Introduction to Monte Carlo Methods

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An Introduction to Monte Carlo Methods

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Abstract

Monte Carlo computer programming is becoming increasingly popular to those who use it, due to the ease with which complex problems may be formulated and solved. However, the growth of MC programming for small projects is inhibited by a frequent misconception of difficulty, inferred from the high level of complexity of problems solved in High Energy and Nuclear Physics using MC methods. In addition, few students of science and engineering are receiving exposure to the basic issues involved in the Monte Carlo process despite the ease with which MC can be used to solve classical physics problems, especially those problems with little symmetry or unusual geometry. Few upper-division or graduate students have begun to exploit this approach, even in research projects. Thus, an introduction to Monte Carlo methods would be valuable, even for the beginning science or engineering student. The present work introduces integration of area and volume, then expands this effort to include surface and volume integrals of scalar and vector functions. Next, integration over unusual geometries introduces programs which convert the geometries defined by CAD (Computer Aided Design) to geometries convenient to the Monte Carlo process. Finally, Gauss's Law uses MC to calculate the size of an asymmetrically positioned charge and a classic example from Sir Isaac Newton uses MC to calculate the effect of a spherically symmetric shell of mass on an exterior field point where the average force components (F_x, F_y, F_z) are calculated. These final examples introduce singularities and convergence problems arising in the Monte Carlo averaging process.

Introduction

Monte Carlo programming would be growing faster today if it were not for the frequent misconception of difficulty inferred from exposure to the huge Monte Carlo programs used to solve problems in High Energy and Nuclear Physics. Examples include complex Monte Carlo modeling programs like GEANT (Roetzel and Braithwaite, 1993) or the need for optimizing parallel computing for MC problems (Byrd et al., 1993). This misconception inhibits the growth of MC programming, which can be extremely useful for much smaller projects than those encountered in High Energy and Nuclear Physics.

Despite these inhibition to newcomers, Monte Carlo computer programming is becoming increasingly popular to its frequent users, due to the ease with which fairly complex problems may be formulated and solved for numerical answers. In many instances, calculational demands of MC are so slight that spreadsheet programming is sufficient to formulate a problem. However, few students of science and engineering receive early exposure to the basic issues involved in the Monte Carlo process. Indeed, upper-division and graduate research projects could be enhanced by using MC, making the introduction to Monte Carlo methods in some tangible examples desirable for beginning science and engineering students (Buslenko et al., 1966; Hammersley and Handscomb, 1986).

Monte Carlo integration has been chosen as the process for introducing Monte Carlo methods, as MC algorithms are useful in solving integral equations (Sabelfield, 1991; Mikhailov, 1992). For applications like integration, the Monte Carlo approach is an averaging process using random numbers to sample the space being integrated. Despite its random nature, the MC averaging process must be set up so as to uniformly sample the space (or domain) being integrated. It is worth noting the Monte Carlo averaging process, as it applies to integration, converges asymptotically ($N \to \infty$) to the exact solution.

The simplest example presented is the calculation of the ratio of the area of a circle inscribed in a square to the area of the square. The ratio, Area(Circle) / Area(Square), is $\pi/4 \approx 0.7854$. The inscribed circle is shown in Fig 1a with Fig. 1b showing 200 (x, y) points each chosen randomly for sampling the square. The procedure used to integrate the area of the circle in units of the square (in which it is inscribed) is to count the number of points falling within the circle (N_{hits}), then divide by the total number of points sampling the square (N_{total}). The ratio N_{hits}/N_{total} is the same as the ratio of areas, Area(Circle) / Area(Square), provided the coordinate pairs of random numbers uniformly sample the square as $N \to \infty$.

