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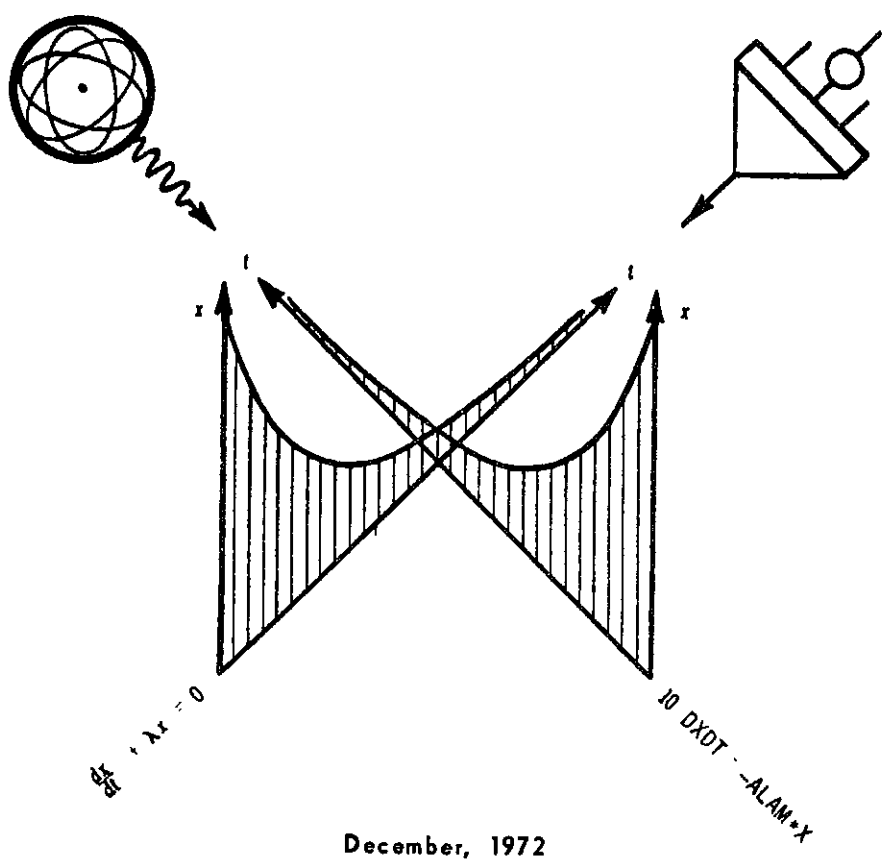
AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS

MATRICES AND NUMERICAL SOLUTION OF LINEAR EQUATIONS

REACTOR PHYSICS, MATHEMATICS AND COMPUTERS

SUMMER SCHOOL FOR TEACHERS

Lecture by G. DOHERTY



December, 1972

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by

G. DOHERTY

ABSTRACT

Matrices and numerical solution of linear equations are introduced through a simple model of a neutron life cycle in a nuclear reactor.

CONTENTS

1. INTRODUCTION

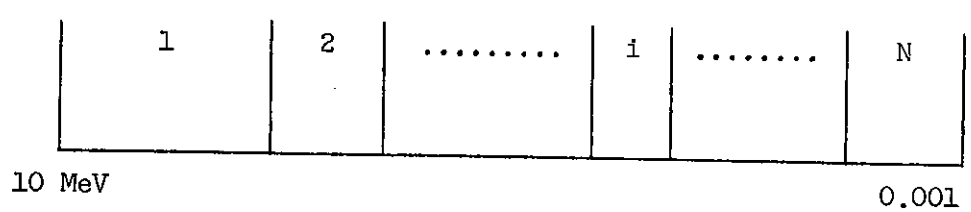
As an example of the kind of simultaneous linear equations which arise in reactor physics we will consider a simple model of the life cycle of a neutron in the reactor. Neutrons produced by the fission process have an average kinetic energy of about 2 MeV or a speed of about 2×10^7 metres per second. Neutron collisions with nuclei result either in absorption or scattering with probabilities which depend on the speed of the neutron and the type of nucleus involved in the collision. Absorption may give rise to further fission if the nucleus is Uranium otherwise the neutron is lost to the fission cycle. The relative probabilities for capture and fission in Uranium again depend on the speed of the neutron.

Neutron scattering collisions at high and low energies are quite different in character. At high energy the speed of the nucleus can be ignored and the neutron scatters as though from a stationary nucleus. If the nucleus is heavy the loss in energy of the neutron is small whatever the angle of scattering. If the nucleus is light then the neutron energy loss depends strongly on the angle of scattering. For example a head-on collision of a neutron with a hydrogen nucleus can reduce the neutron energy almost to zero.

The vibration energy of the atoms themselves is about 0.03 eV which corresponds to a neutron speed of about 2×10^3 metres per second. Once the neutron has slowed down to this sort of speed it is possible for the neutron to gain energy from a collision, so that the neutrons which are not absorbed come into thermal equilibrium with the motion of the scattering atoms.

2. NEUTRON LIFE CYCLE

Throughout the life of the reactor there will be neutrons with energies ranging from a few MeV down to say 10^{-3} eV. To calculate the number at each energy we usually divide the energy range into a number of boxes, called groups, say N, and calculate the number in each group.



The unknown number of neutrons in group i we shall call x_i.

Neutrons from fission are produced at high energies with a distribution which has been measured experimentally. The proportion of neutrons born in

group i we shall denote by y_i. Because no low energy neutrons are produced by fission we have $y_i = 0$ for large values of i.

For each group we calculate, from the measured probabilities for the individual isotopes, an average set of probabilities for each group.

p_{ai} = the probability that collision in group i will result in the neutron being absorbed, and

p_{ji} = the probability that collision in group i will scatter the neutron into group j.

