MONTE CARLO METHODS IN PHYSICS

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ABSTRACT

MONTE CARLO METHODS IN PHYSICS. Method of Monte Carlo integration is reviewed briefly and some of its applications in physics are explained. A numerical experiment on random generators used in the Monte Carlo technique is carried out to show the behavior of the randomness of various methods in generating them. To account for the weight function involved in the Monte Carlo, the metropolis method is used. From the results of the experiment, one can see that there is no regular patterns of the numbers generated, showing that the program generators are reasonably good, while the experimental results, shows a statistical distribution obeying statistical distribution law. Further some applications of The Monte Carlo Method in physics are given. The choice of physical problems are such that the models have available solutions either in exact or approximated values, in which comparisons can be made with the calculations using the Monte Carlo method. Camparisons show that for the models to be considered, good agreement have been obtained.

ABSTRAK

METODA MONTE CARLO DI BIDANG FISIKA. Metoda Monte Carlo disajikan dengan penjelasan aplikasinya di bidang fisika. Suatu eksperimen dengan generator acak yang digunakan dalam Metoda Monte Carlo dilakukan untuk menunjukkan kelakuan keacakan berbagai metoda dalam membangkitkan mereka. Untuk dapat ikut memperhitungkan fungsi bobot yang terlibat dalam metoda Monte Carlo, metoda metropolis digunakan. Dari hasil eksperimen terlihat bahwa tidak adanya pola reguler dari angka-angka terbangkitkan, menunjukkan bahwa program generator cukup baik. Hasil-hasil eksperimen menunjukkan adanya distribusi statistik yang mengikuti aturan distribusi statistik. Selanjutnya beberapa aplikasi dari Monte Carlo dalam fisika diberikan. Pemilihan problema fisika adalah sedemikian, model-model yang diselesaikan mempunyai solusi eksak atau solusi pendekatan, dengan demikian perbandingan hasil kalkulasi dapat dilakukan dengan metoda Monte Carlo. Perbandingan hasil menunjukkan bahwa untuk model-model yang disajikan, hasil-hasil perhitungan sangat berdekatan.

INTRODUCTION

Monte Carlo is a place in Monaco where people come to gamble for money. Gambling is always associated with random numbers.Randomness in this paper is limited to numbers that are generated by deterministic arithmatical process. Monte

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Carlo method solves a certain type of problems through the use of random numbers. There are various methods of generating these numbers eg 'random numbers' (chapter 7, numerical recipes, the art of scientific computing, by William H, Press et.al). Simple example of generating random numbers typically given by

$$x_{n+1} = rx_n \bmod(N) \qquad (1)$$

where an arbitrary number x_n is multiplied by a large constant number r, each product being reduced by modulo N. The sequence $x_0, x_1, x_2 \ldots\ldots$ is distributed fairly evenly over (0,N), if N is large enough. Figure 1 demonstrates the value of random (x_n) as function of n.