The (x, y) points chosen to sample the square come

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from random number pairs each chosen between (-1, +1). Despite expectations that these random (x, y) point-pairs uniformly sample the square as $N \rightarrow \infty$, a small sampling group (like the one in Fig. 1b) looks "spotty" to everyone. How large a sample is needed for the Monte Carlo process to converge to useful results? This important question of convergence is answered qualitatively by repeating the random (x, y) point selection process several more times to see if it reduces the apparent spottiness of the sampling process.
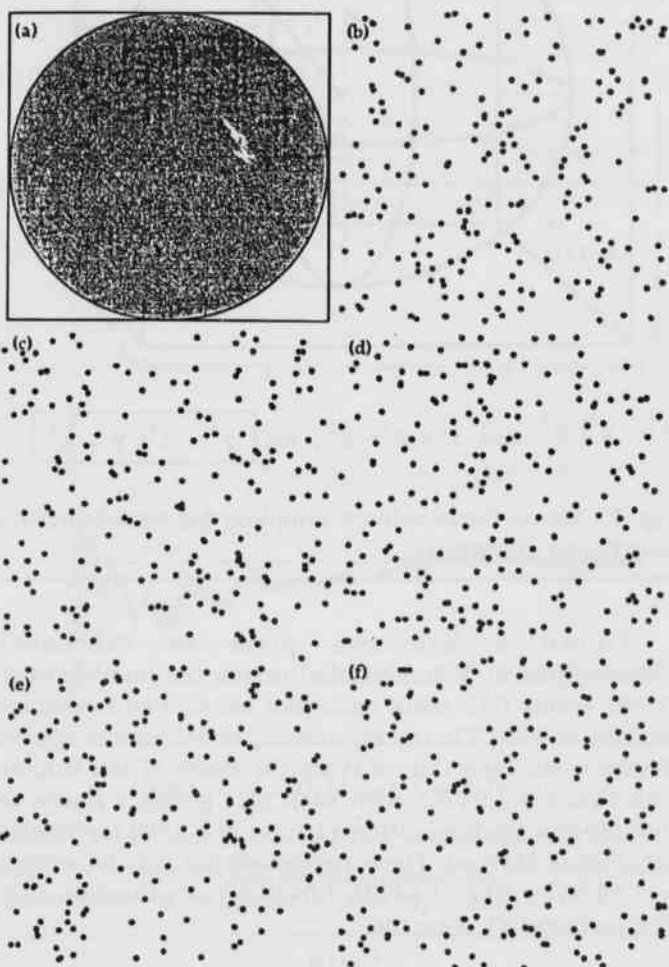

Fig. 1. (a) A "target" Circle is inscribed within a square. (b-f) Five sets of 200 2-D Monte Carlo samplings of the area of the square.

Figure 1c,d,e,f provides graphs showing four additional distinct groups of 200 random (x, y) points where all five groups of 200 points and the "target" circle inscribed within a square (shown in Fig. 1) may be copied to transparencies (with enlargement) and progressively laid one above the other. This progression shows a reduc-
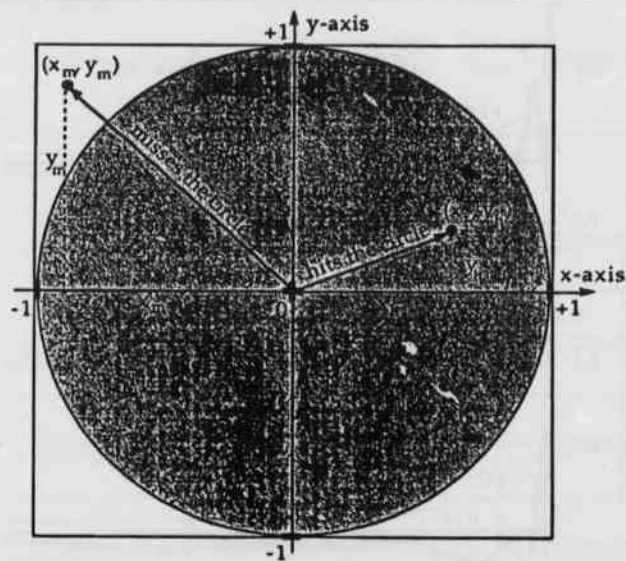
tion of the "spotty" appearance every time the sampling is increased by 200 events. This sampling increase may be accomplished by placing each successive transparency containing 200 events on top of the transparency showing the target circle inscribed in a square.

Fig. 2. Monte Carlo "target" area sampling for visualizing the integration of a circle.

