



Particle transport: Monte Carlo methods versus moment equations

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What is the Monte Carlo method?

Monte Carlo methods have application in a broad array of fields. In this report, I'll focus on one application – particle transport at the atomic level, the foundation of our **GamBet** package for X-ray science. The fundamental issue is how to deal with extremely large numbers of objects. Calculating the history of every particle is beyond the capabilities of even the most powerful computers. Instead, we seek the average properties of large groups.

In the Monte Carlo method, the full set of particles is represented by a calculable set of model particles. In this case, each model particle represents a group. We follow detailed histories of model particles as they undergo random events like collisions with atoms. Characteristically, we use a random-number generator with a known probability distribution to determine the outcomes of the events. In the end, the core assumption is that averages over model particles represent the average behavior of the entire group. The alternative to this approach is the derivation and solution of *moment* (or *transport*) equations. The following section covers this technique.

Instead of an abstract discussion, we'll address a specific example to illustrate the Monte Carlo method. Consider a random walk in a plane. As shown in Fig. 1, particles emerge from a source at the origin with uniform speed v_0 . They move freely over the surface unless they strike an obstacle. The figure represents the obstacles as circles of diameter w . The obstacles are distributed randomly and drift about so we can never be sure of their position. The velocity of obstacles is much smaller than v_0 . If a particle strikes an obstacle, we'll assume it bounces off at a random direction with no change in speed. The obstacles are unaffected by the collisions.

In a few sentences, we have set some important constraints on the physical model:

The nature of the particles (constant speed v_0).

The nature of the obstacles (diameter w , high mass compared to the particles),

The nature of the interaction (elastic collision with isotropic emission from the collision point)

The same type of considerations apply to calculations of radiation transport. The differences are that 1) the model particles have the properties of photons and electrons, 2) the obstacles are the atoms of materials and 3) there are more complex collision models based on experimental data and theory. To continue, we need to firm up the features of the calculation. Let's assume that 10^{10} particles are released at the origin at time $t = 0$. Clearly, there are

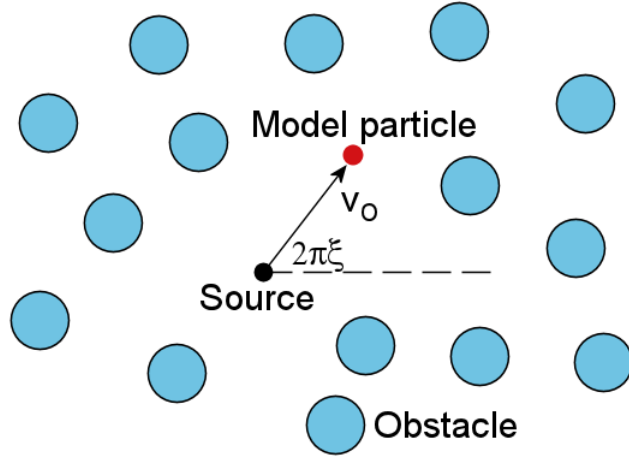


Figure 1: Random walk in a plane.

too many particles to handle on a computer. Instead, we start $N_p = 10,000$ model particles and assume that they will give a good idea of the average behavior. In this case, each model particle represent 10^6 real particles. We want to find the approximate distribution of particle positions after they make N_c collisions. The logic of a Monte Carlo calculation for this problem is straightforward. The first model particle starts from the origin moving in a random direction. We follow its history through N_c collisions and record its final position. We continue with the other $N_p - 1$ model particles and then interpret the resulting distribution of final positions.

The source position is $x = 0, y = 0$. To find the emission direction, we use a random number generator, a component of all programming languages and spreadsheets. Typically, the generator returns a random number ξ equally likely to occur anywhere over the interval

$$0.0 \leq \xi \leq 1.0. \quad (1)$$

Adjusting the range of values to span the range $0 \rightarrow 2\pi$, the initial unit direction vector is

$$u_x = \cos(2\pi\xi), \quad u_y = \sin(2\pi\xi). \quad (2)$$

The particle moves a distance a from its initial position and then has it first collision. The question is, how do we determine a ? It must be a random quantity because we are uncertain how the obstacles are lined up at any time. In this case, we seek the distribution of expectations that the particle has a collision at distance a , where the distance may range from 0 to ∞ . To answer the question, we'll make a brief excursion into probability theory.