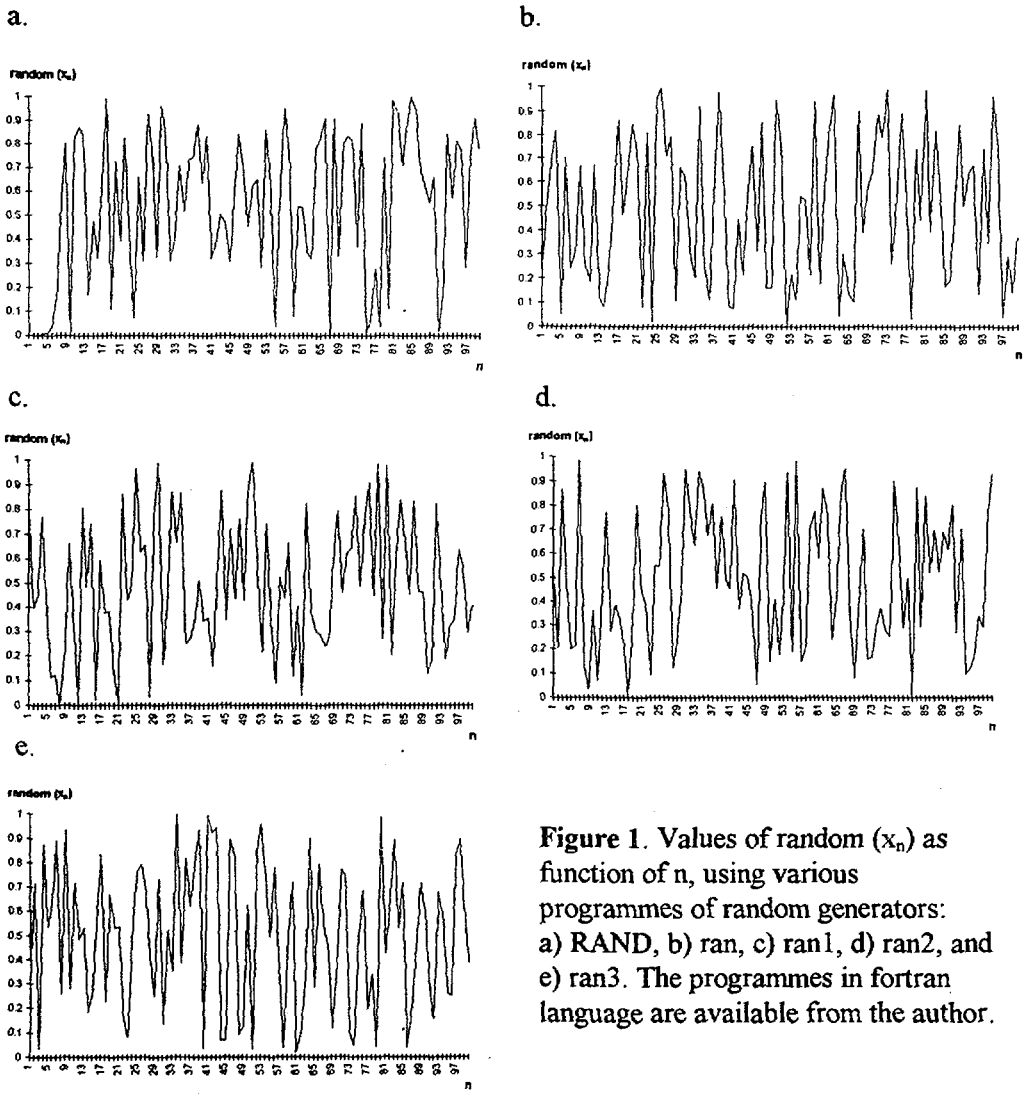

Figure 1. Values of random (x_n) as function of n, using various programmes of random generators: a) RAND, b) ran, c) ran1, d) ran2, and e) ran3. The programmes in fortran language are available from the author.

From the numerical experimental results (figure 2) we can see the behavior of random values generated by different programs. Although they behave differently, the average of their probability in occupying a certain interval are similar in their pattern. This probability should become the same as the number of experiment in increased.

2a. 2b.

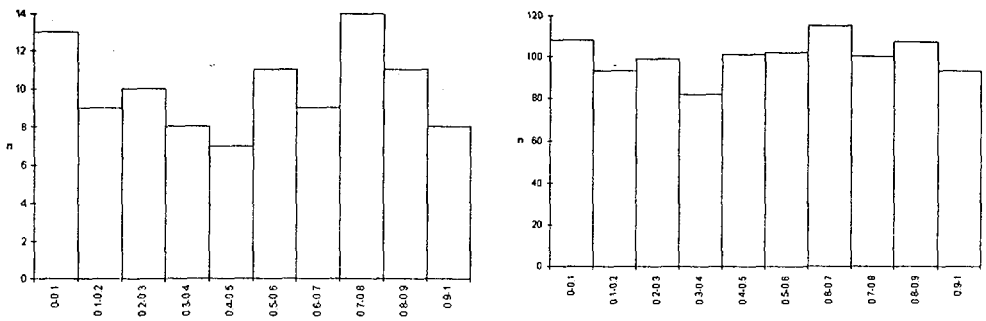

Figure 2. Distribution of P_n : the probability of n times of ran3(x_n) falls between u_n and u_{n+1}. u_n is 0, 0.1, ... , 0.9. Fig 2a is for N=100 generated numbers and fig 2b is for N=1000

Monte Carlo method solves the following integration

$$\int_a^b f(x)\,dx = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i) \qquad (2)$$

by making an average over N of $f(x_i)$ where x_i are selected at random in (a,b). For simple integration such as in single integration, Monte Carlo method is inferior to the trapezoidal and other standard integration procedure. However as the dimensions of integration become larger, the standard procedure becomes more and more impractical if not impossible. Errors introduced in the standard procedure are dependent on the number of numerical operations. The error propagation is becoming bigger as the number of operation is increased. On the other hand, accuracy of the procedure is increased with the increasing number of step length within the same interval, optimization is necessary to get the best result. Monte Carlo method on the other hand introduces errors that follow statistical behavior in nature.

