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UCRL-12170

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Ernest O. Lawrence
Radiation Laboratory

**ON THE CALCULATION OF A COLLISION
DISTANCE WHEN CONDITIONS ALONG
THE PATH ARE CONTINUALLY CHANGING**

Livermore, California

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UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Livermore, California

Contract No. W-7405-eng-48

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J. R. Terrall

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Printed in USA. Price \$1.00. Available from the Clearinghouse for Federal
Scientific and Technical Information, National Bureau of Standards,
U. S. Department of Commerce, Springfield, Virginia.

ON THE CALCULATION OF A COLLISION DISTANCE WHEN CONDITIONS ALONG THE PATH ARE CONTINUALLY CHANGING

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ABSTRACT

In Monte Carlo calculations for transport problems, it is necessary to know how far individual particles are likely to travel between collisions. This is a simple calculation if the collision cross sections do not change as a particle moves through a medium. However if the cross sections are changing because of density variations or because the particles comprising the medium may themselves have velocities which cannot be ignored, the calculation may become quite involved. We suggest here a simple method and several variations on it.

I. THEORY

The decrease in the number of particles which travel a distance ds in a medium is proportional to the number of particles and the probability of a collision:

$$dn = - n \sigma ds \quad (1)$$

where σ is the collision probability per unit of path, evaluated at the particles' present location in space-time and given by the microscopic total cross section multiplied by the numerical density of particles in the medium (or a sum of such products over the various kinds of particles of the medium). Hence the probability that a particle will not have a collision in traveling a distance s is obtained from

$$P = \exp \left(- \int_0^s \sigma ds \right) \quad (2)$$

If the collision probability σ were constant along the path of travel the calculation of a distance to the next collision for a given particle would be extremely simple, once P had been chosen randomly:

$$s = \frac{\ln 1/P}{\sigma} \dots \text{if } \sigma \text{ constant.} \quad (3)$$

Now there are often various circumstances which complicate matters so that (3) cannot be used. The quantity σ may vary along the path because of any one or a combination of the following reasons:

- 1) The density of particles comprising the medium may vary in space.
- 2) The density of particles of the medium may vary in time.
- 3) The particles of the medium may have velocities which are not negligible. This will be important when cross sections vary with incoming particle energy, which is usually the case.
- 4) The velocities of 3) may not only be nonnegligible but also nonconstant.

Circumstances 3) and 4) introduce complications because cross sections are a function of the relative velocity of the incoming and target particles. Consequently the available data on cross sections, usually tabulated against incoming particle velocity, under the assumption that target particle velocities are negligible, may not be usable until the relative velocity has been found.

Thus, in general, the σ in (2) should be written

$$\sigma = \sum N(s, t) \sigma_{\text{total}}(v_{\text{rel}}(s, t)) \text{ with } t = s/v. \quad (4)$$

$N(s, t)$ represents the numerical density of a particular class of particles comprising the medium at position s and time t whose microscopic cross section is σ_{total} . Also, v is the speed of the particle traversing the medium, as measured in the lab system, while v_{rel} is the speed relative to the particles being considered. Happily v , at least, is constant between collisions. For a possible collision with a single target particle we have the following picture:

$$\vec{v}_{rel}(s, t) = \vec{v} - \vec{v}_{target}(s, t)$$

We need both $\vec{v}$ and $\vec{v}_{rel}$ -- $\vec{v}$ to obtain the time and location in space along the path, and $\vec{v}_{rel}$ to obtain the cross sections.

When the distance s to the next collision has been calculated, the location can be obtained from

$$x = x_0 + \alpha s$$

$$y = y_0 + \beta s$$

$$z = z_0 + \gamma s$$

$$t = t_0 + s/v$$

where (x_0, y_0, z_0, t_0) is the initial location and α, β , and γ are the direction cosines of $\vec{v}$.

An interesting case arises when we consider that a particle may not be moving at all in the lab frame of reference. However, while it is just sitting in one spot the particles of the medium may be sweeping past, because of temperature motion and a possible drift motion of the medium. In this situation we want to deal with elapsed time rather than elapsed distance. We could still call this s (for distance in the time dimension). In such a case the location of a collision would be calculated from

$$x = x_0$$

$$y = y_0$$

$$z = z_0$$

$$t = t_0 + s.$$

II. A METHOD

For a practical calculation we propose the following method: Choose a probability P and calculate $\int_0^s \sigma ds$ in finite intervals within which simplifying assumptions may be made; stop when the sum of the contributions equals $\ln 1/P$.