Let $P(a)$ equal the probability that the particle moves a distance a without a collision with an object. By convention, a probability value of 0.0 corresponds to an impossible event and 1.0 indicates a certain event. Therefore, $P(0) = 1.0$ (there is no collision if the particle does not move) and $P(\infty) = 0.0$ (a particle traveling an infinite distance must encounter an object). We can calculate $P(a)$ from the construction of Fig. 2. The probability that a particle reaches $a + \Delta a$ equals the probability that the particle reaches a times the probability that it passes through the layer of thickness Δa without a collision. The second quantity equals 1.0 minus the probability of a collision.

To find the probability of a collision in the layer, consider a segment of height h . If the average surface density of obstacles is N particles/m², then the segment is expected to contain $Nh\Delta a$ obstacles. Each obstacle is a circle of diameter w . The distance range for an interaction with an obstacle is called the cross-section σ . In this case, we will associate the interaction width with the obstacle diameter, or $\sigma = w$. The fraction of the height of the segment obscured by obstacles is

$$F = \frac{N\sigma h\Delta a}{h} = N\sigma\Delta a. \quad (3)$$

The exit probability is given by

$$P(a + \Delta a) = P(a) \times (1 - F) = P(a) \times (1 - N\sigma\Delta a) \quad (4)$$

A first-order Taylor expansion

$$P(a + \Delta a) \cong P(a) + \frac{dP(a)}{da}\Delta a \quad (5)$$

leads to the equation

$$\frac{dP}{da} = -(n\sigma)P = -\Sigma P. \quad (6)$$

Equation 6 defines another useful quantity, the *macroscopic cross section* $\Sigma = n\sigma$ with dimensions m⁻¹. The solution of Eq. 6 is

$$P(a) = \exp[-n\sigma a] = \exp[-\Sigma a] = \exp\left[-\frac{a}{\lambda}\right]. \quad (7)$$

The new quantity is the mean free path, λ . It equals the average value of a for the probability distribution of Eq. 7. The ideas of cross section, macroscopic cross section and mean-free path are central to particle transport.

We can now solidify our procedure for a Monte Carlo calculation. The first step is to emit a particle at the origin in the direction determined by Eq. 2a. Then we move the particle forward a distance a consistent with the

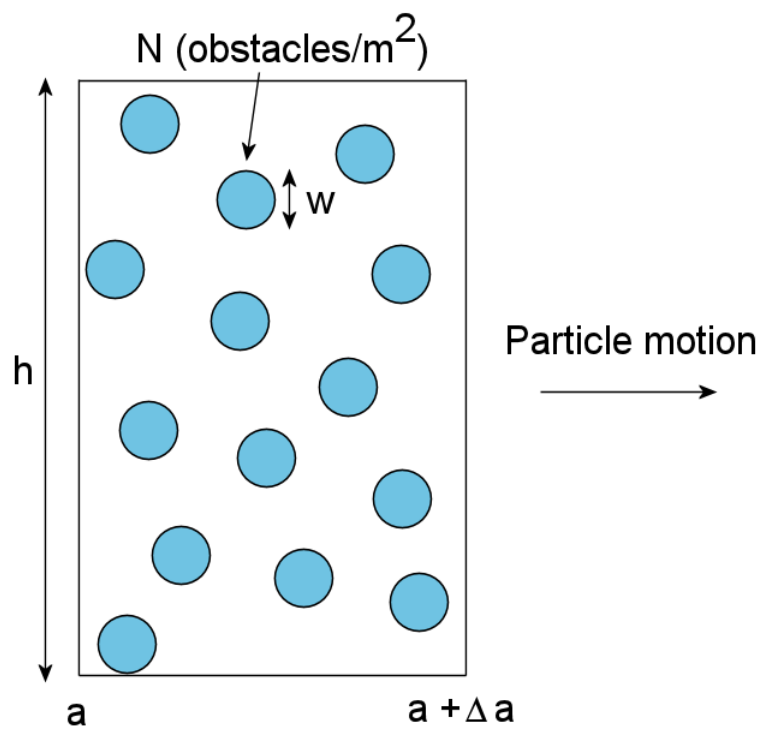


Figure 2: Probability of collision in a differential element.