The area of the square is chosen as 2x2=4, where all (N_{total}) of the (x, y) random number pairs fall within the area of the square, randomly and uniformly sampling the area of the square. Two plots of the ratio Area(Circle) / Area(Square) versus the number of 2-D MC samples are shown in Fig. 3. Most (x, y) points sampling the square also fall within the circle where the Pythagorean Theorem is used to test the "hit" or "miss" status of each (x, y) point. The test is whether $x^2 + y^2 < 1$, if successful, N_{hits} is incremented. The ratio of the area of the inscribed circle to the square is given by:

$$\frac{\text{Area(Circle)}}{\text{Area(Square)}} = \frac{N_{hits}}{N_{hits} + N_{misses}} = \frac{N_{hits}}{N_{total}} \rightarrow \frac{\pi(1)^2}{4} = \frac{\pi}{4} \approx 0.7854.$$

Figures 3 addresses convergence graphically by showing two envelopes labeled as $\pm 1\sigma$. These two envelopes show one standard deviation on each side of the mean (of $\pi/4 = 0.7854$) with the figure of merit being the event fraction lying within $\pm 1\sigma$ (.693 as $N \rightarrow \infty$). The statistical theory of binomial sampling provides formulas for these two $\pm 1\sigma$ envelopes as a function of 2-D samples (N): $0.7854(1\pm\sqrt{(1 - 0.7854)/.7854\,N})$.

The next example of Monte Carlo integration is the calculation of the volume of a sphere inscribed within a cube. All (x, y, z) points fall within the cube with only

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about half of these points falling within the sphere. Analytically, the volume of a sphere is calculated to be $\pi/3$ (≈ 1.0472) times larger than half the volume of the cube.
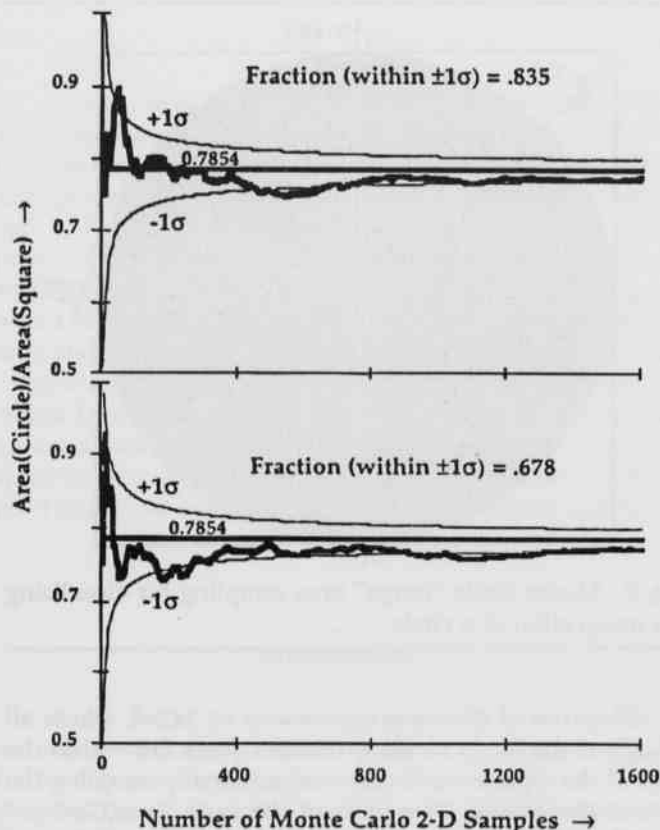

Fig. 3. A Monte Carlo calculation of the area of a circle (inscribed within a square) to the area of the square, as a function of the number of (x, y) samples.

The drawing in Fig. 4 shows an example of an (x, y, z) point on the target sphere. This target picture of the sphere is useful in visualizing the test for integration of a spherical volume by Monte Carlo averaging. The status of each (x, y, z) point is tested using the 3-D Pythagorean Theorem (developed in Fig. 4). This test asks the question: Is $r^2 = x^2 + y^2 + z^2 < 1$? A "yes" is a "hit" within the sphere.

To calculate a volume using Monte Carlo, consider a sampling of (x, y, z) random-triplets, where each is viewed as a coordinate point within the cube. Large numbers of (x, y, z) random triplets are used to uniformly sample the cube; this sampling is used to extract the volume of the sphere inscribed within this cube.