METROPOLIS METHOD

Integration such as in (2) should account for the weight function involved. On a very general way, to produce random variables with a given probability distribution of arbitrary form is known as the Metropolis, Rosenbulth, Teller and Teller algorithm.

The method of Metropolis et al can be implemented in a variety of ways. One simple realization is as follows. Suppose that we want to generate a set of points in space of variables x distributed with probability density w (x). The Metropolis algorithm generates a sequence of points $x_0, x_1, x_2 \ldots\ldots$ such that the next point is connected to previous point approximating closely the desired distribution. If the walker - is presently at x_n then x_{n+1} is generated by random number generator. x_{n+1} is accepted or rejected according to the ratio

$$\mathrm{r} = \frac{W(x_{n+1})}{W(x_n)} \tag{3}$$

If r is larger than one, then x_{n+1} is accepted while if r is less than one, the step is accepted with probability r. This is accomplished by comparing r with a random number η uniformly distributed in the interval (0,1). If $\eta < \mathrm{r}$ then x_{n+1} is also accepted. If x_{n+1} is rejected then x_{n+1} is put equal to x_n. Any arbitrary point x_0 can be used as a the starting point for random walk.

APPLICATION IN PHYSICS

Simple models

In order to be able to verify the validity of the method, it is necessary to apply the Monte Carlo method to simple models where 'exact solutions' are available. This is required for a comparative purposes. Such models that can be chosen are the harmonic oscillator, helium atom and hydrogen molecular energy bounds calculations.

In these system the required energy bounds can be calculated from

$$\varepsilon = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{4}$$

where Ψ satisfies the Hamiltonion eigen function

$$H\Psi_n = \in_n \Psi_n \tag{5}$$

$$H = -\frac{h^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \tag{6}$$

for harmonic oscillator.

$$H = -\frac{h^2}{2m}\nabla_1^2 - \frac{h^2}{2m}\nabla_2^2 - \frac{e^2}{r_{A1}} - \frac{e^2}{r_{A2}} - \frac{e^2}{r_{B1}} - \frac{e^2}{r_{B2}} + \frac{e^2}{r_{12}} + \frac{e^2}{r_{AB}} \tag{7}$$

for hidrogen molecules.

All notations are chosen in a standard way commonly used in Schrodinger equation (e.g. see Davidov, Quantum Mechanics). In the case

$r_{A1} = r_{B1}, r_{A2} = r_{B2}$ *and* $\frac{e^2}{r_{AB}} = 0$, the system becomes an Helium atom.

Except for harmonic oscillator the exact solution for ψ are not known. Approximate solutions can be made using a trial wave functions, where unknown parameter (s) can be introduced. Varying the parameter (s) so as to get the lowest energy bounds, one obtain the solution of Ψ in the variational scheme. As trial function we have chosen $\Psi(x,a) = \exp(-ax^2/2)$ for the harmonic oscillator

$$\Psi(r_1, r_2) = \Psi(r_1)\Psi(r_2)f(r_{12}) \tag{8}$$

where

$$\Psi(r_i) = \exp(-r_{Ai}/\alpha) + \exp(-r_{Bi}/\alpha) \tag{9}$$

$$f(r) = \exp(r/\{\alpha(1+\beta r)\}) \tag{10}$$

$$\alpha = \frac{h^2}{me^2}(1+\exp(-1/\alpha)) \tag{11}$$

For helium atom ($r_{AB} = 0$), it is found that the energy bound computed by the Monte Carlo is - 78,38 eV as compared to - 78,88 eV obtained from experimental value. Other comparative values can be seen in table 1.

Table 1. Comparison with the Monte Carlo Method (MCM)

	exp./exact	MCM
Harmonic oscillator	4.369	4.341
perturbed harmonic osc	3.119	3.143
H_2^+ molecular ($r_{AB} = 1.06A^1$)	-16.4	-17.0
H_2 molecule ($r_{AB} = 0.74A^1$)	-31.95	-31.4

From this comparison it was found that the error in the computation was less than 5%.

More sophisticated problems

In a more sophisticated problem Monte Carlo method can simulate a real system such as fluid system with water like molecules, models of binary spin system, ising model calculations etc.