probability function of Eq. 7. One practical question is, how do we create an exponential distribution with a random number generator that produces only a uniform distribution in the interval $0.0 \leq \xi \leq 1.0$? The plot of the probability distribution of Eq. 7 in Fig. 3a suggests a method. Consider the 10% of particles with collision probabilities between $P(0.3)$ and $P(0.4)$. The corresponding range of paths extends from $a(0.6)/\lambda = -\ln(0.4) = 0.9163$ to $-\ln(0.3) = 1.204$. If we assign path lengths from the uniform random variable according to

$$a = -\lambda \ln(\xi). \quad (8)$$

then we can be assured that on the average 10% will lie in the range $a/\lambda = 0.9163$ to 1.204 . By extension, if we apply the transformation of Eq. 8 to a uniform distribution, the resulting distribution will be exponential. To confirm, Fig. 3 shows a random distribution calculation with 5000 particles.

To continue the Monte Carlo procedure, we stop the particle at a collision point a distance a from the starting point determined by Eq. 8 and then generate a new random number ξ to determine the new direction according to Eq. 2. Another call to the random-number generator gives a new propagation distance a from Eq. 8. The particle is moved to the next collision point. After N_c events, we record the final position and start the next particle. The simple programming task with the choice $\lambda = 1$ is performed by the code excerpt shown in Table 1.

Figure 4 shows the results for $\lambda = 1$ (equivalently, the plot is scaled in units of mean-free-paths). The left-hand side shows the trajectories of 10 particles for $N_c = 100$ steps. With only a few particles, there are large statistical variations, making the distribution in angle skewed. We expect that the distribution will become more uniform as the number of particles increases because there is no preferred emission direction. The right-hand side is a plot of final positions for $N_p = 10,000$ particles. The distribution is relatively symmetric, clustered within roughly 15 mean-free-parts of the origin. In comparison, the average total distance traversed by each particle is 100.

Beyond the visual indication of Fig. 4b, we want quantitative information about how far particles move from the axis. To determine density as a function of radius, we divide the occupied region into radial shells of thickness Δr and count the number of final particle positions in each shell and divide by the area of the shell. Figure 5 shows the results. The circles indicate the relative density of particles in shells of width 0.8λ . Such a plot is called a *histogram* and the individual shells (containers) are called *bins*. Histograms are one of the primary methods of displaying Monte Carlo results. Note that the points follow a smooth variation at large radius, but that they have noticeable statistical variations at small radius. The reason is that the shells

