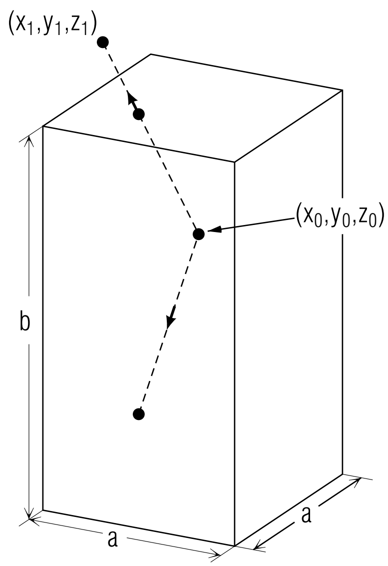
PHYSNET

MISN-0-356

SIMULATION OF A CHAIN REACTION



Project PHYSNET Physics Bldg. Michigan State University East Lansing, MI

SIMULATION OF A CHAIN REACTION

by

Robert Ehrlich

Title: **Simulation of a Chain Reaction**

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Input Skills:

1. Vocabulary: Monte Carlo method (MISN-0-355), random numbers (MISN-0-354).
2. Enter and use a computer program which generates random numbers (MISN-0-354).

Output Skills (Knowledge):

K1. Vocabulary: simulation, half-life, fission, critical mass, generation, survival fraction.

Output Skills (Project):

P1. Enter and run a computer program to generate a computer simulation of a chain reaction. Use it to obtain the critical mass for certain simple rectangular geometries.

P2. Modify the program in P1 to calculate the critical mass of a spherical piece of uranium.

External Resources (Required):

1. A computer with BASIC or FORTRAN.

Post-Options:

1. "The Approach to Equilibrium" (MISN-0-357).

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1. Simulating Physical Processes

1a. Overview. This module introduces the concept of a "simulation" and the use of a simulation to model a nuclear chain reaction. In a simulation the elements of a system are represented by arithmetic and logical processes that can be executed on a computer in order to predict the behavior of the system. In some cases the inner workings of the system are unknown, and the purpose of the simulation is to derive a plausible model of the system by finding one in which the behavior of the simulation and the real system match under specified conditions. In other cases the inner workings of the system may be well-known, and the purpose of the simulation is to predict the behavior of the real system under conditions which it has never experienced, as in the case of a catastrophic reactor accident. Many simulations involve random processes and are, therefore, ideally suited to be studied with the aid of the Monte Carlo method.

1b. Spontaneous Nuclear Fission. The nucleus of an atom of the uranium isotope U^{235} is inherently unstable. By virtue of its instability, the nucleus spontaneously (randomly) disintegrates or "fissions" into a number of fragments. The half-life of a radioactive substance is the amount of time required for half of a large number of nuclei to disintegrate. For example, U^{235} has a half-life of 707 million years. The energy released per atom in the fission process is about a million times greater than the energy release during an ordinary chemical process, such as the burning of wood or coal. However, due to the long half-life, only a relatively small fraction of all nuclei in a piece of uranium undergo fission at any one time, so that the rate at which energy is released may only be sufficient to make the uranium slightly warm to the touch.

1c. Chain Reactions. A chain reaction, which can occur in certain radioactive substances such as uranium, is a random process. The rate at which energy is released is drastically accelerated in the event of a chain reaction, which can lead to a nuclear explosion. In a chain reaction, neutrons which are emitted during one spontaneous fission collide with other U^{235} nuclei. The other U^{235} nuclei absorb the neutrons, which causes them to become highly unstable and very rapidly undergo fission,

thereby emitting more neutrons which trigger more fissions, and so on. We refer to each phase of this process as a "generation." If we assume that two neutrons are emitted during each fission, and that every emitted neutron induces another fission, then starting with N spontaneous fissions, there will be $2N$ induced fissions after one generation, $4N$ after two generations, and 2^nN after n generations. Thus, the number of induced fissions grows exponentially, reaching $2^{30} \approx$ one billion times the original number of spontaneous fissions in only 30 generations.

