NUCLEAR FISSION

AN INTRODUCTION

Heavy nuclei found in the earth's surface have been undergoing spontaneous fission since the being of their creation. Uranium - 238 has an extremely long half-life of approximately 10^{16} years and this is why uranium - 238 is still found within the earth's surface today. This extremely long half-life means that the nuclear activity is very low. Only about 20 uranium nuclei per gram undergo spontaneous fission every hour. Scientists have searched for a method to speed up this process. Such a process was developed in the early 1900's.

The artificial transmutation of elements took a great leap forward in the 1930's when Enrico Fermi realized that neutrons would be the most effective projectiles for causing nuclear reactions and in particular for producing new heavier elements. Because neutrons have no net electric charge, they are not repelled by positively charged nuclei like protons or alpha particles. Hence the probability of a neutron reaching the nucleus and causing a reaction is much greater than for charged projectiles, particularly at low energies. Between 1934 and 1936, Fermi and his co-workers in Rome produced many previously unknown isotopes by bombarding different elements with neutrons. Fermi realized that if the heaviest known element, uranium, were bombarded with neutrons, it might be possible to produce new elements whose atomic numbers were greater than that of uranium. After several years of hard work, it was suspected that two elements had been produced, neptunium (Z = 93) and plutonium (Z = 94). The full confirmation that such "transuranic" elements could be produced came several years later at the University of California, Berkeley. The reactions are shown in the steps below:

Neptunium and plutonium are produced in this series of reactions, after bombardment of uranium -238 by neutrons.

(a) A neutron is captured by the uranium - 238 nucleus

$$ {}^{1}_{0}n + {}^{238}_{92}U \quad {}^{239}_{92}U $$

(b) The uranium - 239 decays by beta decay to neptunium - 239

$$ {}^{239}_{92}U \quad {}^{239}_{93}Np + {}^{0}_{-1}e + \bar{\upsilon} $$

(c) The neptunium, which is radioactive with a half-life of only 2.35 days, decays by beta decay to produce plutonium - 239, and the plutonium is also radioactive with a half-life of 24,360 years.

$$ {}^{239}_{93}Np \quad {}^{239}_{94}Pu + {}^{0}_{-1}e + \bar{\upsilon} $$

In 1938, the German scientists Otto Hahn and Fritz Strassmann made an amazing discovery. Following up on Fermi's work, they found that uranium bombarded by neutrons sometimes produced smaller nuclei which were roughly half the size of the original uranium nucleus. Lise Meitner and Otto Frisch, two refugees from Nazi Germany working in Scandinavia, quickly realized what had happened: the uranium nucleus, after absorbing a neutron, actually had split into two roughly equal pieces. This was startling, for until then the known nuclear reactions involved knocking out only a tiny fragment (for example, n, p, or α) from a nucleus.

This new phenomenon was named "nuclear fission" because of its resemblance to biological fission (cell division). It occurs much more readily for ${}^{235}_{92}U$ than for the more common ${}^{238}_{92}U$. The process can be visualized by imagining the uranium nucleus to be like a liquid drop. According to this "liquid-drop model", the neutron absorbed by the ${}^{235}_{92}U$ nucleus gives the nucleus extra internal energy (like heating a drop of water). This intermediate state, or "compound nucleus", is ${}^{236}_{92}U$, (because of the absorbed neutron). The extra energy of this nucleus--it is in an excited state--appears as increased motion of the individual nucleons which causes the nucleus to take on abnormal elongated shapes. When the nucleus elongates into the elongated shape the attraction of the two ends via the short-range nuclear force is greatly weakened by the excess separation distance, but the electric repulsive force is weakened only slightly and becomes predominant; so the nucleus splits in two. The two resulting nuclei, N_1 and N_2, are called "fission fragments", and in the process a number of neutrons (typically two or three) are also given off. The reaction can be written

$$ {}^{1}_{0}n + {}^{235}_{92}U \rightarrow {}^{236}_{92}U \rightarrow N_1 + N_2 + neutrons \qquad (1)$$

The compound nucleus, ${}^{236}_{92}U$, exists for less than 10^{-12} s, so the process occurs very quickly. The two fission fragments have roughly half the mass of the uranium, although rarely are they exactly equal in mass. A typical fission reaction is

$$ {}^{1}_{0}n + {}^{235}_{92}U \rightarrow {}^{141}_{56}Ba + {}^{92}_{36}Kr + 3{}^{1}_{0}n \qquad (2)$$

or

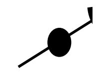
$$ {}^{1}_{0}n + {}^{235}_{92}U \quad {}^{236}_{92}U^{*} \quad {}^{140}_{54}Xe + {}^{94}_{38}Sr + 2{}^{1}_{0}n \qquad (2a)$$

and many others also occur.