The increasingly uniform sampling of a square with increasing sample size, using (x, y) random pairs, was seen in the 2-D example presented above. Convergence in

this earlier 2-D work is reassuring to a new MC user as it relates to the 3-D problem; it corresponds to examining each face of the cube from a position of normal incidence.

$$\rho^2 = x^2 + y^2 \quad \text{and} \quad r^2 = \rho^2 + z^2, \text{ so:} \quad \boxed{r^2 = x^2 + y^2 + z^2}$$
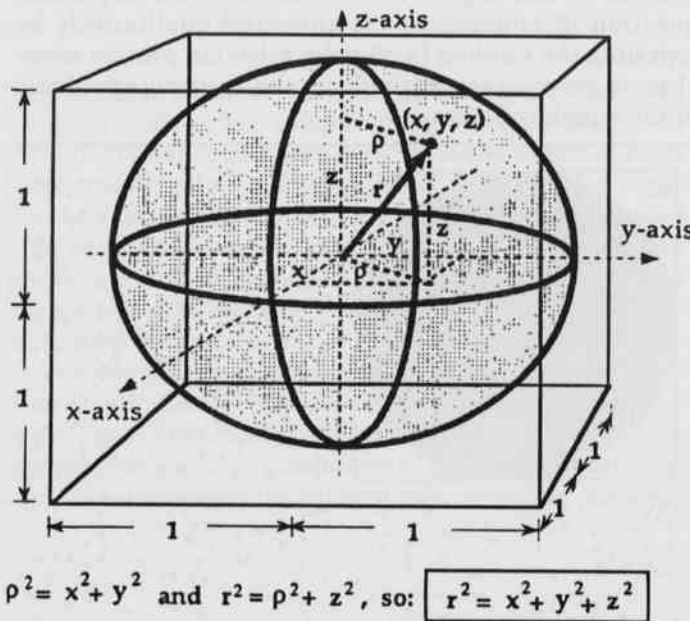
Fig. 4. Monte Carlo volume sampling for visualizing the integration of a sphere.

Figure 5 has two plots of calculated Volume(Sphere)/Volume(Cube) versus the number of 3-D MC events (N). Also, each plot shows two envelopes labeled at $\pm 1\sigma$. These two envelopes are one standard deviation on each side of twice the mean of the volume ratios ($\pi/3 = 1.0472$), with each plot giving a figure of merit (event fraction within $\pm 1\sigma$) for N = 1600 (approaching .693 as N $\rightarrow \infty$). These two envelopes may be written as $1.0472(1 \pm \sqrt{(2 - 1.0472)/1.0472 N})$ as a function of 3-D samplings (N). Note the

$$\frac{\text{Volume(Sphere)}}{\text{Volume(Cube)}} = \frac{N_{hit}}{N_{total}} \rightarrow \frac{\frac{4}{3}\pi(1)^3}{8} = \frac{1}{2}\frac{\pi}{3} = \frac{1}{2}(1.0472...) \approx 50\%.$$

This second example uses a spreadsheet with graphics to calculate 1600 volume samplings of the cube. Figure 6 displays a matrix of 20 distinct MC calculations of the volume of the sphere versus N [the number of (x, y, z) triplets of random samples]. Each plot has two envelopes indicating one standard deviation from $\pi/3$ as a function of N. The number in each calculation is the figure of merit indicating the event fraction lying within this ± 1 standard deviation for each set of 1600 samples.

