

MONACO
A MONTE CARLO TRAJECTORY FORTRAN IV SUBROUTINE
FOR HIGH-ENERGY PROTONS IN BULK MATERIAL

J. MacLachlan, T. Borak, and M. Awschalom

May 14, 1970

INTRODUCTION

An important problem in accelerator and experimental-area design is the determination of the fate of high-energy particles after they collide with something.

A high-energy proton or, in general, a high-energy hadron undergoes different interactions with the medium as it traverses an element of path length in it. Both the sequence and location, as well as the nature and intensity of the interactions, occur randomly but under reasonably well-known probabilities along any element of path length. Hence, a convenient way to estimate the trajectory and fate of a high-energy proton entering a block of material is by following it through a sequence of small steps wherein all possible interactions are chosen randomly according to known probabilities.

MONACO is a computer subroutine of the Monte-Carlo type which can be easily incorporated with other codes to investigate problems such as accelerator particle losses at scrapers, septa and abort systems, beam-slit efficiencies, etc. With minor changes it may also be used to calculate muon trajectories.



The listing given in the Appendix shows the simplicity of this subroutine. This simplicity also forces the disregard of fine details for the sake of mathematical compactness and time savings in the calculations. Of course, the simplifications imply some limitations in the applicability of the results. However, it is felt that the general nature of the results is not affected by the simplifications.

The main limitations of the program are

1. Neglect of proton energy losses by collisions
2. Material thicknesses > 0.1 radiation length
3. Neglect of secondary particles resulting from nonelastic events.

MONACO has its origins in several of the subroutines of the extra-nuclear cascade program TRANSK¹ written by J. Ranft in CERN.

Program Specification

MONACO is a FORTRAN-coded subroutine which follows a single proton through a block of material. The physical processes calculated are multiple coulomb scattering (MCS), nuclear elastic scattering, and nonelastic events as a whole. The energy loss dE/dX to ionization and recoil are not calculated. The block is specified by its length, width, height, density, atomic weight, and atomic number. The general flow of the program is diagrammed in Fig. 1.

An entry is made at MONACO to calculate material constants such as radiation length, nuclear cross sections, etc., as functions of atomic

weight, atomic number, and density. Any of these quantities for which the user has particular values, e.g. experimental values, may be entered as data by placing them in common storage prior to calling MONACO. Any of the three processes, MCS, nuclear scattering, or inelastic interaction, may be left out of the calculation by setting the parameters INHIBT (I) (I = 1, 2, 3) equal to 'TRUE'. A check is made that the given step length ΔZ lies between $1/4$ radiation length and $1/2$ interaction length. An entry is made at FATE for each proton which is to be followed.

A length to a nuclear interaction point is chosen. If this length is greater than the step size, no nuclear event occurs in the step, and MCS only is calculated. The MCS angle θ is chosen and a sine and cosine of a random azimuth are used to get projected values, θ_X and θ_Y , of the polar scattering angle. Transverse drifts proportional to the projections are added to the x and y coordinates. The projected angles are added to the existing angles for the path. The coordinates are then checked to see that they lie within the block. If they do not, the subroutine returns to the calling program with the particle coordinates at the end of the interval. If the particle is still in the block, a new step is taken. If a nuclear interaction point lies within the interval, the MCS results are calculated to that point. A choice is made between an elastic or nonelastic strong interaction by comparing a random number to the ratio $\sigma_{el} / \sigma_{tot}$. If the interaction is nonelastic, the subroutine returns the event coordinates to the calling program. If the

event is elastic, a choice between coherent and incoherent scattering determines the formula for the differential cross section. The random projections of this angle are added to the existing projected angles for the path and then the MCS calculation is carried from the interaction point to the end of the step.