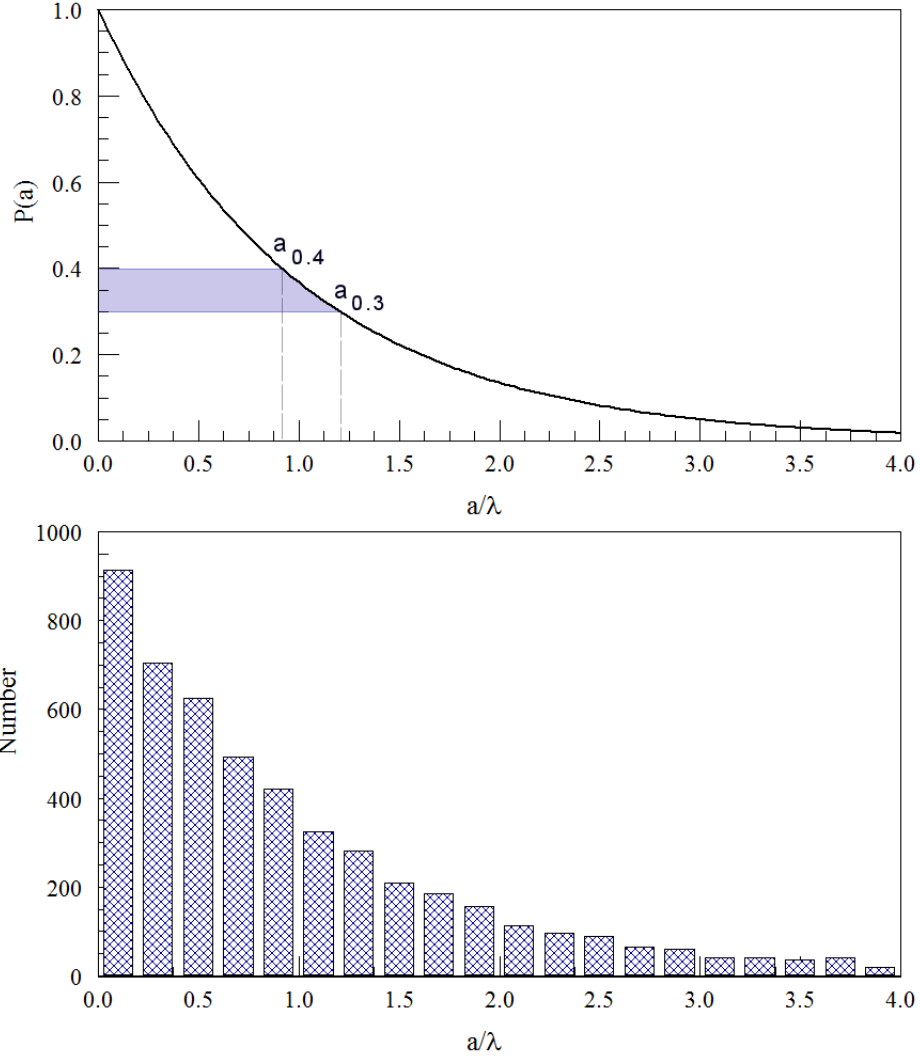


Figure 3: Exponential distribution. a) Relationship between intervals of $P(a)$ and a . b) Testing assignment of the collision distance, 5000 particles with a/λ assigned according to Eq. 8.

Table 1: Core code for a random walk in a plane

```

DO Np=1,NShower
! Start from center
  XOld = 0.0
  YOld = 0.0
! Loop over steps
  DO Nc=1,NStep
! Random direction
    CALL RANDOM_NUMBER(Xi)
    Angle = DTwoPi*Xi
! Random length
    CALL RANDOM_NUMBER(Xi)
    Length = -LOG(Xi)
! Add the vector
    X = XOld + Length*COS(Angle)
    Y = YOld + Length*SIN(Angle)
    XOld = X
    YOld = Y
  END DO
END DO

```

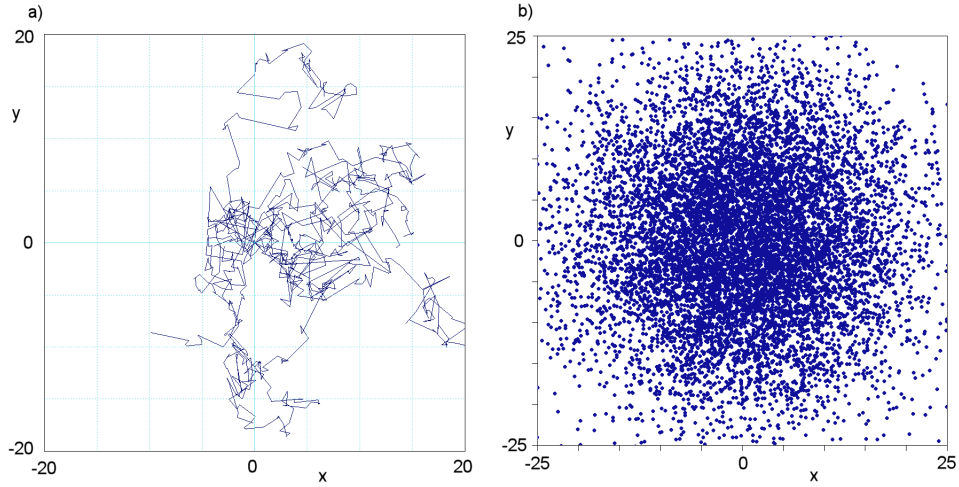


Figure 4: Random walk in a plane, $\lambda = 1$ and $N_c = 100$. *a)* Sample trajectories for 10 model particle trajectories. *b)* Final positions of 10,000 model particles.