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Figure 6 shows the large variation in MC predictions for repeated calculations as a function of N. Envelopes of $\pm 1\sigma$ generally show the convergent trend as the number N (of 3-D MC events) increases to 1600. Despite this convergent trend, large variations are observed in repeated calculations of volume as the calculation process is repeated over-and-over; each calculation could be available graphically in seconds using modern Workstations.
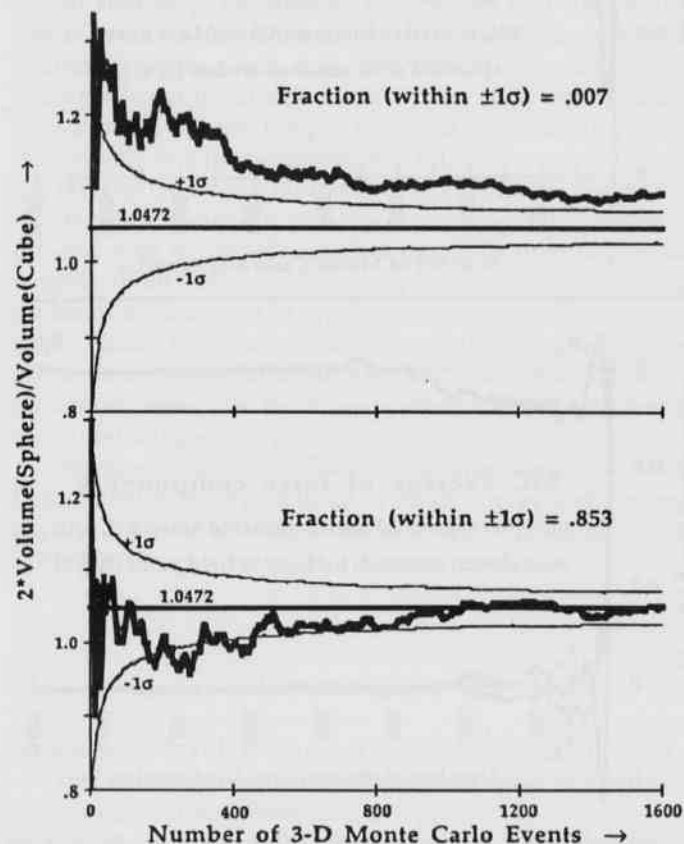

Fig. 5. A MC calculation of the volume of the sphere inscribed within a cube to the volume of the cube as a function of N, the number of (x, y, z) samples.

Results and Discussion

Integration of area may be expanded to include surface integrals of scalar and vector functions. First consider integrating a scalar function f(x, y) over a circle (inscribed within a square) using MC. Little change in procedure is needed from that used to integrate the area of the circle. For each "hit" (defined above) form a running sum of the evaluated $f(x_h, y_h)$, but ignore the sum for a "miss." If a spreadsheet like EXCEL is used, the logical IF statement is a function subroutine which returns a 1 (true) or a 0 (false) which can be multiplied by the func-

tion f(x, y) for R2 <1 [R2 = r^2 = $x^2 + y^2$]. Using a statement like S2=S1+ IF(R2<1,1,0)*f(x, y), effectively removes it from the sum in the "fill-down" (S1 is 0). In FORTRAN an expression like sum = sum + $f(x_h, y_h)$ is evaluated for a "hit," but skipped over for a "miss" (with sum initially 0). In summary:

$$\iint f(x,y)\,dx\,dy = \text{average}[f(x_h,y_h)] \cdot A(\text{Circle}) \rightarrow \frac{\text{sum}}{N_{hit}} \cdot \frac{N_{hit}}{N_{total}}\,\text{Area(Square)}.$$
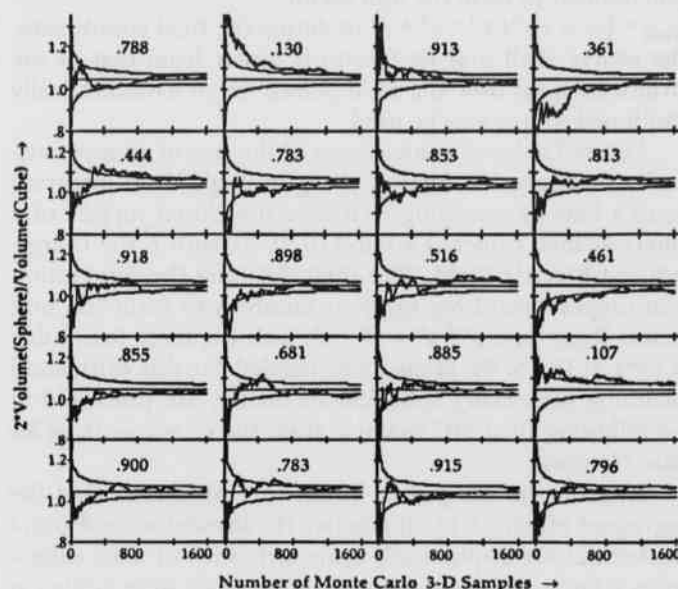

Fig. 6. 20 spherical-volume calculations each with two $\pm\sigma$ envelopes as a function of N and the event fraction lying within $\pm\sigma$ at N=1600 (asymptotically .683).