Multiple Coulomb Scattering

The scattering produced by many soft coulomb interactions with nuclei and electrons is represented by a Gaussian distribution with standard deviation given by²

$$\sqrt{\langle \theta^2 \rangle} = \sqrt{L/L_0} (1 + \epsilon), \quad (1)$$

where $\beta = v/c$, p is proton momentum in MeV/c, $\langle \theta^2 \rangle$ is the mean squared scattering angle, L is the thickness of the scatterer, and L_0 is the radiation length. The formula used to calculate L_0 is¹

$$L_0 = \frac{137 \text{ Me}^2 \text{C}^4 \text{A}}{4e^4 N_0 \ln(183Z^{-1/3}) Z(Z + 1.39 - 0.095 \log_{10} Z)} \quad (2)$$

The quantity $\epsilon < 0$ is a thickness correction which reflects the fact that the condition³

$$L > 6 \left(\frac{137}{Z} \right) \frac{\text{A}^{1/3}}{\rho} \text{ (cm)}, \quad (3)$$

for the validity of Eq. (1) with $\epsilon = 0$ is not met. However, for

$$L > 0.1 L_0, \quad |\epsilon| < 0.1.^2$$

More exact formulae are known, but formula (1) has the advantage of computational simplicity. Relativistic corrections and non-Gaussian statistics affect the results by less than 10%. The formula (2) for radiation length is used in absence of a user supplied value.

The MCS angular distribution probability is³

$$p(\theta) d\Omega = k d\phi \sin \theta d\theta \exp(-\theta^2 / \langle \theta^2 \rangle) \quad (4)$$

where

$$k = \left[\int_0^\pi d\phi \sin \theta d\theta \exp(-\theta^2 / \langle \theta^2 \rangle) \right]^{-1}. \quad (5)$$

Some people are initially disconcerted about the interpretation of $\langle \theta^2 \rangle$ as the mean square angle of scattering and the absence of a 2 in the denominator of the exponent. The difference between the one dimensional Gaussian

$$P(x) = (\text{const}) \exp(-x^2 / 2\sigma^2) \quad (6)$$

where $\langle x^2 \rangle = \sigma^2$, and the Gaussian given in Eq. (4) follows from the different type of "space differential," namely, dx in Eq. (6) and $\sin \theta d\theta$ in Eq. (4).

It is trivial to show the correctness of Eq. (4) in the small-angle approximation through straight forward integration. Recall that

$$\int_0^\pi x \exp(-x^2 / L^2) dx = \frac{L^2}{2}, \quad (7)$$

and
$$\int_0^{\pi} x^3 \exp(-x^2/L^2) dx = \frac{L^4}{2}. \quad (7)$$

Hence,

$$\langle x^2 \rangle = \frac{\int_0^{\pi} x^2 * x dx * \exp(-x^2/L^2)}{\int_0^{\pi} x dx * \exp(-x^2/L^2)} = \frac{\frac{L^4}{2}}{\frac{L^2}{2}} = L^2, \quad (8)$$

or the mean-square angle equals the denominator of the exponential function.

To make a random choice of scattering angle according to the differential probability (4) one notes that the integrated probability for a scattering at angle $\leq \theta$ is

$$P(\theta) = \int_0^{\theta} p(\theta') d\theta' = 1 - \exp(-\theta^2/\langle \theta^2 \rangle). \quad (9)$$

Thus, a random choice of integrated probability (i. e., a number from a uniform random distribution between 0 and 1) leads to θ distributed according to the differential probability $p(\theta)$. This may be seen from a consideration of a $P(\theta)$ vs θ plot with a uniform distribution of points along the P axis with separation ΔP . The corresponding points along the θ axis will have separation

$$\Delta \theta = \Delta P / \frac{dP}{d\theta} = p(\theta) \Delta P. \quad (10)$$

Thus, there is no need to calculate numbers distributed according to (4) directly. One need only set $P(\theta)$ equal to a random number and solve for θ .

$$\theta_{\text{rand}} = \sqrt{-\langle \theta^2 \rangle \log N_{\text{rand}}}, \quad (11)$$

where the substitution 1-random number = another random number.

Although the scattering angles are small, the azimuth may have any value; therefore, only the projected angles can be summed from step to step. MONACO uses an algorithm due to van Neuman⁴ to choose the sine and cosine of a random azimuth without use of the sine and cosine routines. If two random numbers x and y are chosen such that

$$x^2 + y^2 \leq 1, \quad (12)$$

they represent a random complex number in the first quadrant of the unit circle. This number is interpreted as the square root of a random number Z

$$Z = r^2 e^{i\phi}, \quad (13)$$

so that

$$x + iy = re^{i\phi/2}, \quad (14)$$

and

$$Z = x^2 - 2ixy - y^2 = (x^2 + y^2) (\cos \phi + i \sin \phi). \quad (15)$$

Thus,

$$\cos \phi = (x^2 - y^2) / (x^2 + y^2) \quad (16)$$

$$\sin \phi = (\text{random}) \pm 2xy / (x^2 + y^2). \quad (17)$$

The squaring of $x + iy$ covers the second quadrant from the first; the random choice of sign covers the third and fourth quadrants. The squaring destroys the uniform distribution in radius but not in phase.

