Chapter 5

MATHEMATICAL SIMULATION MONTE CARLO

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5.1 INTRODUCTION

In many situations, the physical phenomena under investigation can be described by a mathematical formula in the form of an integral, a linear system of equations, a differential equation, or an integral equation. In this case it becomes possible to directly solve the mathematical description of the problem accounting for different boundary and initial conditions. The Monte Carlo method in this case would solve the formulated mathematical problem rather than attempting the solution in an analog fashion. It should be expected in general that a mathematical formulation would lead to a more efficient solution of the problem by the fact that more information and knowledge are injected into the solution.

Instead of using a direct analog simulation of needle dropping like in the Pascal's solution to the Buffon Needle's problem, or dart throwing at a board, we use the method of integral calculus to derive a mathematical description to the value of π in the form of an integral. The mathematical expression is then used in conjunction with a Monte Carlo estimator, to estimate its value.

The validity of a mathematical versus an analog simulation in different applications is discussed in terms of the Knudsen Number.

5.2 MATHEMATICAL FORMULATION

Considering the quadrant of radius R shown in Fig. 1, an element of area dA can be expressed as:

$$dA = ydx. \quad (1)$$

Integrating over x, the area of the quadrant is:

$$A = \int dA = \int ydx \quad (2)$$

Using the Pythagorean Theorem, and substituting the limits of integration over x from 0 to the radius R, we get for the area of the quadrant:

$$A = \int_0^R (R^2 - x^2)^{1/2} dx \quad (3)$$

Substituting for the area of the quadrant as:

$$A = \frac{\pi R^2}{4}, \tag{4}$$

in Eqn. 3, we get:

$$\frac{\pi R^2}{4} = \int_0^R (R^2 - x^2)^{1/2}\, dx \tag{5}$$

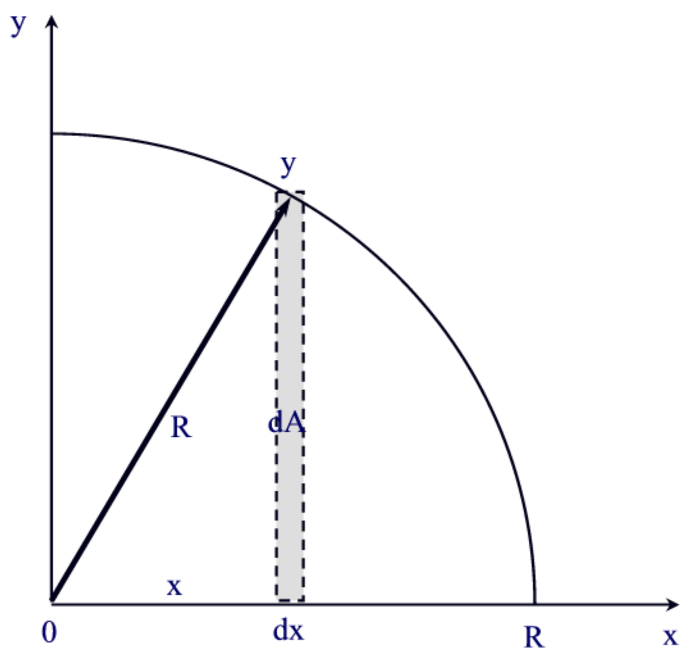

Figure 1. Geometrical model for the integral calculus expression of π.

One can then estimate the value of π from the mathematical expression:

$$\pi = \frac{4}{R^2}\int_0^R (R^2 - x^2)^{1/2}\, dx \tag{6}$$

5.3 MONTE CARLO ESTIMATORS

A simplified form of Eqn. 6 can be used by substituting R = 1 as:

$$\pi = 4\int_0^1 (1 - x^2)^{1/2}\, dx, \tag{7}$$

which is an integral over the unit interval to be used to estimate the value of π.

A flow diagram of the process is shown in Fig. 2. It shows a structure that is much simpler than in the case of direct analog simulation.