That is, obtain s by solving

$$\sum_{i=1}^{I-1} \int_{s_{i-1}}^{s_i} \sigma ds + \int_{s_{I-1}}^s \sigma ds = \ln 1/P, \quad s_{I-1} \leq s. \quad (5)$$

The idea is simple, straightforward and obvious, and hardly seems worthwhile writing about, except that there are certain questions which must be faced.

If the intervals $s_i - s_{i-1} = (\delta s)_i$ are small enough that $\sigma(s)$ may be approximated by a linear function (different for each interval of course) then

$$\int_{s_{i-1}}^{s_i} \sigma ds = \sigma_i (\delta s)_i \quad (6)$$

where σ_i is the value of σ computed at the midpoint of the interval, using the relative speed. The calculation of the relative speed may be the hardest part of the whole business.

There is a question of how big to make the intervals. The answer is quite arbitrary without a prior knowledge of how the particle travels through the medium. However, something appealing suggests itself when we observe that if δs were constant and (6) used in (5) we would have just a sum of σ -values until the last step:

$$\sum_{i=1}^{I-1} \sigma_i + \left(\frac{s - s_{I-1}}{\delta s} \right) \sigma_I = \frac{\ln 1/P}{\delta s} \quad (7)$$

This is true because, under our assumption of the linearity of σ in each interval, the area of the final interval is just the fraction $(s - s_{I-1})/(s_I - s_{I-1})$ of the total area $(s_I - s_{I-1}) \cdot \sigma_I$. Hence we have only to sum the σ_i until, when the next contribution is added in, the quantity

$$\Delta = \sum \sigma_i - \frac{\ln 1/P}{\delta s} \quad (8)$$

exceeds zero. We then back off for our final computation:

$$\begin{aligned} s &= s_I - \frac{(\Delta - 0)}{\sigma_I} \delta s \\ &= s_I - \left[\sum_{i=1}^I \sigma_i - (\ln 1/P)/\delta s \right] \frac{\delta s}{\sigma_I} \end{aligned} \quad (9)$$

We write $\Delta - 0$ because it is the excess which must be gotten rid of.

The appeal of this method is that, at each step along the way we merely add in a new quantity and stop when the running sum changes from negative to positive.

$$\Delta_0 = - \frac{\ln 1/P}{\delta s} < 0$$

$$\Delta_1 = \sigma_1 + \Delta_0$$

$$\Delta_2 = \sigma_2 + \Delta_1$$

The interval width δs might be taken as some fraction of the mean free path at the start of the flight:

$$\delta s = \frac{\ln 1/P}{10 \sigma_0} \text{ for example.}$$

The foregoing method has the disadvantage that if the cross section changes drastically along the flight (and perhaps suddenly, as at a boundary between different media) the original estimate of δs might be too coarse. Or it may become too fine, causing extra work to be done in the calculation. An a priori method of adjusting δs suggests itself, wherein the path is broken into zones, each with its separate δs . This would be one way to handle boundary crossings, with the new δs obtained in the ratio of the mean free paths at the start of a new zone, for example. Thus we might take

$$\sum_{i=1}^I \sigma_i (\delta s)_i = \sum_{i=1}^{I_1} \sigma_i (\delta s)_i + \sum_{i=1}^{I_2} \sigma_i (\delta s)_i + \dots$$

$$= (\delta s)_1 \sum_{i=1}^{I_1} \sigma_i + (\delta s)_2 \sum_{i=1}^{I_2} \sigma_i + \dots, \text{ if } \delta s \text{ constant in each zone,}$$

and we have the equation $\left(\text{with } \Sigma_k \equiv \sum_{i=1}^{I_k} \sigma_i \right)$

$$\Sigma_1 \delta s_1 + \Sigma_2 \delta s_2 + \dots + \underbrace{\text{last contribution}}_{\text{contains } s} = \ln 1/P. \quad (5')$$