The multiple scattering leads to a drift of the particle trajectory which is strongly correlated with the scattering angle. Because the angle is built up from many small scatterings, the particle travels some distance as the angle is accumulating. Under the small angle approximation, not even a few soft scatterings will change the angle substantially. Approximately one would say that the particles' drift should be about half the step size times the accumulated angle as though the entire angle came from a scattering at the center of the step. It is demonstrated by Rossi³ that the result is actually

$$\Delta x = \theta_x \Delta z / \sqrt{3}, \quad (18)$$

where Δx is the transverse displacement accumulated in traveling a step Δz of scatterer in which the projected scattering angle is θ_x .

Nuclear Scattering

The probability of a proton surviving strong interactions while penetrating a block of material of length Z is

$$P(Z) = ke^{-Z/\lambda}, \quad (18)$$

where λ is the nuclear collision mean-free path related to the total cross sections by

$$\lambda = 1/N\sigma(A), \quad (19)$$

where

N = number of nuclei/g = N_0/A

N_0 = Avagadro's number

A = atomic weight of the material

σ = total nuclear cross section = $\sigma_{\text{elastic}} + \sigma_{\text{nonelastic}}$

This cross section is assumed to be independent of proton energy.

The value of σ can be read into common storage if it is explicitly known. For materials where the total cross section has not been measured, the cross section is calculated using the interpolation

$$\sigma_{\text{tot}} = 0.059 A^{0.64} \text{ barns.} \quad (20)$$

Equation (20) represents a fit to the cross section measurements at 19.3 GeV/c by Bellettini et al.⁵

A length to a strong interaction is randomly chosen by a technique similar to that used to obtain formula (14) for multiple coulomb scattering. Using Eq. (18) we get

$$Z = -\log (N_{\text{Random}}) * \lambda. \quad (21)$$

If Z is less than the step length, a nuclear collision occurs and the proton is transported to the point of collision undergoing MCS. The ensuing interaction can be either elastic or nonelastic. A decision is made by comparing a random number to the ratio of cross sections. If

$$N_{\text{Random}} < \sigma_{\text{el}} / \sigma_{\text{tot}}, \quad (22)$$

then an elastic process occurs. The elastic cross section is obtained from a fit to the Bellettini data at 19.3 GeV/c:⁵

$$\sigma_{el} = 0.0064 A^{1.04} \text{ barns.} \quad (23)$$

The elastic scattering cross section of protons on nuclei at high energies has two distinct components. One is the coherent scattering by the whole nucleus and the other is incoherent scattering of the protons on the individual nucleons of the nucleus (quasi-elastic). The coherent scattering predominates at small angles and the incoherent at large angles.

For a given material atomic weight less than 62, the differential cross section can be approximated by the sum of two exponential terms of the form⁶

$$\begin{aligned} \frac{d\sigma}{d\Omega} = & 0.036A^{1.63} p^2 \exp(-14.5A^{0.66} |t|) \\ & + 0.047A^{0.33} p^2 \exp(-10 |t|), \end{aligned} \quad (24)$$

where p is the momentum of the incident proton and t is the four momentum transfer to the scattered proton. For elastic scattering

$$|t| = -2p^2 (1 - \cos \theta). \quad (25)$$

Since the scattering is dominated by angles less than 15 mrad, $|t|$ can be approximated by

$$t \approx p^2 \theta^2. \quad (26)$$

Equation (24) is then just a sum of two gaussians which are compatible with the previously discussed Monte-Carlo method for selecting scattering angles.

The two components can conveniently be integrated over all angles to obtain the relative rate for each contribution. The decision on which elastic process occurs is made by comparing a random number with the ratio of $\sigma_{\text{coherent-elastic}} / \sigma_{\text{elastic}}$.