Similarly, integration of volume can be expanded to include surface or volume integrals of scalar and vector functions. First consider integrating the function f(x, y, z) over the sphere (inscribed within a cube) using MC with little change in procedure from that used to integrate the volume of the sphere. In similar fashion to the integral of the 2-D f(x, y) outlined above for each 3-D "hit," form a running sum of the evaluated function $f(x_h, y_h, z_h)$, but ignore the sum for a "miss." Spreadsheet and FORTRAN procedures are essentially the same as outlined for the 2-D integral above. In summary:

$$\iiint f(x,y,z)\,dx\,dy\,dz = \text{average}[f(s_h,y_h,z_h)] \cdot \text{Vol(Sphere)} \rightarrow \frac{\text{sum}}{N_{hit}} \cdot \frac{N_{hit}}{N_{total}}\,\text{Vol(Cube)}.$$

Integration of a function over an unusual volume, such as a closed "teapot" in a rectangular box, would follow similar procedures once the MC geometry is defined. Programs are available for converting CAD (Computer Aided Design)

geometries to geometries to geometries convenient to Monte Carlo (Cloth and Sterzenbach, 1993). An example of this type of program is OCTAGON (Dragovitsch et al., 1992), a program for converting CAD geometries defined in the drawing of High Energy Physics detector elements to geometries compatible with CERN's Monte Carlo detector modeling (GEANT, 1994).

Gauss' Law may be used with MC where the field point is replaced by another spherical shell which is used to define the surface integral over a sphere. This shell uses three random number to form the unit vector: $\vec{R}_{field} = (x, y, z)/\sqrt{x^2 + y^2 + z^2}$ to define the field coordinates. The source shell may be taken off center from that of the surface integral over the field-points, or an asymmetrically positioned source may be used.

Figure 7a shows a calculation of the size of an asymmetrically positioned source of charge using MC to integrate Gauss's Law by averaging $\vec{E} \cdot \hat{n}$ over the closed surface of a spherical shell centered around (0, 0, 0), with $\vec{E}$ the charge-induced Electric Field. The shell defining the integration coordinates uses three random numbers to form the unit vector: $\vec{R}_{field}=(x,y,z)/\sqrt{x^2 + y^2 + z^2}$, with the force found due to Q=1 at (0, .5, 0). Many ideas needed for this calculation including preserving spherical symmetry, are presented in the following final MC example from the classic work of Sir Isaac Newton.

Newton was obliged to invent the calculus to find the aggregate effect of earth's mass. He showed a field point located outside a spherically symmetric shell of mass experiences a force as though the mass of the shell were located at its symmetry center, with the net force being zero for a field point located inside the spherical shell of mass.

The shell providing the source of mass is defined using three random numbers $\vec{R}_{source} = r*(x,y,z)/\sqrt{x^2 + y^2 + z^2}$, where (the scalar) r is the distance of the source shell from its symmetry center. Spherical symmetry is preserved in the MC 3-D sampling of $\vec{R}_{source}$ provided only random number triplets with $x^2 + y^2 + z^2 < 1$ are used. The field point is located *outside* the shell for r < 1, and MC sampling of $1/|\vec{R}_{source} - \vec{R}_{field}|^2$ converges to 1, provided a sufficiently large MC sampling is taken when "r" is near one. The vector integral is calculated for the force (F_x, F_y, F_z). Figure 7b shows results of a spreadsheet calculation of each force component (for G=1) when the unit-vector field point is taken along the axis $\vec{R}_{field}$ = (0, 1, 0), (0, 1, 0). The fixed field point is easily changed to any of these three unit vectors or to any other (x, y, z) unit-vector.

The graph for any force component may be presented in a different color on a computer display, so changing the unit vector field assignment to another coordinate axis changes the color of the force component averaging to 1, with color of the graph of the original force component now averaging to 0 (along with a third graph). The display will change when any other arbitrary unit vector field point is chosen such as:

$(1,1,1)/\sqrt{3}$. In this case all 3 components converge (as N increases) to the same value.
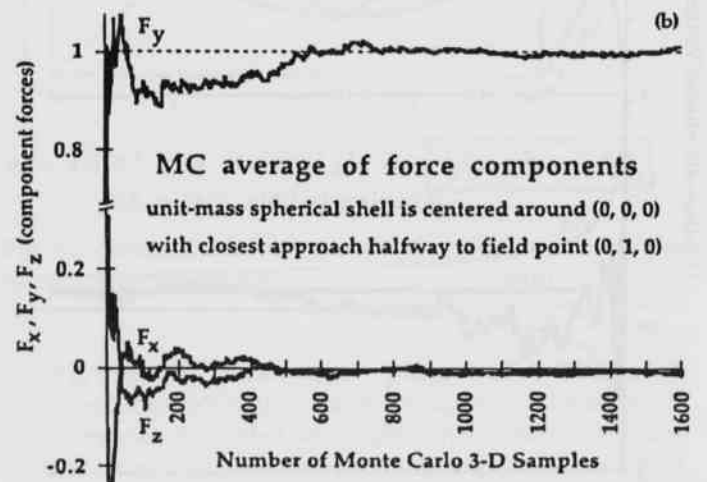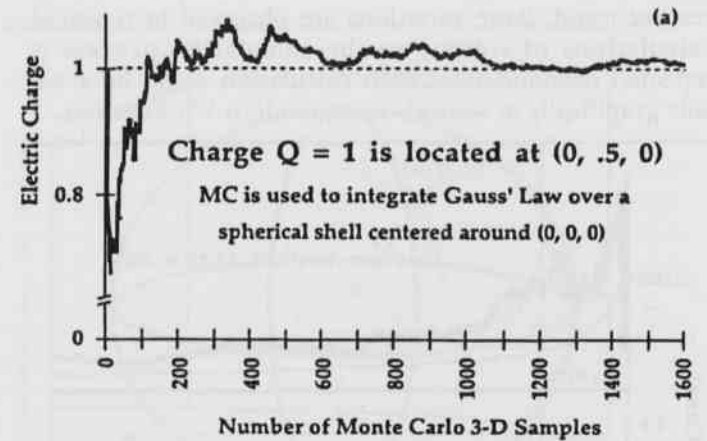

(a)

Charge Q = 1 is located at (0, .5, 0)

MC is used to integrate Gauss' Law over a spherical shell centered around (0, 0, 0)

Number of Monte Carlo 3-D Samples

(b)

MC average of force components

unit-mass spherical shell is centered around (0, 0, 0) with closest approach halfway to field point (0, 1, 0)

Number of Monte Carlo 3-D Samples

Fig. 7. (a) MC is used to integrate Gauss' Law by averaging $\vec{E} \cdot \hat{n}$ over a spherical shell. $\vec{E}$ is due to a unit charge located off-center from the spherical shell. (b) MC averaging provides the vector integral of the force (F_x, F_y, F_z) at the field point (0, 1, 0) due to a spherically symmetric unit-mass shell at r = 0.5.

To appreciate the problem of convergence, consider r=1 where the MC weighting term is singular, as $|\vec{R}_{source} - \vec{R}_{field}|^2 \rightarrow 0$ at closest approach of source to the field point so the MC calculation cannot converge. At r = 0.90, the closest approach point of the source shell (of mass) is 0.1, and the weighting term in the MC is 100. In contrast, weighting for force contributions from the far side of the source shell is ≈ 0.277, about 400 times smaller. This means that for r = 0.9 (or 1.1) a sampling of 1600 MC triplets is insufficient and a

much larger value of N must be used. Students are asked to estimate how many MC samplings are needed of r = 0.95 and for r = 0.99, etc. This example allows students the opportunity to explore near singularities and their effect on the convergence of the Monte Carlo averaging process. Rough estimates are useful in determining N, the number of MC samplings which will be sufficient to assure reasonable convergence; for r = 0.9 a safe but unduly large estimate of N is 100*1600.

In summary, the present work shows that the calculational demands of Monte Carlo methods for many simple problems are so slight that spreadsheet programming is often sufficient to provide useful results (e.g., when evaluating surface or volume integrals of scalar or vector functions). An example of a near-singularity in MC was presented where the remedy requires a substantial increase in the number of MC samples. Examples presented above were indicative of the ease with which MC calculations can be used to provide tangible results when solving many science and engineering problems encountered in upper division or graduate coursework. Monte Carlo methods can complement the formal mathematics by providing an easy way to arrive at a numerical answer, especially for those problems with little symmetry or unusual geometry.

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