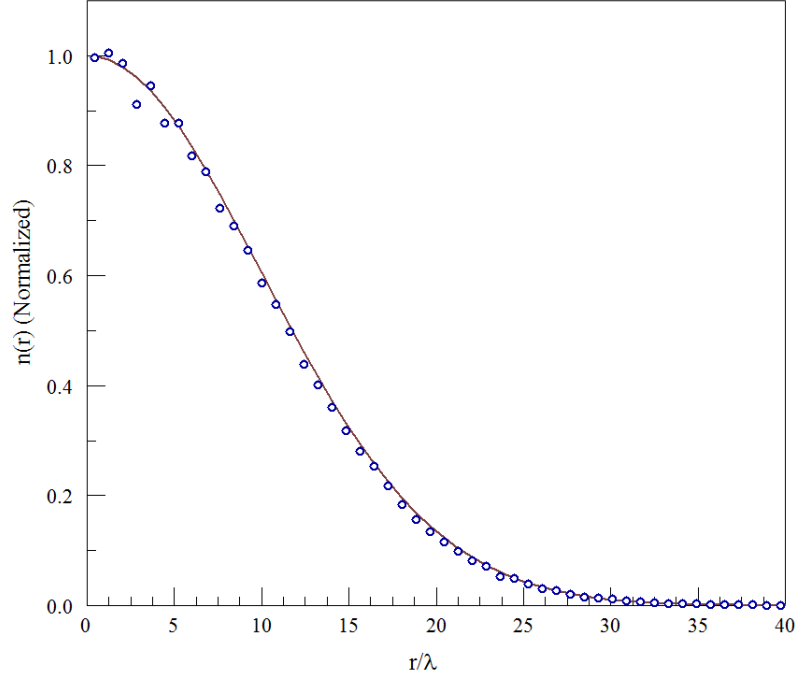


Figure 5: Particle density as a function of radius (distance from the source), $\lambda = 1$ and $N_c = 100$. The solid line is the solution of the two-dimensional diffusion equation and the points are the results of the Monte Carlo solution.

near the origin have smaller area, and therefore contain fewer particles to contribute to the average. Statistical variations are the prime concern for the accuracy of Monte Carlo calculations.

Transport equation solution

The alternative to the Monte Carlo treatment of the two-dimensional random walk is to derive and to solve a *transport equation*. Here, we define an appropriate quantity averaged over a random distribution of particles and seek a differential equation that describes how the quantity varies. For this calculation, the quantity is the average density of particles $n(x, y, t)$ with units of number/m²) (the quantity plotted in Fig. 5). To make a direct comparison with the Monte Carlo results, we must carefully set model constraints:

Although the density may vary in space, the distribution of particle velocities is the same at all points. Particles all have constant speed v_0 and there is an isotropic distribution of direction vectors.

There is a uniform-random background density of scattering objects.

Equation 8 gives the probability distribution of a (the distance particles travel between collisions) in terms of the mean-free-path λ .

We want to find how the density changes as particles perform their random walk. Changes occur if, on the average, there is a flow of particles (a *flux*) from one region of space to another. If the density n is uniform, the same number of particles flow in one direction as the other, so the average flux is zero. Therefore, we expect that fluxes depend on gradients of the particle density. We can find the dependence using the construction of Fig. 6. Assume that the particle density varies in x near a point x_0 . Using a coordinate system with origin at x_0 , the first order density variation is:

$$n(x) \cong n(0) + \frac{dn(0)}{dx} x. \quad (9)$$

The goal is to find an expression for the number of particles per second passing through the line element Δy . To carry out derivation, we assume the following two conditions:

The material is homogeneous. Equivalently, λ has the same value everywhere.

Over scale length λ , relative changes in n are small.

Using the polar coordinates shown centered on the line element, consider an element in the plane of area $(r\Delta\theta)(\Delta r)$. We want to find how many particles per second originating from this region pass through Δy . We can write the quantity as the product $J_x \Delta y$, where J_x is the linear flow density in units of particles/m-s. On the average, every particle in the calculation volume has the same average number of collisions per second:

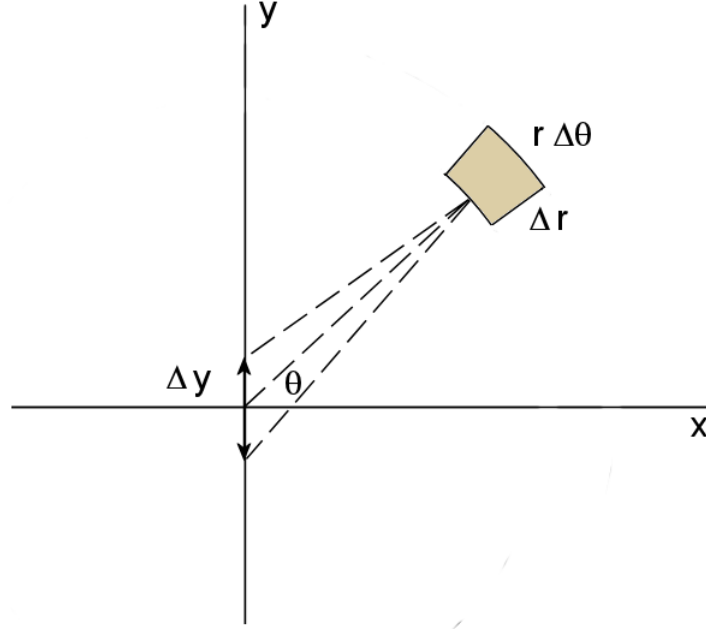


Figure 6: Geometry to calculate flux in a plane from a density gradient in x .

$$\nu = \frac{v_0}{\lambda}. \quad (10)$$

The rate of scattering events in the area element equals ν times the number of particles in the area:

$$n(x) \nu (r \Delta r \Delta \theta). \quad (11)$$

The fraction of scattered particles aimed at the segment is

$$\frac{\Delta y \cos(\theta)}{2\pi r}. \quad (12)$$

Finally, the probability that a particle scattered out of the area element reaches the line element is given by Eq. 7 as $\exp(-r/\lambda)$. Combining this expression with Eqs. 11 and 12, we can determine the current density from all elements surrounding the line segment. Taking the density variation in the form:

$$n(x) = n(0) + \frac{dn(0)}{dx} r \cos(\theta). \quad (13)$$

leads to the expression:

$$J_x \cong - \int_0^{2\pi} d\theta \int_0^\infty dr \frac{\nu}{2\pi} \exp(-r/\lambda) \left[n(0) \cos(\theta) + \frac{dn(0)}{dx} r \cos^2(\theta) \right] \quad (14)$$

The integral of the first term in brackets equals zero, so that only the term proportional to the density gradient contributes. Carrying out the integrals, the linear current density is

$$J_x \cong -D \frac{dn}{dx}, \quad (15)$$

where the planar *diffusion coefficient* (with units m²/s) is given by

$$D = \frac{\lambda^2 \nu}{2} = \frac{\lambda v_0}{2}. \quad (16)$$

Generalizing to possible variations in both x and y , can write Eq. 15 as

$$\mathbf{J} = -D \nabla n. \quad (17)$$

This relationship between the vector current density and the gradient of density is called Fick's first law. Fick's second law, a statement of conservation of particles, states that:

$$\frac{\partial n}{\partial t} = -\nabla \cdot \mathbf{J} + S = -\nabla \cdot D \nabla n + S. \quad (18)$$

The quantity $\nabla \cdot \mathbf{J}$ is the divergence of flux from a point and S is the source of particles at that point (particles/m²-s). Equation 18 is the *diffusion equation* for particles in a plane. It states that the density at a point changes in time if there is a divergence of flux or a source or sink.

We are now ready to compare the predictions of the model with the Monte Carlo results of the previous section. The solution to the diffusion equation for particles emission from the origin of the plane is

$$n(r, t) = \frac{A}{Dt} \exp\left(\frac{-r^2}{4Dt}\right), \quad (19)$$

where $r = \sqrt{x^2 + y^2}$. We can verify Eq. 19 by direct substitution by using the cylindrical form of the divergence and gradient operators and taking D as uniform in space. In order to make a comparison with the Monte Carlo calculation, we pick a time value $t_0 = N_c \lambda / v_0$ and evaluate A in Eq. 19 based on the condition that

$$\int_0^\infty 2\pi r dr n(r, t) = N_p. \quad (20)$$

The resulting expression for the density at time t_0 is

$$n(r, t_0) = \frac{N_p}{2\pi N_c \lambda^2} \exp\left(\frac{-r^2}{2N_c \lambda^2}\right), \quad (21)$$

The prediction of Eq. 21 is plotted as the solid line in Fig. 5. The results from the two methods show close absolute agreement.

Finally, we can determine the theoretical 1/e radius of the particle cloud from Eq. 21 as

$$r_e = \sqrt{2N_c} \lambda. \quad (22)$$

In a random walk, the particle spread increases as the square root of the number of transits between collisions. For $N_c = 100$, the value is $r_e/\lambda \cong 14.1$

Comparing the methods

The demonstration calculations give a basis for comparing the relative benefits and drawbacks of the Monte Carlo and transport equation approaches. We have seen that both strategies are based on averages over random distributions of particles whose statistical properties are known. Both methods give the same result in the limit of a large number of model particles. The main difference is that the averaging process is performed at the beginning of the transport equation calculation but at the end of the Monte Carlo solution.