Above atomic weight of 62 the measured differential cross sections show distinct secondary diffraction maximum and minimum. A general expression describing the elastic scattering is quite complicated. So, for mathematical convenience the following sum of two exponents is also used for high-Z materials:

$$\begin{aligned} \frac{d\sigma}{d\Omega} = & 0.134A^{1.33} p^2 \exp(-60A^{0.33} |t|) \\ & + 0.054A^{0.40} p^2 \exp(-10 |t|). \end{aligned} \tag{27}$$

Since secondary diffraction structure is missing, the scattering angles for heavy materials may be underestimated.

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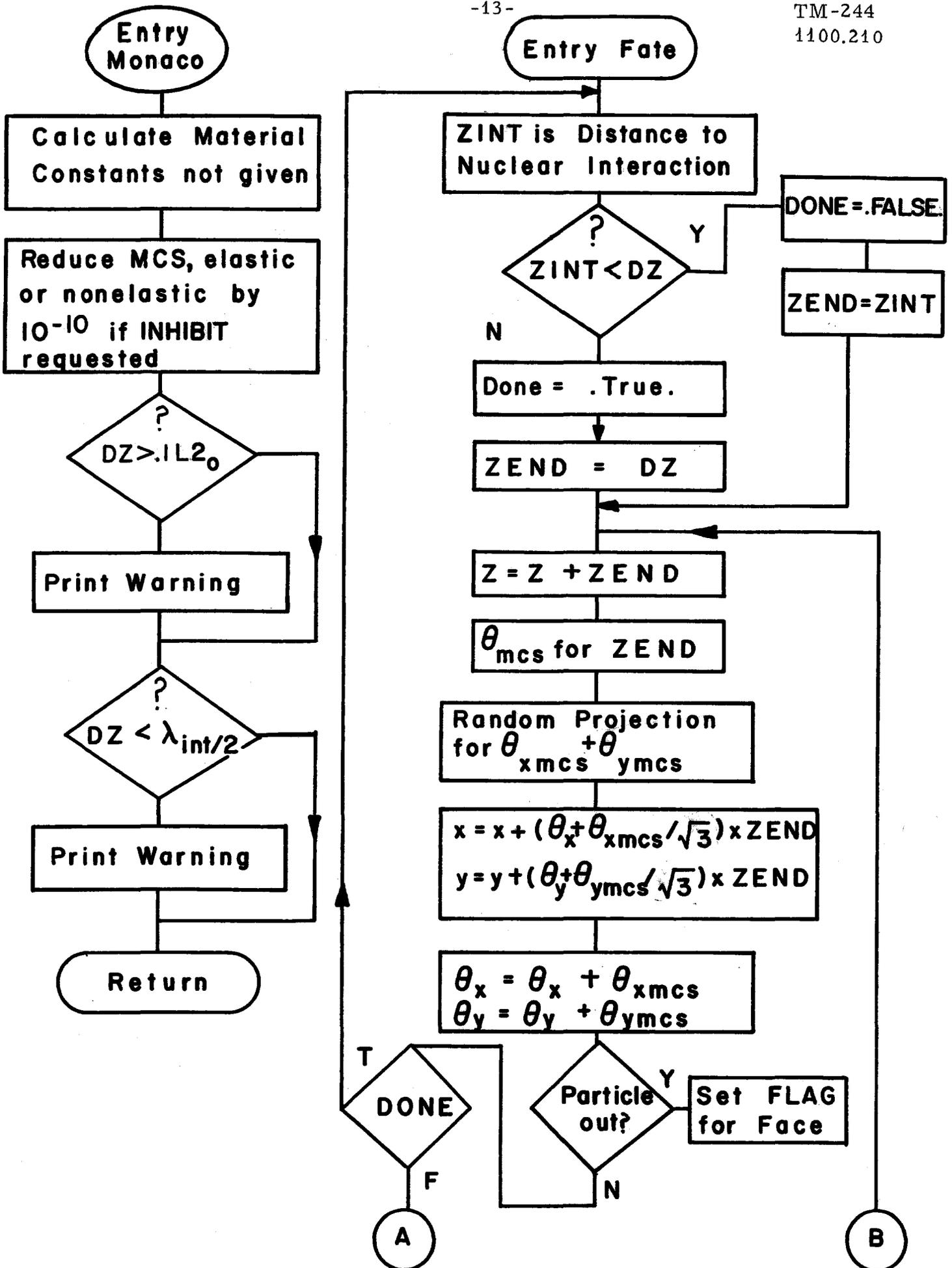


Fig. 1. Flow chart.