A tremendous amount of energy is released in a fission reaction because the mass of ${}^{235}_{92}U$ is considerably greater than that of the fission fragments. This can be seen from the binding-energy-per-nucleon curve; the binding energy per nucleon for uranium is about **7.6 MeV/nucleon**, but for fission fragments that have intermediate mass (in the center portion of the graph, Z ≈ 100), the average binding energy per nucleon is about **8.5 MeV/nucleon.** Since the fission fragments are more tightly bound, they have less mass. The difference in mass (or energy) between the original uranium nucleus and the fission fragments is about **8.5 - 7.6 = 0.9 MeV per nucleon**. Since there are 236 nucleons involved in each fission, the total energy released per fission is

$$(0.9 \text{ MeV/nucleon}) (236 \text{ nucleons}) \approx 200 \text{ MeV}.$$

This is an enormous amount of energy on the nuclear scale. At a practical level, the energy from one fission is, of course, tiny. However, a great deal of energy at the macroscopic level would be available if many such fissions could occur at once. A number of physicists, including Fermi, recognized that the neutrons released in each fission (Eq. 1 or 2) could be used to create a chain reaction; one neutron initially causes one fission of a uranium nucleus; the two or three neutrons released can go on to cause additional fissions, so the process multiplies as shown schematically in Fig. 2. If a self-sustaining chain reaction was actually possible in practice, the enormous energy available in fission could be released. Fermi and his co-workers (at the University of Chicago) showed it was possible by constructing the first nuclear reactor in 1942.



