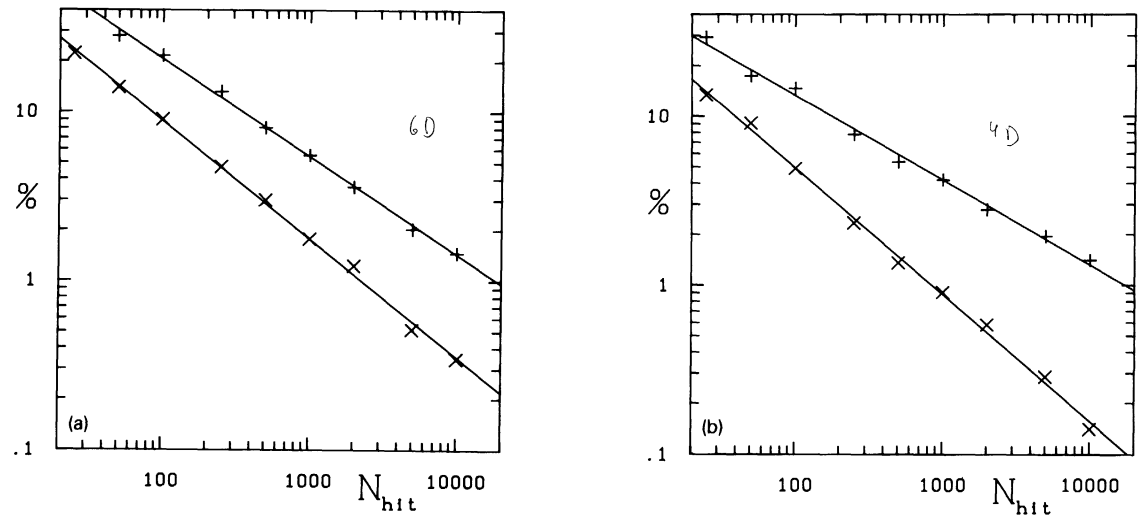

Fig. 3. Monte Carlo integration of the phase-space volume of the molecule H_3^+ at $E = +1.05$ eV, $J = 25$. The relative standard deviation within groups of 10 integrations, each with N_{hit} hits, has been averaged over 36 values of the coordinate R at which the integral was taken. For details see the text. The markers are: + = pseudo-random numbers, × = Halton-type quasi-random numbers. (a) Six-dimensional continuous integrand, the fitted exponents a_2 are −0.579 (pseudo-random) and −0.699 (Halton). (b) Further pre-integration has made the integral four-dimensional, see the text. The fitted exponents a_2 are now −0.502 (pseudo-random) and −0.749 (Halton).

Table 2
Results from the collinear anharmonic molecular model (eq. (3), with $k = 0$) at $E = 0.9$ computed with pseudo-random and quasi-random (Halton) numbers. N_{hit} is the number of hits in each single integration (the number of trials is about 7.70 N_{hit}). vol is the average phase-space volume from 10 integrations (the exact value is 3.134787×10^{-1}). std-dev is the relative standard deviation within the groups of 10 integrations. err is the relative error of the mean of 10 integrations, i.e. the error of an integration with 10 N_{hit} hits. c_1 is the column average of $x\sqrt{N}_{hit}$ (where x = std-dev or |err|), i.e. the constant c_1 in a fit of x (N_{hit}) to $c_1/\sqrt{N}_{hit}$. a_2 is the exponent in a fit to a power law x = constant $\times N_{hit}^{a_2}$ (where x = std-dev or |err|)

N_{hit}	Pseudo-random			Quasi-random		
	vol (10^{-1})	std-dev (%)	err (%)	vol (10^{-1})	std-dev (%)	err (%)
100	3.163	6.89	0.914	3.1323	4.72	−8.08E-2
200	3.167	4.15	1.026	3.1176	2.08	−5.45E-1
400	3.227	3.85	2.933	3.1341	0.895	−2.24E-2
1000	3.194	2.34	1.398	3.1312	0.712	−1.20E-1
2000	3.176	1.55	1.302	3.1326	0.622	−6.91E-2
4000	3.1497	1.41	0.474	3.1369	0.425	6.68E-2
10000	3.1454	0.946	0.339	3.13614	0.259	4.25E-2
20000	3.1407	0.696	0.188	3.13665	0.155	5.94E-2
40000	3.1365	0.356	0.0548	3.13517	0.123	1.21E-2
100000	3.1340	0.243	−0.0249	3.13504	3.99E-2	8.30E-3
200000	3.13822	0.256	0.110	3.13458	4.11E-2	−6.60E-3
400000	3.13836	8.10E-2	0.114	3.13477	2.45E-2	−5.31E-4
1E6	3.13559	0.112	2.52E-2	3.13485	1.18E-2	2.19E-3
2E6	3.13534	8.89E-2	1.78E-2	3.13479	8.89E-3	9.54E-5
4E6	3.13536	5.87E-2	1.83E-2	3.13478	3.00E-3	1.0E-5
c_1 (%)		84	32		22.5	0.365
a_2		−0.459	−0.477		−0.598	−0.622

the standard deviation of a group of otherwise similar integrations, shows that the distribution of errors in the quasi-random case is not a normal distribution. A look on a few histograms revealed that the error distribution is nearly triangular, so the probability for small errors peaks much higher than in a normal distribution of the same standard deviation. The reasons are not clear, however. The suspicion that it might be a consequence of the correlations between different components of the quasi-random vectors as discussed by Braaten and Weller [18] did not substantiate, since scrambled Halton sequences show the same behaviour.