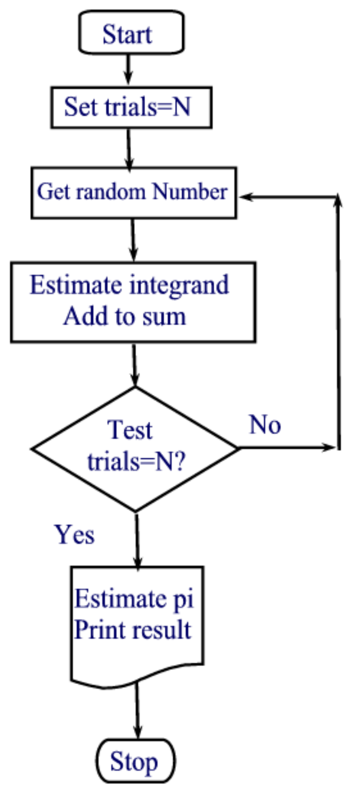

Figure 2. Flow Chart for estimating π using a finite integral.

For pseudo-random numbers ρ_i uniformly distributed over the interval [0, 1]:

$$\rho_i \in [0,1]$$

the positions x_i are taken as:

$$x_i = \rho_i, \; i = 1, 2, ..., N \tag{8}$$

A Monte Carlo "estimator" for the value of π becomes:

$$\mu_\pi = 4\left(\frac{\sum_{i=1}^{N} (1 - x_i^2)^{1/2}}{N} \right) \tag{9}$$

Similar estimators can be written to estimate the higher moments of the distribution. These would allow the estimation of other statistical parameters such as the variance, the coefficient of kurtosis, and confidence intervals.

The solution algorithm becomes much simpler than the algorithms using analog Monte Carlo, and the programming of the procedure becomes also simpler as shown in Fig. 3. A single call to the pseudorandom number generator is needed to provide a sampled value of x for an estimation of the integrand. The process is repeated N times, and the average value of the integrand constitutes its estimate.

```
!	mathematical_monte_carlo for
!	Mathematical Monte Carlo
!	Estimation of the value of pi using Mathematical Monte Carlo
!	M. Ragheb
	program mathematical_monte_carlo
	real(8) mean,f,score,x
	integer trials
	real :: xtrials=1.0E+03
!	Define sampled function, integral is from 0 to 1
	g(x) = dsqrt(1.0-x*x)
!	Initialize score
	score = 0.0
!	Sample points on unit
	trials = xtrials
	do i=1,trials
		call random(rr)
		f=g(rr)
		score =score + f
	end do
!	Estimate mean value
	mean=4.0*(score/xtrials)
!	Write results
	write(*,*) mean, trials
	end
```

Figure 3. Procedure for the estimation of π through Monte Carlo estimation of integral.

Table 1 provides a comparison of the estimated of π carried out by Laplace's Buffon needle problem, the darts throwing algorithm, and the integral estimation of π. It can be observed that the analog approach requires a larger number of histories to sample the whole space and start capturing the correct value of π. At the larger number of histories the two approaches estimate the value of π to the same degree of accuracy.

Table 1. Comparison of estimates of the value of π, for different numbers of histories N.

Number of trials,	Estimate of π	Estimate of π	Estimate of π

N	Laplace's Buffon Needle Monte Carlo	Darts throwing, Analog Monte Carlo.	Integral Estimation Monte Carlo.
10^1	4.999999	2.8000000	3.155703
10^2	3.703704	3.3200000	3.108870
10^3	3.194888	3.1480000	3.139951
10^4	3.193868	3.1344000	3.139084
10^5	3.147326	3.1474000	3.143803
10^6	3.138978	3.1442680	3.142643
10^7	3.140663	3.1425804	3.142193
10^8	3.141302	3.1416612	3.141712
10^9	3.141682	3.1416093	3.141627

5.4 VALIDITY OF MATHEMATICAL AND ANALOG APPROACHES, THE KNUDSEN NUMBER

Even though the mathematical approach to Monte Carlo is simple, elegant and attractive, one must be extremely cautious that the formulation must be physically valid. This is another software engineering gigo (garbage in, garbage out) trap. No amount of simulations will lead to a meaningful result, unless the formulation of the problem is valid in the first place.

Usually a mathematical formulation entails an ensemble average of the behavior of the individual components involved in the simulation: photons, electrons, atoms, ions, molecules, neutrons, cars in traffic, investors, or bacteria. Under some conditions, using these ensemble averages are totally invalid, leading to simulation results that are totally meaningless, and an analog approach using the individuals particles or individuals is mandated to obtain valid results.

