Use of tabulated cumulative density functions to generate pseudorandom numbers obeying specific distributions for Monte Carlo simulations

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A new method for the generation of pseudorandom numbers, which obey a specific statistical distribution, is presented. As an example the generation of the scattering angle θ for Monte Carlo light-scattering simulations is shown, using real, peaked, scattering phase functions.

When the theory or the geometry of a physical experiment is too tedious, computer simulations may be performed to understand the process. These simulations need pseudorandom numbers that obey a specific probability density function PDF(x). If the PDF is simple and analytically invertible, the inverse distribution method may be used. In other cases the well-known rejection technique is mostly used, but this technique is inefficient when the PDF is sharply peaked. Both techniques are clearly explained by Lux and Koblinger.[1]

Recently, Walker[2] described how a sharply peaked PDF can be dealt with by using a mesh of x points with an x-dependent density, which is obtained with an adaptive quadrature method.

In this Note we propose to deal with a sharply peaked PDF(x) by using a tabulated density function. Let x be a variable between x_1 and x_2. The cumulative PDF (CPDF) can be calculated with

$$\mathrm{CPDF}(x) = \int_{x_1}^{x} \mathrm{PDF}(x')\mathrm{d}x' \qquad (1)$$

and normalized so that $\mathrm{CPDF}(x_2) = 1$; CPDF is stored in an array. The inverted CPDF (ICPDF) can be calculated and stored in the array ICPDF[k] as follows. For all k the two values of CPDF(x) that most closely correspond to the index value k are looked up in the array CPDF, and an appropriate interpolation technique has to be performed. From a random number *RND* the corresponding index of the array ICPDF can be calculated, and the pseudorandom value of x is given by the value of the corresponding element of the array ICPDF[k].

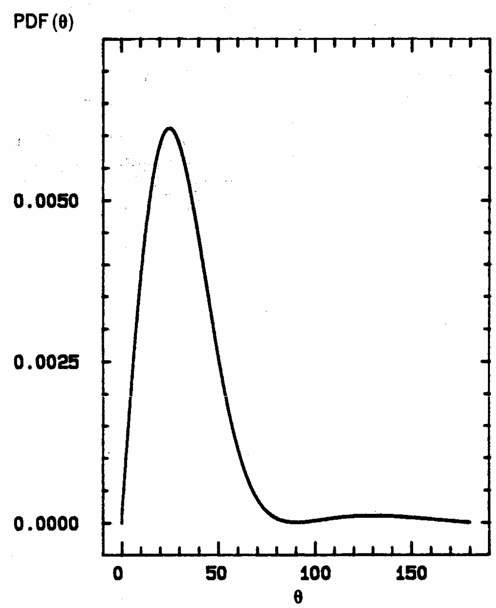

Fig. 1. Probability density function (PDF) of θ obeying the Mie phase function (size parameter $x = 3.1$, relative refractive index $m = 1.050$, anisotropy factor $g = 0.8$).

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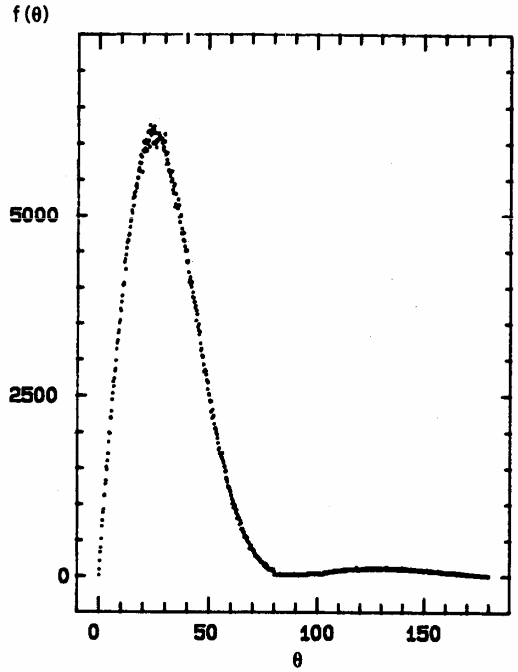

Fig. 2. Distribution of 1,000,000 generated values of θ. The fluctuations in the frequency $f(\theta)$ are equal to the expected statistical noise.

As an example we show generation of pseudorandom angles θ in a Monte Carlo calculation, simulating a light-scattering process. We use a tabulated real scattering phase function, one of a sphere calculated by Mie theory, as clearly explained by van de Hulst[3]; the function is available with a resolution of 0.25° and is stored in an array with 720 elements. The CPDF(θ) is calculated and inverted by performing Lagrange interpolations to give an ICPDF array having 1000 elements. We stored the values of cos(θ) in the ICPDF array. The cos(θ) can be generated from a linear interpolation between the array elements whose index is given by the rounded value of (1000*RND*) and (1000*RND*) + 1.

Table 1. Average Time Needed to Generate a Value of cos(θ) (in Microseconds)[a]

Phase Function	Analytical Inverted Function	Rejection Technique	Presented Method
Isotrope	11	70	41
Henyey–Greenstein ($g = 0.8$)	30	186	41
Mie ($x = 3.1, m = 1.050, g = 0.8$)	—	143	41
Mie ($x = 11.2, m = 1.500, g = 0.8$)	—	307	41

[a]All problems were programmed in Turbo Pascal and executed on an 80486/33 MHz personal computer.

The averaged times needed to generate a value of cos(θ) are shown in Table 1. The time needed to generate a value of cos(θ) by the presented method is a fraction longer than the time needed by the analytical inverted Henyey–Greenstein phase function. This difference is reducing if θ is generated instead of cos(θ). Figures 1 and 2 show the theoretical and the generated distribution functions of θ, respectively.

We conclude that the presented method is an accurate and fast method for the generation of pseudorandom numbers that have to obey a known statistical distribution.

References

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2. P. L. Walker, "Modification of Monte Carlo codes for use with sharply peaked phase functions," Appl. Opt. **32**, 2730–2733 (1993).
3. H. C. van de Hulst, *Light Scattering by Small Particles* (Dover, New York, 1981), Chap. 9, p. 114.