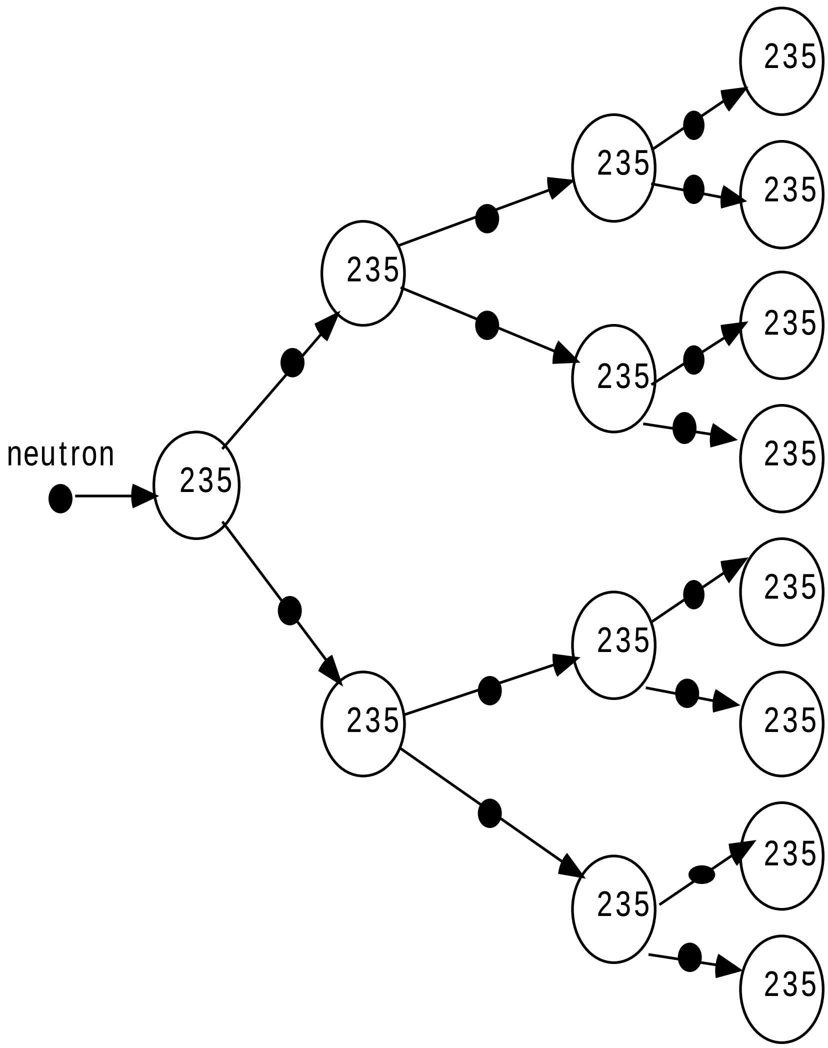


Figure 2: Chain Reaction

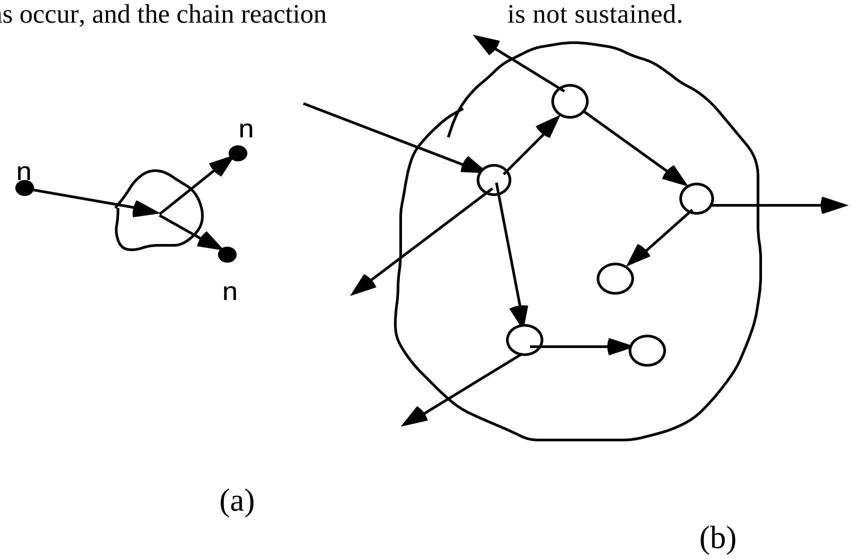
Several Problems have to be overcome in any nuclear reactor:

- 1. **First**, the probability that a ${}^{235}_{92}U$ nucleus will absorb a neutron is large only for slow neutrons, but the neutrons emitted during a fission, and which are needed to sustain a chain reaction, are moving very fast. A substance known as a "moderator" must be used to slow down the neutrons. The most effective moderator will consist of atoms whose mass is as close as possible to that of the neutrons. (To see why this is true, a billiard ball striking an equal mass at rest can itself be stopped in one collision; but a billiard ball striking a heavy object bounces off with nearly the same speed it had). The best moderator would thus contain ${}^{1}_{1}H$ atoms; unfortunately, ${}^{1}_{1}H$ tends to absorb neutrons; but deuterium, ${}^{2}_{1}H$, does not absorb many neutrons and is thus an almost ideal moderator. Either ${}^{1}_{1}H$ or ${}^{2}_{1}H$ can be used in the form of water; in the latter case, it is heavy water, where the hydrogen atoms have been replaced by deuterium. Another common moderator is "graphite", which consists of ${}^{12}_{6}C$ atoms.

- 2. A **second** problem is that the neutrons produced in one fission may be absorbed and produce other nuclear reactions with other nuclei in the reactor, rather than produce further fissions. In a "light water" reactor the ${}^{1}_{1}H$ nuclei absorbed neutrons, as does ${}^{238}_{92}U$ to form ${}^{239}_{92}U$ in the reaction n + ${}^{238}_{92}U \rightarrow {}^{239}_{92}U +$. Naturally occurring uranium contains 99.3 percent ${}^{238}_{92}U$ and only 0.7 percent fissionable ${}^{235}_{92}U$. To increase the probability of fission of ${}^{235}_{92}U$ nuclei, natural uranium is often enriched to increase the percentage of ${}^{235}_{92}U$ using processes such as diffusion or centrifugation.

- 3. The **third** problem is that some neutrons will escape through the surface of the reactor core before they cause further fissions (Fig. 4). Thus the mass of fuel must be sufficiently large for a self-sustaining chain reaction to take place. The minimum mass of uranium needed is called the "critical mass". The value of the critical mass depends on the moderator, the fuel (${}^{239}_{92}Pu$ may be used instead of ${}^{235}_{92}U$), and how much the fuel is enriched, if at all. Typical values are on the order of a few kilograms (Note: that is, not grams nor thousands of kilograms).

Figure 3
If the amount of uranium exceeds the critical mass, as in (b), a sustained chain reaction is possible. If the mass is less than critical, as in (a), most neutrons escape before additional fissions occur, and the chain reaction is not sustained.