1d. Critical Mass. In view of the preceding discussion, you may wonder why a chain reaction doesn't always result from spontaneous fissions. The answer is related to the notion of "critical mass," which is the smallest mass of uranium or other fissionable material in which a self-sustaining chain reaction can occur. Due to the small size of the uranium nucleus, neutrons emitted during nuclear fission have to travel, on the average, appreciable distances (on the order of centimeters) before interacting with other nuclei and inducing them to fission. Thus, for a small piece of uranium even if two neutrons are emitted during a spontaneous fission one or possibly both neutrons may leave the piece before encountering another uranium nucleus. In that case the average number of induced fissions caused by each spontaneous fission would be a number less than two. Let us define the quantity $f = N_{in}/N$, where N_{in} is the number of fissions induced by neutrons emitted in N fissions during the preceding generation. We shall refer to f as the "survival fraction." Starting with N fissions in the first generation, there will be (fN) fissions in the next generation, (f^2N) fissions in the one after that, and f^nN fissions in the n^{th} generation. Only for $f \geq 1$ will exponential growth in the released energy occur from generation to generation. The value of f for a particular piece of uranium is determined by its mass, shape, and purity. A piece of uranium for which $f = 1.0$ is said to have a critical mass. If a piece of uranium has a mass greater than the critical mass M_c, it will spontaneously undergo a chain reaction and possibly cause a nuclear explosion. To create such an explosion, one need only bring together two pieces of uranium whose combined mass exceeds the critical mass. It is clearly very important to be able to determine the value of the critical mass theoretically, as the experimental determination is a bit risky. In the early days of the nuclear age (before the first bomb was built) several brave scientists actually did attempt this experimental determination – a process that was aptly called "tickling the dragon's tail."

2. Calculation of the Critical Mass

2a. Overview. We can empirically calculate the critical mass for a block of uranium by finding the survival fraction for a range of masses and shapes (recall that a block has the critical mass provided the survival fraction has the value $f = 1.0$). The procedure we shall use to find the value of f for a block of specified size and shape involves generating a large number (N) of simulated random fissions, and keeping a count of the number (N_{in}) of induced fissions which are caused by the emitted neutrons.

2b. Simulation of the Fission Process. The first step in generating a random fission is to choose the location of the nucleus undergoing fission to be a random point (x_0, y_0, z_0), lying within the boundaries of the piece of uranium (see Fig. 1). If we assume that the piece of uranium is a rectangular block of dimensions $a \times a \times b$, then we must choose random values for the coordinates x_0, y_0, and z_0, subject to the conditions

$$-\frac{a}{2} < x_0 < +\frac{a}{2},$$

$$-\frac{a}{2} < y_0 < +\frac{a}{2},$$

$$-\frac{b}{2} < z_0 < +\frac{b}{2}.$$

The only fission fragments that we are concerned with are the neutrons, since the heavy nuclear fragments play no part in the chain reaction mechanism. The two neutrons emitted during the fission process may travel in many directions.[1] A direction in three dimensions can be specified by two angles: θ, the polar angle, and ϕ, the azimuth. If the emitted neutrons have an "isotropic" distribution, i.e., all directions are equally likely, then the probability of a neutron emitted from the point (x_0, y_0, z_0) hitting any area on a surrounding unit sphere depends only on the size of the area. This implies that the azimuth ϕ is uniformly distributed between 0 and 2π, and that $\cos\theta$, is uniformly distributed between -1 and 1. Note that it is $\cos\theta$, not θ itself, which is uniformly distributed due to the fact that equal intervals in $\cos\theta$ contain the same surface area on a sphere of unit radius. Whether an emitted neutron hits another nucleus before leaving the block depends only on the distance along its

[1] We shall ignore the fact that the number of emitted neutrons is not always two, and we shall also ignore possible correlations between the two neutron directions.

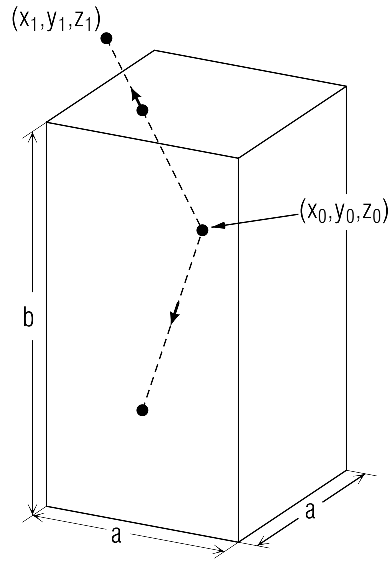

Figure 1. A fission is assumed to occur at a randomly located point giving rise to two neutrons travelling along random directions indicated by the dotted lines.