As an example, if we consider that the flow of a gas or a fluid is a continuum, a mathematical description in terms of the Navier-Stokes equations is totally valid. If the fluid cannot be considered as a continuum, then an analog approach considering the discrete individual molecules making up the fluid, or aggregates of them is necessary to obtain meaningful results.

If the fluid is contained in a region of characteristic length L, and if λ is the mean free path of a fluid molecule, then the dimensionless Knudsen number:

$$K_n = \frac{\lambda}{L}, \qquad (10)$$

determines whether the continuum of particles description is the appropriate approach or not. The characteristic length L could be for instance the diameter of a pipe, or the geometrical dimension of a cavity containing the fluid such as the poloidal radius of a Tokamak or a Stellarator fusion plasma.

In general, if:

$$K_n \geq 0.1, \tag{11}$$

then the continuum description breaks down and the discrete nature of the fluid becomes important. That is to say that if the mean free path is larger than one tenth the characteristic dimension of the enclosure:

$$\lambda \geq \frac{L}{10} \tag{12}$$

then an analog simulation is mandated.

At atmospheric pressure in air, the mean free path of the nitrogen and oxygen molecules is:

$$\lambda_{molecules} \approx 50 \times 10^{-9} [m],$$

which is comparable to the wavelength of light. The dimension of the atmosphere is a few kilometers with:

$$L_{atmosphere} \approx 10 \times 10^{3} [m],$$

leading to a Knudsen number:

$$K_n \approx \frac{50 \times 10^{-9}}{10 \times 10^{3}} = 5 \times 10^{-12} < 0.1$$

So, for most applications, the atmosphere can be adequately described as a continuum using the Navier-Stokes equations.

On the other hand, the gap between the head and the platter of a disk drive is:

$$L_{gap} \approx 50 \times 10^{-9} [m],$$

meaning that:

$$K_n \approx \frac{50 \times 10^{-9}}{50 \times 10^{-9}} = 1 > 0.1,$$

necessitating a particle description of the problem.

Another application is to space vehicles in the upper atmosphere. The mean free path of air molecules increases with height above the surface of the Earth where the air is more rarefied than at the surface. The space shuttle enters the atmosphere at an altitude of about 120 km, developing a bow shock wave in front of its nose cone. At this altitude the mean free path of an air molecule is a few meters:

$$\lambda_{\substack{molecules \\ upper\,atmosphere}} \approx 10[m]$$

And the size of the space ship is also of the order of meters:

$$L_{spaceship} = 10[m]$$

Hence the Knudsen Number can be estimated as:

$$K_n = \frac{10}{10} = 1 > 0.1,$$

and the continuum approach is no more adequate to model the shock wave and must be replaced by a particle approach.

In the simulation of fusion plasmas, the ions and electrons may have a mean free path larger than the size of the evacuated enclosure. In this case the use of the techniques of Molecular Dynamics (MD) or Direct Simulation Monte Carlo (DSMC) are mandated for a meaningful analysis of the problem.

5.5 CONCLUSIONS

Analog simulations are not the only approach to the application of Monte Carlo method. Whenever a mathematical description of the problem can be obtained as an integral, a linear system of equations, a differential equation, or an integral equation, this should be tried. The result can be expected to lead to a simpler algorithm that is easier to program on a computational platform. In addition, for a small number of simulations, the mathematical approach should capture the solution earlier than the analog approach.

In general, injection of analytical knowledge into a Monte Carlo problem, whenever possible can always be expected to result in more effective solutions. A pitfall must here be avoided: the validity of a mathematical versus an analog simulation should always be checked in terms of the Knudsen number before embarking on a major simulation of a physical system.

EXERCISES

1. Derive an "estimator", then write a Monte Carlo procedure that estimates the value of π using the integral:

$$\pi = 4\int_0^1 \frac{1}{1+x^2}dx$$

Plot the estimated value of π and its absolute relative deviation as a function of the number of trials N.

2. Apply the Knudsen criterion to examples from your respective fields of interest, e. g. plasmas, heat transfer, fluid flow, electron transport, electromagnetism, gamma and

neutron transport, to decide whether an analog microscopic or a mathematical macroscopic description of a potential simulation is the most appropriate approach to be adopted.