To have a self-sustaining chain reaction, it is clear that on average at least one neutron produced in each fission must go on to produce another fission. The average number of neutrons per each fission that do go on to produce further fissions is called the "multiplication factor", f. For a self-sustaining chain reaction we must have $f \geq 1$. If $f < 1$, the reactor is "sub-critical"; $f > 1$, it is "super-critical". Reactors are equipped with movable control rods (usually of cadmium or boron), whose function is to absorb neutrons and maintain the reactor at just barely "critical", $f = 1$.

Nuclear reactors have been built for use in research and to produce electric power. Fission produces many neutrons and a "research reactor" is basically an intense source of neutrons. These neutrons can be used as projectiles in nuclear reactions to produce nuclides not found in nature, including isotopes used as tracers and for medical therapy. A "power reactor" is used to produce electricity. The energy released in the fission process appears as heat, which is used to boil water and produce steam to drive a turbine connected to an electric generator. The core of a nuclear reactor consists of the fuel and a moderator (water in most U.S. commercial reactors). The fuel is usually uranium enriched so that it contains 2 to 4 percent $^{235}_{92}U$. Water or other liquid (such as liquid sodium) is allowed to flow through the core. The thermal energy absorbed is used to produce steam in the heat exchanger, so the fissionable fuel acts as the heat input for a heat engine.

Many problems are associated with nuclear power plants. There is, of course, the usual thermal pollution associated with any heat engine. But probably the most serious problems are associated with the radioactive fission fragments produced in the reactor, plus radioactive nuclides produced by neutrons interacting with the structural parts of the reactor. Fission fragments, like their uranium or plutonium parents, have about 50 percent more neutrons than protons. Nuclei with atomic number in the typical range for fission fragments ($Z \approx 30$ to 60) are stable only if they have more nearly equal numbers of protons and neutrons (see Fig. 2). Hence the highly neutron-rich fission fragments are very unstable and decay radioactively. The accidental release of highly radioactive fission fragments into the atmosphere poses a serious threat to human health. Also a serious problem is the disposal of the spilt fuel, which contains highly radioactive fission fragments. Leakage of radioactive wastes is possible and has in fact occurred. Indeed, a satisfactory method of disposal is still not at hand. Finally, the lifetime of nuclear power plants is limited to some 30 years, due to buildup of radioactivity and the fact that the structural materials themselves are weakened by the intense conditions inside. Decommissioning of a power plant will be a major undertaking, and could take on a number of forms. The cost of any methods of decommissioning a large plant will probably be extremely large.

So-called breeder reactors have the same problems, but were proposed as a solution to the problem of limited supplies of fissionable uranium. A breeder reactor is one in which some of the neutrons produced in the fission of $^{235}_{92}U$ are absorbed by $^{238}_{92}U$ and $^{238}_{92}Pu$ is produced via the set of reactions shown in Fig. 1. $^{239}_{94}Pu$ is fissionable with slow neutrons, so after separation it can be used as a fuel in a nuclear reactor. Thus a breeder reactor "breeds" new fuel ($^{239}_{94}Pu$) from otherwise useless $^{238}_{92}U$. Since natural uranium is 99.3 percent $^{238}_{92}U$, this means that the supply of fissionable fuel could be increased by more than a factor of 100. But breeder reactors present additional problems. First, plutonium has a very long half-life of 24,000 years, and is a highly toxic substance that poses a serious danger to health. Also important is the fact that plutonium produced can readily be used in a bomb. Thus the use of a breeder reactor, even more than a conventional uranium reactor, presents the danger of nuclear proliferation: even poor nations might be able to produce nuclear bombs. And the possibility of theft of fuel by terrorists who could produce a bomb further increases the probability of nuclear holocaust.

NUCLEAR SCIENCE

SIMULATION OF A CHAIN REACTION

Introduction

A chain reaction, which can occur in certain radioactive substances such as uranium, is a random process that can be studied with the aid of the **"Monte Carlo"** method. The nucleus of an atom of the uranium isotope U^{235} is inherently unstable. By virtue of its instability, the nucleus spontaneously 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; 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 released during an ordinary chemical process, such as burning 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.

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, the starting with N spontaneous fissions, there will be 2N induced fissions after one generation, 4N after two generations, and 2^n N after n generations. Thus, the number of induced fissions grows exponentially, reaching 2^{30} (about one billion) times the original number of spontaneous fissions in only 30 generations.