line of flight to the boundary of the block. We shall assume (unrealistically) that a neutron emitted during fission can hit another nucleus after it travels any distance between 0 and 1 centimeters, with equal probability. For example, if a neutron travels along a direction such that it would leave the block after traveling only 0.3 cm, then there is a 30% chance of it hitting a nucleus in the block. Our procedure, therefore, is to choose a random number between 0 and 1 for d, the distance traveled by each neutron. Since the neutron starts at the point (x_0, y_0, z_0) and travels along a direction (θ, ϕ), we can find the coordinates of the point (x_1, y_1, z_1) where the neutron would hit another nucleus using the geometrical relations:

$$\begin{aligned} x_1 &= x_0 + d\,\sin\theta\cos\phi\,, \\ y_1 &= y_0 + d\,\sin\theta\sin\phi\,, \\ z_1 &= x_0 + d\,\cos\theta. \end{aligned} \qquad (1)$$

Whether the neutron actually hits a nucleus at the point (x_1, y_1, z_1) and causes it to fission depends on whether the point lies within the block.

2c. Calculation Of The Survival Fraction. To calculate the survival fraction, we need only generate a large number of random fissions (N) and keep a count of the number of neutron endpoints (N_{in}) which lie inside the block. To generate each random fission, we need nine random numbers r_1, r_2, ...,r_9, which lie between 0 and 1. The nine quantities needed for each random fission are obtained from the random numbers r_1, r_2, ..., r_9 according to the following equations:

$$\left.\begin{aligned} x_0 &= a\left(r_1 - \frac{1}{2}\right) \\ y_0 &= a\left(r_2 - \frac{1}{2}\right) \\ z_0 &= b\left(r_3 - \frac{1}{2}\right) \end{aligned}\right\} \textit{coordinates of the nucleus undergoing fission}$$

$$\left.\begin{aligned} \phi &= 2\pi r_4 \\ \cos\theta &= 2\left(r_5 - \frac{1}{2}\right) \end{aligned}\right\} \textit{two angles for one emitted neutron}$$

$$\left.\begin{aligned} \phi' &= 2\pi r_6 \\ \cos\theta' &= 2\left(r_7 - \frac{1}{2}\right) \end{aligned}\right\} \textit{two angles for the other emitted neutron}$$

$$\left.\begin{aligned} d &= r_8 \\ d' &= r_9 \end{aligned}\right\} \textit{distance traveled by each neutron}$$

These formulas insure that each of the nine parameters will lie within the proper range. For each neutron from a random fission we need to calculate the neutron endpoint from Eq. (1), and then test whether the point be inside or outside the block. The survival fraction f is then given by $f = N_{in}/N$. In using the Monte Carlo method to find the survival fraction f, we are actually integrating a function F of nine variables:

$$F = F(x_0, y_0, z_0, \phi, \theta, d, \phi', \theta', d'),$$

which represents the number of fissions induced by two emitted neutrons for particular values of the variables x_0, y_0, ..., d'. The value of F is zero, one, or two, depending on these variables. In order to obtain the survival fraction f, we, must integrate the function F over all nine variables. The advantages of the Monte Carlo technique over conventional integration techniques are quite apparent in a case such as this. In order to evaluate a nine-dimensional integral using a finite sum, each of the nine variables must be allowed to take on some number of values. If only two values are used for each variable, it becomes necessary to evaluate the function at $2^9 = 512$ points.

2d. Dependence of Critical Mass on Shape of Object. For simplicity we calculate the critical mass of rectangular blocks of dimensions $a \times a \times b$. To calculate the critical mass for a given shape we want to

keep the ratio $S = a/b$ fixed and vary the mass of the block, M, until the survival fraction f has the value 1.0. We can then vary the ratio $S = a/b$, to find the critical mass for each shape. It is to be expected that we should find that cubic blocks ($S = a/b = 1$) yield the smallest critical mass for blocks having a generally rectangular shape. It would further be expected that if the calculation were done using a sphere this would have the smallest critical mass of all.

3. Program for the Survival Fraction

3a. Input. The input variable are:

M = mass of the block
S = ratio of the dimensions a/b
N = number of random points to use

It is assumed that the block has unit density so that its dimensions a and b can easily be found in terms of S and M[S − 1].