Then we make the final assumption that the system is stationary with respect to time, i.e. the number of neutrons entering each group by fission or scattering is the same as the number leaving by absorption or scattering. If we consider group i,

y_i are produced from fission,

$p_{ij} x_j$ are scattered into group i from group j,

therefore, the total number entering the group is

$$y_i + \sum_j p_{ij} x_j \quad .$$

$p_{ai} x_i$ are absorbed in the group,

$p_{ji} x_i$ are scattered from group i into group j,

therefore, the total number leaving the group is

$$p_{ai} x_i + (\sum_j p_{ji}) x_i \quad .$$

Thus the equation for group i can be written

$$y_i + \sum_j p_{ij} x_j = p_{ai} x_i + (\sum_j p_{ji}) x_i \quad . \qquad \ldots(1)$$

A similar equation exists for each group so that to solve for the number of neutrons in each group we have only to obtain the solution of a set of simultaneous equations in x_i.

3. A SIMPLE EXAMPLE

To see what the equations look like we will suppose that there are only three groups. In practice, of course, many more groups are often used and one of our programmes uses 100,000 groups. With three groups we have three

equations. The equation for group 1 is

$$y_1 + p_{11} x_1 + p_{12} x_2 + p_{13} x_3 = p_{a1} x_1 + p_{11} x_1 + p_{21} x_1 + p_{31} x_1 \; . \qquad \ldots(2)$$

The first thing you will notice is that $p_{11} x_1$ is common to both sides so we may cancel it out. Equation (2) may be rearranged as follows:

$$(p_{a1} + p_{21} + p_{31}) x_1 - p_{12} x_2 - p_{13} x_3 = y_1 \; . \qquad \ldots(3)$$

Similarly the equations for the other two groups can be written

$$- p_{21} x_1 + (p_{a2} + p_{12} + p_{32}) x_2 - p_{23} x_3 = y_2 \qquad \ldots(4)$$

$$- p_{31} x_1 - p_{32} x_2 + (p_{a3} + p_{13} + p_{23}) x_3 = y_3 \; . \qquad \ldots(5)$$

With the appropriate assignment of coefficients a_{ij} we may write this set as

$$a_{11} x_1 + a_{22} x_2 + a_{13} x_3 = y_1 \qquad \ldots(6)$$

$$a_{21} x_1 + a_{22} x_2 + a_{23} x_3 = y_2 \qquad \ldots(7)$$

$$a_{31} x_1 + a_{32} x_2 + a_{33} x_3 = y_3 \qquad \ldots(8)$$

or in the matrix notation as

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{33} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \qquad \ldots(9)$$

4. SOLUTION METHODS

A variety of methods have been developed for solving sets of simultaneous equations and here we will briefly mention two. The first is systematic

elimination which will be familiar to all of you.

Subtract a_{21}/a_{11} times equation 6 from equation 7 and a_{31}/a_{11} times equation 6 from equation 8.

$$a_{11} x_1 + a_{12} x_2 + a_{13} x_3 = y_1 \quad \ldots(10)$$

$$a'_{22} x_2 + a'_{23} x_3 = y'_2 \quad \ldots(11)$$

$$a'_{32} x_2 + a'_{33} x_3 = y'_3 \quad \ldots(12)$$

where the coefficients with primes are

$$a'_{22} = a_{22} - \frac{a_{21}}{a_{11}} a_{12} \text{ etc.} \quad \ldots(13)$$

On the computer the matrix of coefficients is destroyed in the process of solution because we store a'_{22} in the same core location that previously assigned to a_{22}.

The next step is to subtract a'_{32}/a'_{22} times equation 11 from equation 12 so that the final result is

$$a_{11} x_1 + a_{12} x_2 + a_{13} x_3 = y_1 \quad \ldots(14)$$

$$a'_{22} x_2 + a'_{23} x_3 = y'_2 \quad \ldots(15)$$

$$a''_{33} x_3 = y''_3 \quad \ldots(16)$$

Then x_3, x_2, x_1 are obtained in turn from equations 16, 15 and 14.

The other method which we shall discuss is an iterative method. For this method we rewrite equations 6, 7, 8 in the form.

$$x_1 = \frac{1}{a_{11}} (y_1 - a_{12} x_2 - a_{13} x_3) \quad \ldots(17)$$

$$x_2 = \frac{1}{a_{22}} (y_2 - a_{21} x_1 - a_{23} x_3) \quad \ldots(18)$$

$$x_3 = \frac{1}{a_{33}} (y_3 - a_{31} x_1 - a_{32} x_2) \quad \ldots(19)$$

Then we start with trial values for x_2 and x_3 and solve equation 17. Using the result for x_1 and the trial value for x_3, equation 18 gives a new estimate of x_2. Then equation 19 gives a new estimate of x_3 and we begin again at equation 17.

This method is called Gauss Seidel iteration. It will not converge for some sets of coefficients and we do not have time to examine the convergence properties in detail. A sufficient condition is that

$$\left| a_{ii} \right| > \sum_{j \neq i} \left| a_{ji} \right|$$

which you can see is satisfied for the original set of equations 3, 4, 5. The rate of convergence is roughly determined by the magnitude of the ratio

$$\frac{\left| a_{ii} \right| - \sum_{j \neq i} \left| a_{ji} \right|}{\left| a_{ii} \right|}$$

The larger this ratio, the faster the method converges.

Large systems of equations were solved using variants of this method before computers were available. The iterative methods have the particular advantage that an isolated numerical mistake will be corrected by further iteration whereas similar mistakes in the elimination method would be fatal. We do not expect mistakes on the computer but in a large manual calculation they are almost inevitable.