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 introducing them to fission. Thus, for a small piece of uranium, even though two neutrons may be emitted in each spontaneous fission, the average number of induced fissions f caused by the neutrons is some number less than two. Let us define the factor f more precisely. Suppose N nuclei undergo spontaneous fission thereby emitting 2N neutrons, of which N_{in} induce other nuclei in the piece of uranium to fission. (The remaining neutrons leave the piece of uranium before colliding with a nucleus.) During the first generation, the fractional change in the number of nuclei undergoing fission is given by:

$$f = \frac{N_{IN}}{N} \qquad (1)$$

which we shall refer to as the survival fraction. After two generations, the number of induced fissions is given by f^2N, and after "n" generations, the number is f^nN. Thus, the number of induced fissions grows exponentially if and only if "f" is greater than 1.0.

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, an **explosion** occurs. 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.**

Theory: Calculation of the Critical Mass

We can calculate the critical mass for a block of uranium "experimentally", by finding the survival fraction f for a range of masses and shapes. (Recall that a block has the critical mass provided f = 1.0.) The computer 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. We illustrate the procedure by giving the steps necessary to generate one random fission, shown schematically in the following figure.

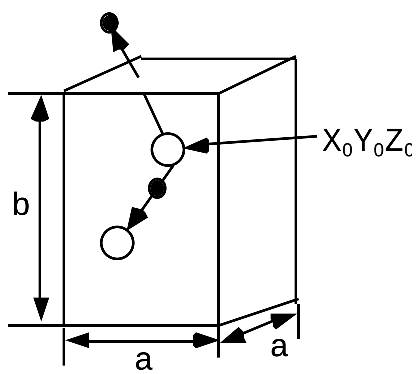


Figure 1
Two neutrons emitted during a random fission

We first choose the location of the nucleus undergoing fission to be a random point (x_o, y_o, z_o), lying within the boundaries of the piece of uranium. If we assume that the piece of uranium is a rectangular block of dimensions a,a,b; (see figure) then we must choose random values for the coordinates x_o, y_o and z_o, subject to the conditions

$$-\frac{a}{2} < X_o < +\frac{a}{2}$$

$$-\frac{a}{2} < Y_o < +\frac{a}{2} \qquad (2)$$

$$-\frac{b}{2} < Z_o < +\frac{b}{2} \, .$$

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. (We shall ignore the fact that the number of emitter neutrons is not always two; and we shall also ignore possible correlations between the two neutron directions.) A direction in three dimensions can be specified by two angles: θ, the polar angle, and φ, the azimuth (see Figure 2). 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_o, y_o, z_o) hitting any area on a surrounding unit sphere depends only on the size of the area. This implies that the azimuth angle is uniformly distributed between 0 and 2π, and that cosθ is uniformly distributed between -1 and +1. **Note that it is cosθ, and not θ,** which is uniformly distributed, due to the fact that equal intervals in cosθ contain the same 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 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.

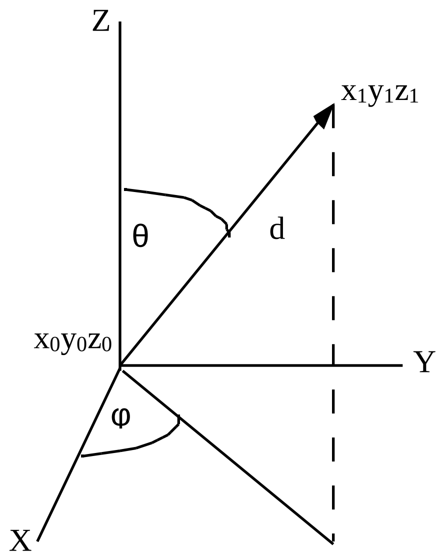


Figure 2

A neutron emitted at the point (xo, yo, zo) travels along a direction specified by the angles theta and phi.

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:

$$x_1 = x_o + d \sin(\theta) \cos(\varphi)$$

$$y_1 = y_o + d \sin(\theta) \sin(\varphi) \qquad (3)$$

$$z_1 = z_o + d \cos(\theta).$$

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. If we count the total number of times "N_{in}" that the neutron endpoints (x_1,y_1,z_1 like within the block for all N random fissions, we can compute the survival fraction f, using $f = N_{in}/N$.