3b. Output. The output shown below was obtained using the following values:

	M	S	N
1^{st} set	1.0	1.0	100.0
2^{nd} set	1.0	1.0	100.0
3^{rd} set	1.0	16.0	100.0

Different values for f when identical values for the parameters M, S, and N are used is indicative of the statistical fluctuations present in all Monte Carlo calculations (see output for first two cases). The accuracy of the calculation can be increased by using a larger value for N.

```
M = 1.0000  S = 1.0000   N = 100.0000  F = .85
M = 1.0000  S = 1.0000   N = 100.0000  F = .94
M = 1.0000  S = 16.0000  N = 100.0000  F = .50
```

4. Procedures

4a. Calculation of the Critical Mass for a Cube. Determine the critical mass for a cube ($a/b = 1.0$) by running the program using S = 1.0, and a range of values for the mass of the block M. You can let N = 100 for all runs. You can find the critical mass by making a plot of the calculated value of f against the mass M and then drawing a smooth curve through the data points. Remember that since you are dealing with random numbers the points will not lie exactly on the curve but some will be above and some below. The critical mass is that value of M where the hand-drawn curve crosses $f = 1$. You should also estimate a value for the uncertainty in the critical mass M_c by bracketing your hand-drawn curve with a curve on either side that includes all the data points. You can then see for what values of M the bracketing curves cross the $f = 1$ line and express your final result in the form: $M_c \pm \Delta M_c$.

4b. Critical Mass as Function of Shape. To calculate the critical mass for non-cubic rectangular blocks you will need to repeat the procedure in paragraph 4a using values of S other than one. Try using S $= 0.25, 0.50, 0.75, 1.00, 1.25, 1.50,$ and 1.75. Once you have found the critical mass corresponding to each of these shapes make a graph of the critical mass versus S. Where should the minimum be?

4c. Critical Mass for a Spherical Piece of Uranium. Modify the program so that the random fissions occur inside a spherical piece of uranium. Use the same technique as in the present version of the program to calculate the survival fraction f. Run the modified version of the program to calculate f for a range of masses, and determine the critical mass for a sphere. Compare the result with what you found for the rectangular block.

Acknowledgments

Preparation of this module was supported in part by the National Science Foundation, Division of Science Education Development and Research, through Grant #SED 74-20088 to Michigan State University.

Glossary

- **critical mass**: the smallest amount of fissionable material in which a self sustaining chain reaction can occur.
- **fission**: the disintegration of a nucleus into two or more fragments.
- **generation**: individual stages in the process where by neutrons emitted by a fissioning nucleus are absorbed by other nuclei, inducing these nuclei to fission.

- **half-life**: the amount of time required for half of a large number of nuclei to disintegrate.
- **simulation**: the representation of elements of a system by logical and arithmetic processes that can be executed on a computer in order to predict the behavior of a system.
- **survival fraction**: the ratio of the number of fissions induced in a generation to the number of fissions in the previous generation.

A. Fortran, Basic, C++ Programs

All programs are at

`http://www.physnet.org/home/modules/support_programs`

which can be navigated to from the home page at

`http://www.physnet.org`

by following the links: → `modules` → `support programs`, where the programs are:

`m356p1f.for`, Fortran;
`m356p1b.bas`, Basic;
`m356p1c.cpp`, C++;
`lib351.h`, needed Library for C++ program;

MODEL EXAM

1. See Output Skills K1.

> **Examinee**:
> On your computer output sheet(s):
>
> (i) Mark page numbers in the upper right corners of all sheets.
>
> (ii) Label all output, including all axes on all graphs.
>
> On your Exam Answer Sheet(s), for each of the following parts of items (below this box), show:
>
> (i) a reference to your annotated output; and
>
> (ii) a blank area for grader comments.
>
> When finished, staple together your sheets as usual, but include the original of your annotated output sheets just behind the Exam Answer Sheet.

2. Submit your hand-annotated output for determining the critical mass of a cube of U^{235}. Make sure that it shows:

   a. that you used a cube and that you followed 100 fissions for each of a number of values for the mass of the block;

   b. your smoothly-drawn curve on your plot of survival fraction versus mass, with a pointer to the critical value;

   c. your central critical value and its uncertainty (its "error"), along with an explanation of how you deduced the error from the plot.

3. Submit your hand-annotated output for determining the critical masses of non-cubic rectangular blocks of U^{235}. Make sure that it shows:

   a. that you used a cube and six different non-cubic rectangular blocks and that you followed 100 fissions for each of the masses used to find the critical mass for each shape;

   b. your smoothly-drawn curve on your plot of shape parameter versus critical mass, with a pointer to the minimum value;

   c. a discussion of the extent to the minimum in the plot in b) agrees with expectations.

4. Submit your hand-annotated output for finding the critical mass for a sphere of U^{235}. Be sure that it shows:

   a. that you calculated the survival fraction for a range of masses and determined the critical mass from it.

   b. a comparison with the values from the rectangular blocks.

INSTRUCTIONS TO GRADER

If the student has submitted copies rather than originals of the computer output, state that on the exam answer sheet and **immediately stop grading the exam and give it a grade of zero.**