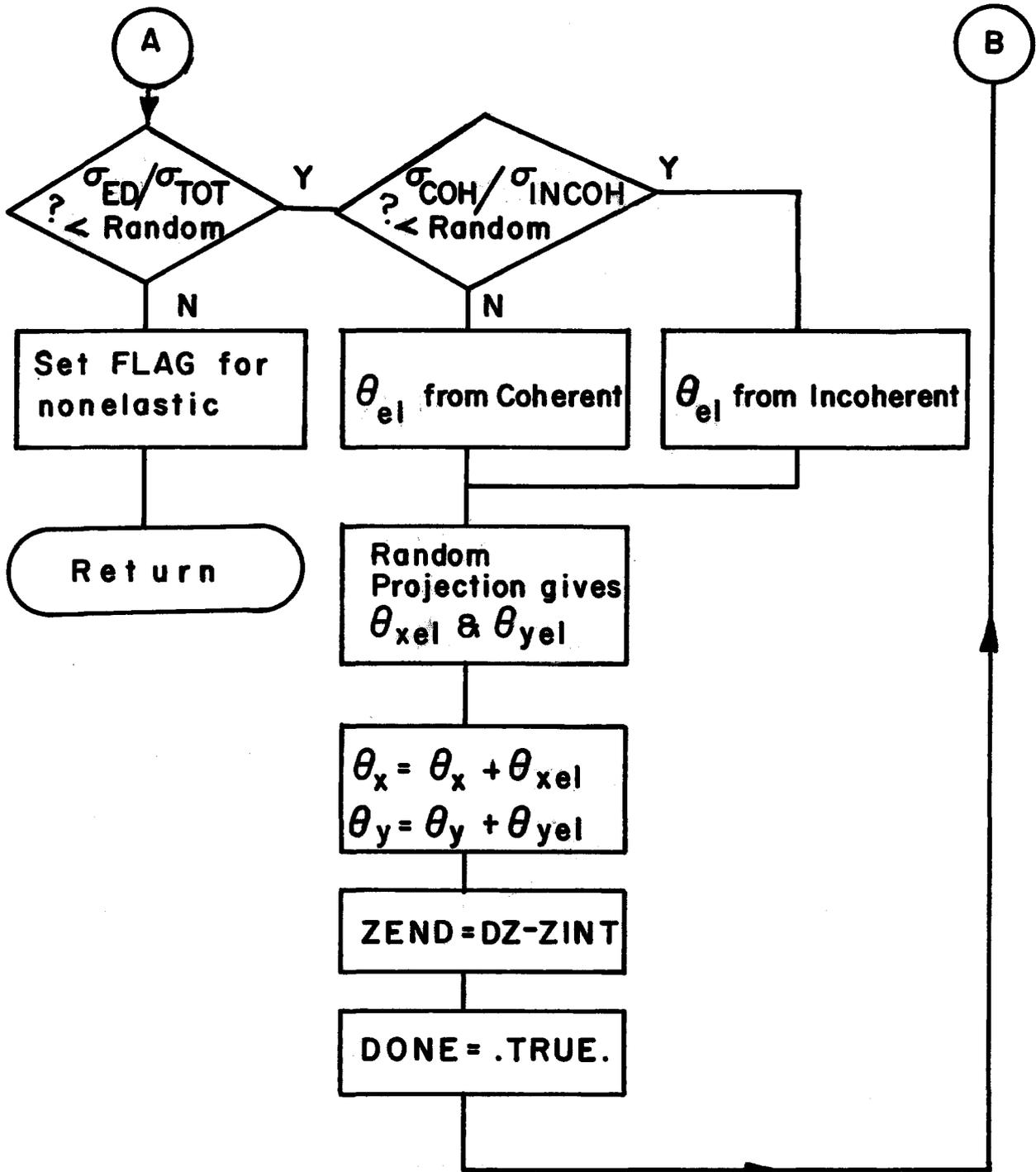


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