Table 3
Results from the collinear anharmonic molecular model (eq. (3), with $k = 0$) averaged over nine calculations at energies $E = 0.1$ (0.1) 0.9, computed with pseudo-random and quasi-random (Halton) numbers. Each calculation consists of 10 integrations with $N_{hit} = 2000$. ⟨std-dev⟩ is the average of the relative standard deviations (in %) from the nine calculations. ⟨err⟩ the average relative error (in %) of these calculations, i.e. it belongs to one integration with $N_{hit} = 20000$

	⟨std-dev⟩	⟨err⟩
Expected	2.236 ± 0.527	0.707 ± 0.236
Pseudo-random	1.644 ± 0.352	1.109 ± 0.278
Quasi-random (Halton)	0.597 ± 0.092	0.073 ± 0.110
Improvement	2.75	15.2

The final example comes from our production runs. The phase-space volume of H_3^+ at energy $E = +1.05$ eV and total angular momentum $J = 25$ has been computed at 36 values of the reaction coordinate R. Each integration was done 10 times with prescribed N_{hit}, and the standard deviation σ determined. The true errors are no longer known. For the purpose of this paper, we further averaged the relative standard deviations σ/Γ over the set of 36 R's. Figure 3a shows the results from the integration of a continuous integrand in 6 dimensions as described in section 2. Both data sets fit well to a power law (with powers given in the

figure caption), and conform well to expectations. Again the standard deviation of a group of integrations is about three times less with quasi-random numbers than with pseudo-random numbers, and this improvement increases with N_{hit}, i.e. with the needed accuracy. A further analytical pre-integration discussed elsewhere [19] allows to do the same integrals with only a 4-dimensional Monte Carlo step. These results are shown in fig. 3b, and the conclusions are as above. The gain in accuracy by the use of quasi-random numbers seems to be even higher than in fig. 3a.

5. General recommendations and conclusions

At least for an integration task of the type demonstrated here, which is characterized by the integrand being not smooth, a rather simple integration domain, an accuracy level of the order of 10^{-2}–10^{-4}, and dimensions between 4 and (say) 12, the lesson to learn from our experience and the examples shown in this paper is obvious: use quasi-random numbers and save one or two orders of computer time! We also showed that d-dimensional quasi-random points of the Halton type can be easily produced in sufficient numbers by a portable program. Whether Sobol numbers (or Faure numbers [20], or the new Niederreiter numbers [21], to be sure) are any better has to be found out; it can neither be decided from tests which use only a few thousand trials, nor is it important what the mathematically asymptotic behaviour is, if this asymptotic region is only reached with 10^{20} trials!

The use of quasi-random points can, of course, be combined with methods of variance reduction well known [4,5] under the labels importance sampling and stratified sampling. Such and other methods will certainly be needed if one wants to do integrals in higher dimensions, which is the proper realm of Monte Carlo integration [5]. Molecular dynamicists would, e.g., like to integrate phase-space volumes of four- and five-atomic molecules with $d = 18$ and 24, respectively. From our experience, in addition to the use of quasi-random numbers we recommend:

(a) Do as many integrations as possible before the Monte Carlo step. This is generally nontrivial, and we found, e.g., only recently [11,19] that under many circumstances even for a rotating molecule the whole momentum part of the molecular phase space can be pre-integrated analytically, saving $3N_{\text{atoms}} - 3$ dimensions in the Monte Carlo part.

(b) On integrating a step function $\Theta(E - H)$, where $H = H_1 + H_2 + H_3 + \cdots$ consists of different summands, one may save much computer time by arranging the H_i according to descending values and stopping the computation of H as soon as the *partial sum* exceeds E. Similar "breaks" could be programmed also for continuous integrands.

(c) It may also be advantageous to set aside one (or even two) dimensions of the integrand for a final integration by standard numerical methods. I.e. compute a Monte Carlo integral $\Gamma_{\text{MC}}(x_i)$, which depends parameter-wise on one coordinate x_i, and integrate $\int \Gamma_{\text{MC}}(x_i)\,\mathrm{d}x_i$ by some high-order integration rule. The error of this integration may easily be as small as $\mathcal{O}(N^{-6})$ in one or $\mathcal{O}(N^{-3})$ in two dimensions, where N is the number of points $\{x_i\}$ or $\{x_i, x_j\}$, respectively. This seems to contradict the philosophy of the Monte Carlo scheme, but it has been shown already in ref. [5] that low-dimensional integrations are better not done by Monte Carlo, and there is no reason against combining the advantages of both methods.