In the transport equation approach, the idea is to seek average quantities n or \mathbf{J} and to find relationships between them (like Fick's first and second laws). These relationships are accurate when there are large numbers of particles. To illustrate the meaning of large, note that the number of electrons in one cubic micrometer of aluminum equals 3×10^{15} . When averages are taken over such large numbers, the transport equations are effectively deterministic.

In the Monte Carlo method, the idea is to follow individual particles based on a knowledge of their interaction mechanisms. A practical computer simulation may involve millions of model particles, orders of magnitude below the actual particle number. Therefore, each model particle represents the average behavior of a large group of actual particles. In contrast to transport equations, the accuracy of Monte Carlo calculations is determined by statistic variations, evident in Fig. 5.

An additional benefit of transport equations is that they often have closed-form solutions that lead to scaling relationships like Eq. 22. We could extract an approximation to the relationship from Monte Carlo results, although at the expense of some labor.

Despite the apparently favorable features of the transport equations, Monte Carlo is the primary tool for electron/photon transport. Let's understand why. One advantage is apparent comparing the relative effort in the demonstration solutions – the Monte Carlo calculation is much easier to understand. A clear definition of physical properties of particle collisions was combined with a few simple rules. The only derivation required was that for the mean free path. The entire physical model was contained in the 14 lines of code of Table 1. In contrast, the transport model required considerable insight and derivation of several equations. In addition, it was necessary to introduce additional results like the divergence theorem. Most of us feel more comfortable staying close to the physics with a minimum of intervening mathematical constructions. This attitude represents good strategy, not laziness. Less abstraction means less chance for error. A computer calculation

that closely adheres to the physics is called a *simulation*. Program managers and funding agents have a warm feeling for simulations.

Beyond the emotional appeal, there is an over-riding practical reason to apply Monte Carlo to electron/photon transport in matter. Transport equations become untenable when the interaction physics becomes complex. For example, consider the following scenario for a demonstration calculation:

In 20% of collisions, a particle splits into two particles with velocity $0.5v_0$ and $0.2v_0$. The two particles are emitted at a random angles separated by 60° . Each secondary particle has its own cross section for interaction with the background obstacles.

It would be relatively easy to modify the code of Table 1 to represent this history and even more complex ones. On the other hand, it would be require consider effort and theoretical insight to modify a transport equation. As a second example, suppose the medium were not uniform but had inclusions with different cross sections and with dimensions less than λ . In this case, the derivation of Fick's first law is invalid. A much more complex relationship would be needed. Again, it would relatively simple to incorporate such a change in a Monte Carlo model. Although these scenarios may sound arbitrary, they are precisely the type of processes that occur in electron/photon showers.

In summary, the goal in collective physics is to describe behavior of huge numbers of particles. We have discussed two approaches:

Monte Carlo method. Define a large but reasonable set of model particles, where each model particle represents the behavior of a group of real particles with similar properties. Propagate the model particles as single particles using known physics and probabilities of interactions. Then, take averages to infer the group behavior.

Transport equation method. Define macroscopic quantities, averages over particle distributions. Derive and solve differential equations that describe the behavior of the macroscopic quantities.

The choice of method depends on the nature of the particles and the interaction mechanisms. Often, practical calculations usually use a combination of the two approaches. For example, consider the three types of calculations required for the design of X-ray devices (supported in our **Xenos** package):

Radiation transport in matter. Photons may be treated with the Monte Carlo technique, but mixed methods are necessary for electrons and positrons. In addition to discrete events (hard interactions) like

Compton scattering, energetic electrons in matter undergo small angle scattering and energy loss with a vast number of background electrons (soft interactions). It would be impossible to model each interaction individually. Instead, averages based on transport calculations are used.

Heat transfer. Here, a *particle* is the energy transferred from one atom to an adjacent one. Because the interaction model is simple and the mean-free-path is extremely small, transport equations are clearly the best choice.

Electric and magnetic fields. The standard approach is through the Maxwell equations. They are transport type equations, derived by taking averages over a large number of charges. On the other other hand, we do employ Monte-Carlo-type methods to treat contributions to fields from high-current electron beams.