Fluid System with Waterlike Molecules

In the equilibrium state the pressure can be calculated from the virial function defined as

$$_{vir} = -\frac{1}{2} < \sum V_{kl} . F_{kl} > \tag{12}$$

This can be done since in all configurations all V_{kl} and F_{kl} are known (the interaction force $F = -\nabla . E_2$ for pairwise interaction, where E_2 is the Lennard Jones model given by

$$E_2 = 4\in((\frac{\delta}{r_{kl}})^{12} - (\frac{\delta}{r_{kl}})^{6}) \tag{13}$$

r_{kl} is the internuclear distance of two particles k and l, δ is the diameter of the particles and $\in$ is the absolute value of energy in the minimum of the potential curve. The pressure is related to the virial function with the equation:

$$\frac{PV}{NkT} = 1 - \frac{2}{3}\frac{V_{vir}}{NkT} \tag{14}$$

An the excess free energy can be calculated from the equation

$$\frac{A^1}{NkT} - \int_{\rho=0}^{\rho} (\frac{P}{\rho kT} - 1)\frac{d\rho}{\rho} \tag{15}$$

Where $\rho = N/V$ and A^1 is the excess free energy, that is the difference between the free energy of the system and of the ideal gas with the same temperature and the same ρ.

Table 2 shows the results of the calculation by W. Bol (1979) of configuration space in a fluid of hard sphere with density 0.6. For N= 2 the result is obtained analytically and for N = 1 is trivial solution.

Table 2. Values of $\frac{A^1}{NkT}$ as function of N

N	Total number of Monte Carlo steps	$\frac{A^1}{NkT}$
1	-	1.149
2	-	1,495
3	0.18×10^6	1.651
20	1.63×10^6	1.981
44	2.9×10^6	2.014
91	1.77×10^6	2.029
172	1.67×10^6	2.035

The ising model in two dimensions

The ising models simplifies models in which the degrees of freedom reside on a lattice and interact locally. These arise in several areas of condensed matter physics and field theory.

A model of solid magnetization using the ising model consists of a set of spin degrees of freedom interacting with each other and with external magnetic field. We can consider the magnetic moments of atom in a solid, in wich in two spatial dimensions spin are located on sites of an $N_x \times N_y$ square lattice. The spins should be labelled (S_α) where i and j are the indices for two spatial direction while α is a generic site label ($S_\alpha = +1$ is "up" and $S_\alpha = -1$ is down). The Hamiltonion for the system is conventionally written as

$$H = -J\sum_{\langle\alpha\beta\rangle} S_\alpha S_\beta - B\sum_\alpha S_\alpha \tag{16}$$

where the notation $\langle\alpha\beta\rangle$ is understood as the sum over nearest neighbour pair of spin, J is the coupling strength constant, B is the external magnetic field.

Interest of the system is on the thermodynamic properties such as the magnetization.

$$M = \sum_s w(S)(\sum_\alpha S_\alpha) \tag{17}$$

the susceptibility

$$\chi = \sum_s w(S)(\sum_\alpha S_\alpha)^2 - M^2 \tag{18}$$

the energy

$$E = \sum_s w(S)H(S) \tag{19}$$

and the specific heat at constant field

$$C_B = \sum_s w(S)H^2(S) - E^2 \tag{20}$$

and where :

$$w(S) = \frac{e^{-H(S)}}{Z} \tag{21}$$

Z is the partition function:

$$Z(J,B) = \sum_S e^{-H(S)} \tag{22}$$

The ising model is soluable in the limit of $N_{x,y} \rightarrow \infty$
For B= 0 in this limit, the energy is given by

$$E = -N_s J(\coth 2J)(1 + \frac{2}{\pi}\kappa' K_1(\kappa)) \tag{23}$$

the specific heat is :

$$C_B = N_S \frac{2}{\pi}(J \coth 2J)^2 (2K_1(\kappa) - 2E_1(\kappa) - (1-\kappa')\left[\frac{\pi}{2} + \kappa' K_1(\kappa)\right] \tag{24}$$

While the magnetization is given:

$$M = \pm N_S \frac{(1+z^2)^{1/4}(1-6z^2+z^4)^{1/8}}{(1-z^2)^{1/2}} \tag{25}$$

for $J > J_c$ and varushes for $J < J_c$. In these expressions

$$\kappa = 2\frac{\sinh 2J}{\cosh\ 2J} \leq 1, \kappa' = 2\tanh^2 2J - 1 \text{ and } z = e^{-2J}. \tag{26}$$

Figure 3 ilustrates the results of the Monte Carlo calculations good behaviors has been shown from the result of these calculations Monte Carlo methods have also been extensively used in neutronic calculations.