(d) A word of warning is due against using components of Halton vectors in situations where absence of any kind of correlation is needed. We encountered such a case, when we alternately sampled from the horizontal and vertical "legs" of a T-shaped domain, and used the component with $p = 2$ of the Halton vector to sample one of the coordinates. Since the Halton sequence $H_p(n)$ with $p = 2$ lies alternately in the intervals $\{0.0, 0.5\}$ and $\{0.5, 1.0\}$, the coordinate corresponding to $p = 2$ was now restricted to the first interval in one leg of the T, and to the second in the other leg. This produced an an appreciable bias!

We did not, however, see in our calculations any harm by the correlation between pairs of vector components discussed in ref. [18]. This effect apparently dies out for large N_{trial}, and is only important if one uses large p_i concurrently with

small N_{trial}. Some of our test calculations were repeated with scrambled Halton numbers, and did not show any significant difference.

Concluding, there is strong reason to use quasi-random numbers in Monte Carlo integration, even if certain questions must still be answered: Which are the best quasi-random sequences for a given problem? Are there problems in which it really pays to scramble the Halton sequences? Under which circumstances are Sobol or Faure or the improved Niederreiter sequences better? Is the method also useful in Markov chain ("Metropolis"-) sampling? Finally: even the mathematical question of whether one can find still better quasi-random sequences seems to be an open one.

Acknowledgements

The support of the Deutsche Forschungsgemeinschaft (Schwerpunktprogramm Atom- und Molekültheorie and SFB 276) is gratefully acknowledged C.S. wants also to acknowledge the hospitality of the Fritz Haber Research Center for Molecular Dynamics at the Hebrew University, Jerusalem, Israel, where the first integrations with Halton numbers were performed.

References

[1] H. Niederreiter, Quasi Monte Carlo methods and pseudo-random numbers, Bull. Am. Math. Soc. 84 (1978) 957.
[2] G. Marsaglia, Random numbers fall mainly in the planes, Proc. Nat. Acad. Sci. USA 61 (1968) 25.
[3] A.H. Stroud, Approximate Calculation of Multiple Integrals (Prentice-Hall, Englewood Cliffs, NJ, 1971).
[4] P.J. Davis and P. Rabinowitz, Methods of Numerical Integration, 2nd ed. (Academic, New York, 1984).
[5] F. James, Monte Carlo theory and practice, Rep. Prog. Phys. 43 (1980) 1145.
[6] M. Berblinger, E. Pollak and Ch. Schlier, Bound states embedded in the continuum of H_3^+, J. Chem. Phys. 88 (1988) 5643.
[7] J.H. Halton, On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals, Numer. Math. 2 (1960) 84, 196.
[8] P.K. Sarkar and M.A. Prasad, A comparative study of pseudo- and quasi-random sequences for the solution of integral equations, J. Comput. Phys. 68 (1987) 66.
[9] P. Bratley and B.L. Fox, Implementing Sobol's quasirandom generator, Algorithm 659, ACM Trans. Math. Software 14 (1988) 88.
[10] W.H. Press and S.A. Teukolsky, Quasi- (that is, sub-) random numbers, Comput. Phys. 3 (1989) 76.
[11] S.C. Farantos, J.N. Murrell and J.C. Hajduk, Monte Carlo calculations of classical density of states for non-separable polyatomic potential energy surfaces, Chem. Phys. 68 (1982) 109.
[12] F. James, A review of pseudorandom number generators, Comput. Phys. Commun. 60 (1990) 329.
[13] P.J. Robinson and K.A. Holbrook, Unimolecular Reactions (Wiley, New York, 1972).
[14] W.L. Hase, Dynamics of unimolecular reactions, Dynamics of Molecular Collisions, Vol. B, in: W.H. Miller, ed. (Plenum, New York, 1976) p. 156.
[15] J.G. van der Corput, Verteilungsfunktionen I und II, Proc. K. Ned. Akad. Wet. 38 (1935) 813, 1058.
[16] J.H. Halton and G.B. Smith, Radical inverse quasi-random point sequence, Algorithm 247, Commun. ACM 7 (1964) 701.
[17] P. L'Ecuyer, Efficient and portable combined random number generator, Commun. ACM 31 (1988) 742.
[18] E. Braaten and G. Weller, An improved low-discrepancy sequence for multidimensional quasi Monte Carlo integration, J. Comput. Phys. 33 (1979) 249.
[19] M. Berblinger, Thesis, Universität Freiburg (1991).
[20] H. Faure, Discrépance de suites associées à une système de numération (en dimension s), Acta Arith. 41 (1982) 337.
[21] H. Niederreiter, Low-discrepancy and low-dispersion sequences, J. Number Theor. 30 (1988) 51.