Critical Mass

- If the mass of a fissionable material is less than the critical mass, the chain reaction will die out.
- Consider a neutron produced by spontaneous fission in a sphere of fissionable material. If the radius of the sphere is increased, the neutron can make more collisions with atoms before it reaches the surface, therefore, the probability of fission is increased.
- However, when the radius of the sphere is increased, the surface area of the sphere is increased, and the probability that the neutron will escape is increased. Thus, there are two competing effects.
- Increasing the volume raises the probability of fission, while increasing the surface area raises the probability of escape.
- Since volume is proportional to R^3 and the surface area to R^2, the volume increases more rapidly than the surface.
- For one value of R, the two effects are equal, and the neutrons causing fission just equal those lost at the surface.

Program to Calculate the Survival Fraction f

The objective of this computer simulation project is to develop a computer program that calculates the survival fraction "f" for a block of uranium of specified size and shape. The program will use numerical input data for the parameters M, S, and N, where:

- **M** = mass of the uranium block
- **S** = **a/b** (the ratio of the lengths of two of the sides of the block)
- **N** = number of random fissions to use in calculating f.

The program then finds the dimensions of the block (a and b) from the values of M and S. (The reason for inputting the values of M and S instead of a and b directly is to make it easier to study the dependence of the survival fraction f on the mass and shape of the block separately.) It is to be assumed that the units are such that the **density** of the block is equal to **one**, so that the mass and volume of the block are numerically equal. The mass or the volume of the sample can be expressed in terms of "a" and "b":

$$M = V = a^2 b = \frac{a^3}{S} = b^3 S^2 \,, \qquad (4)$$

where S = a/b. Using equation (2), an expression can be found for a and b in terms of M and S only:

$$a = (MS)^{1/3} \qquad\qquad b = \left(\frac{M}{S^2}\right)^{1/3} \;. \qquad (5)$$

The program proceeds to generate N random fissions, as explained in the previous section. To generate each random fission, it will be necessary to define nine random numbers $r_1, r_2, \ldots, r_9$ which lie between 0 and 1. The nine quantities needed for each random fission are obtained from the random numbers $r_1, r_2, \ldots, r_9$ according to the following equations:

$$x_0 = a(r_1 - \tfrac{1}{2})$$
$$y_0 = a(r_2 - \tfrac{1}{2}) \qquad \text{coordinates of the nucleus undergoing fission}$$
$$z_0 = a(r_3 - \tfrac{1}{2})$$

$$\varphi = 2\pi r_4 \;\text{ and }\; \cos(\theta) = 2(r_5 - 1/2) \qquad \text{two angles for one emitted neutron}$$

$$\varphi' = 2\pi r_6 \;\text{ and }\; \cos(\theta') = 2(r_7 - 1/2) \qquad \text{two angles for the other emitted neutron}$$

$$d = r_8 \;\text{ and }\; d' = r_9 \qquad \text{distances traveled by each neutron}$$

These formulas give the proper range for each of the nine parameters. The program computes the neutron endpoint using equation (1) and determines whether the point (x_1, y_1, z_1) lies within the block, in which case it adds 1 to the value of N_{in}, the number of induced fissions. After generating N random fissions, it computes the survival fraction $f = N_{in}/N$ and prints the result.

In finding the survival fraction f, we are actually integrating a function F of nine variables:

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

which represents the number of fissions induced by two emitted neutrons for particular values of the variables $x_0, y_0, \ldots d'$. 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 sun, 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 2^9 times or 512 calculations.

Procedure

1. Write a computer algorithm to calculate the critical mass as was described above.

2. 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** and the number of random fissions **N**. The critical mass is that mass for which the computed survival fraction "f" is equal to 1.0. A good strategy might be to use a relatively small value for N, say N = 100, until the computed values for "f" are in the vicinity of 1.0, and then use larger values for N to attain greater accuracy.

3. Find the critical mass using a number of values of S both less than one and greater than one. At least try s = 0.50 and s = 1.50. Explain the dependence you observe of the critical mass on the parameter S = a/b. It will be helpful to derive a relationship for the ratio of surface area to volume in terms of S.

4. Modify the program so that random fissions occur inside a spherical piece of uranium. Let the radius of the sphere be "a/2", half the base of the cube in part A. The density is still one, so the mass is equal to the volume. In this example there is no "S" ratio. The radius of the sphere will be determined from the value of the mass that is selected. Use the same technique as in the present version of the program to calculate the survival fraction "f", however, the positions of the atoms and neutrons will be compared to the radius of the sphere. Determine the critical mass of a sphere for a range of masses until the survival fraction is equal to one.