We mean each Σ_k to stand for a different zone, each with its own number of intervals I_k . We would compute

$$\sum^{(1)} \sigma_i - \frac{\ln 1/P}{\delta s_1}$$

where $\sum^{(1)}$ is the running sum in zone 1, and if this stayed negative in the first zone then we would compute

$$\sum^{(2)} \sigma_i + \frac{\delta s_1}{\delta s_2} \Delta_1 = \sum^{(2)} \sigma_i + \frac{\delta s_1}{\delta s_2} \Sigma_1 - \frac{(\ln 1/P)}{\delta s_2}$$

where $\Delta_1 = \Sigma_1 - (\ln 1/P)/\delta s_1$. If this stayed negative for $i = I_2$ we would compute

$$\begin{aligned} \sum^{(3)} \sigma_i + \frac{\delta s_2}{\delta s_3} \Delta_2 &= \sum^{(3)} \sigma_i + \frac{\delta s_2}{\delta s_3} \Sigma_2 + \frac{\delta s_1}{\delta s_3} \Delta_1 \\ &= \sum^{(3)} \sigma_i + \frac{\delta s_2}{\delta s_3} \Sigma_2 + \frac{\delta s_1}{\delta s_3} \Sigma_1 - \frac{\ln 1/P}{\delta s_3} \end{aligned}$$

where $\Delta_2 = \Sigma_2 + (\delta s_1/\delta s_2)\Delta_1$. We would continue on and finally stop when

$$\sum^{(\kappa)} \sigma_i + \frac{\delta s_{\kappa-1}}{\delta s_{\kappa}} \Delta_{\kappa-1}$$

turned positive, and then back off as before. At the final step we would have

$$\sum^{(k)} \sigma_i + \frac{\delta s_{k-1}}{\delta s_k} \Sigma_{k-1} + \dots + \frac{\delta s_1}{\delta s_k} \Sigma_1 - \frac{\ln 1/P}{\delta s_k} > 0,$$

and s would be obtained from the first positive value for Δ :

$$\begin{aligned} s &= s_{I_k} - \frac{\Delta}{\sigma_{I_k}} \delta s_k \\ &= s_{I_k} - \left[\sum_{i=1}^{I_k} \sigma_i - \frac{\ln 1/P}{\delta s_k} \right] \frac{\delta s_k}{\sigma_{I_k}} \end{aligned} \quad (9')$$

This procedure is like that for the single zone case except that now, starting with

$$\Delta_0 = - \frac{\ln 1/P}{\delta s_1},$$

we have zonal deltas:

$$\begin{aligned} \Delta_1 &= \Sigma_1 + \Delta_0 \\ \Delta_2 &= \Sigma_2 + \frac{\delta s_1}{\delta s_2} \Delta_1 \\ \Delta_3 &= \Sigma_3 + \frac{\delta s_2}{\delta s_3} \Delta_2 \\ &\vdots \end{aligned}$$

Each of the Σ 's is carried only to the zone boundary and the last contribution at the boundary may be from only a fraction of the δs for that zone.

Another way is to adjust the δs continually, at each new step, instead of leaving it constant for a whole set of steps. Thus, we might take a new δs as a fraction of the mean free path in the interval immediately preceding, which we have just computed:

$$(\delta s)_i = c \cdot \frac{1}{\sigma_{i-1}}, \text{ with } c = \text{const} < 1.$$

Then we would have, as the equation for s ,

$$\sum_{i=1}^I c \frac{\sigma_i}{\sigma_{i-1}} = \frac{s_I - s}{s_I - s_{I-1}} \cdot c \cdot \frac{\sigma_I}{\sigma_{I-1}} = \ln 1/P. \quad (5'')$$

But, since $s_I - s_{I-1} = (\delta s)_I = c/\sigma_{I-1}$, we find, on solving for s ,

$$s = s_I - \left[\sum_{i=1}^I (\sigma_i/\sigma_{i-1}) - \frac{\ln 1/P}{c} \right] \frac{c}{\sigma_I}. \quad (9'')$$

This is just like (9) except that the constant c takes the place of the constant δs before and our sum is a bit more complicated to compute, involving a division for each new interval. However, the advantage of this method is that we continually take account of the changes in mean free path, using larger intervals as the mfp increases and smaller intervals as it decreases. In this last method our Δ 's would be

$$\Delta_1 = \sigma_1/\sigma_0 - \frac{\ln 1/P}{c}$$

$$\Delta_2 = \sigma_2/\sigma_1 + \Delta_1$$

$$\Delta_3 = \sigma_3/\sigma_2 + \Delta_2, \text{ etc.}$$

where σ_0 is the cross section at the start of the flight.

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