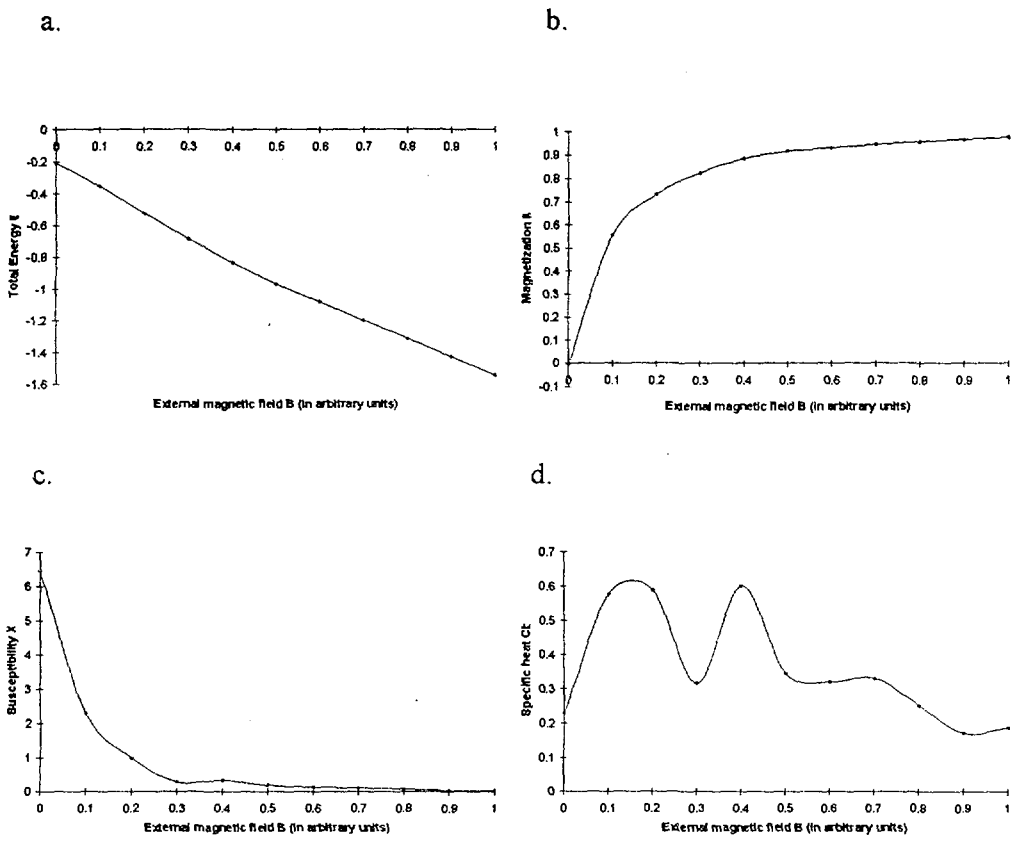

Figure 3. Total energy, Magnetization, Susceptibility and Specific heat as function of B.

CONCLUSIONS

In conclusions we have demonstrated the potensial method of the Monte Carlo technique to physical system that otherwise could not be possible to compute using conventional procedure.

REFERENCE

1. DAVIDOV, A.S., *"Quantum Mechanics"*, Pergamon Press, London 1965

2. HOOGENBOOM, J.E.. *"Adpoint Monte Carlo Methods in Neutron Transport Calculations"*, Delft University Press, Delft 1977

3. BOL, W. *"Monte Carlo Simulations of Fluid Systems with Waterlike Molecules"*, doctoral thesis, Technische Hogeschool, Eindoven 1979

4. KONIN, STEVEN *"Computational Physics"*, Addison - Wesley Publ. Comp. Inc, N.Y. 1986

5. KRANENDONK, W. *"Computer Simulations of Models for Colloidal Systems"*, doctoral thesis, University of Utrecht, 1990

6. SANTOSO, BUDI *"Monte Carlo Methods in Quantum Energy Bounds Variational Calculations"*, Proceedings, Institut Teknologi Bandung, vol. 25, no 1, 1993

7. HUANG, H. *"Statistical Mechanics"* John Wiley and Sons, New York, 1963

8. FLANNERG, BRIAN P. ; TEUKOLSKY, SAUL A.; VETTERLING, WILLIAM T., *"Numerical Recipes, The Art of Scientific Computing, William H. Press"* Press Syndicate of the University of Cambridge, 1986