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(U) Neutronics for Novices

XCP Summer Workshop 2018

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Los Alamos National Laboratory

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Part I: Particles, Reactions, and Cross Sections

LAP

- ▶ Fundamental Particles of Interest
- ▶ Basic Reactions
- ▶ Microscopic Cross Sections
- ▶ Macroscopic Cross Sections
- ▶ Cross Section Characteristics

Fundamental Particles of Interest

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Name	Charge	Rest Mass	Comment
Proton	+1	938.3 MeV	
Neutron	0	939.6 MeV	
Electron	-1	0.511 MeV	
Photon (γ)	0	0	$E = \hbar\nu$
β^- particle	-1	0.511 MeV	electron
β^+ particle	+1	0.511 MeV	positron, anti-electron
α particle	+2	3727.4 MeV	positron, anti-electron

$$1 \text{ amu} = \frac{1}{12} m(^{12}\text{C}) = 931.5 \text{ MeV} = 1.66 \times 10^{-27} \text{ kg}$$

Nuclear Notation

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Chemical symbol = X

Atomic number (proton count) = Z

Mass number (proton + neutron count) = A

Energetically excited = $*$

A Whole Lotta Nothin'

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- ▶ Nuclear radius is about $1.25 \times 10^{-13} A^{\frac{1}{3}}$ cm, so the volume per nucleon is constant.
- ▶ Atomic radius is about 2×10^{-8} cm
- ▶ An iron atom ($A=56$) is only about 1.4×10^{-14} “stuff”

Binding Energy

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Theory asserts and measurement confirms that the nuclear mass

$$m\left({}^A_ZX\right) < (A - Z) m_n + Z m_p$$

The difference is known as the *mass defect* and indicates conversion of some of the nucleons' mass into *binding energy* that holds the nucleus together against the Coulombic repulsion of its protons. The binding energy is the amount of energy that would be required to separate the nucleus completely into free protons and neutrons.

Binding Energy

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A plot of binding energy per nucleon as a function of nucleon count shows the tendency of light nuclei to fuse and heavy nuclei to fission:

Nuclear Stability

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If we plot the nuclides in $N = A - Z$ and Z space (next slide), we see that a *band of stability* exists.

For light nuclei, stability occurs when $N : Z$ is about 1. As nuclei grow heavier the ratio for stability rises to about 1.5.

Outside the band of stability, nuclei transition to stable states through a number of mechanisms.

Nuclear Stability

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Common Radioactive Decay Modes

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Mode	Notation	Comments
Photon emission	${}^A_ZX^* \rightarrow {}^A_ZX + \gamma$	Discrete energy
α decay	${}^A_ZX \rightarrow {}^{A-4}_{Z-2}Y + \alpha$	Discrete energy
β^- decay	${}^A_ZX \rightarrow {}^A_{Z+1}Y + \beta^-$	Continuous energy
β^+ decay	${}^A_ZX \rightarrow {}^A_{Z-1}Y + \beta^+$	Continuous energy
K-capture	${}^A_ZX + e^- \rightarrow {}^A_{Z-1}Y^+$	Continuous energy

- ▶ α decay is typical of heavier-than-lead isotopes
- ▶ β^- decay is typical of neutron-rich isotopes
- ▶ β^+ decay is typical of neutron-deficient isotopes
- ▶ K-capture competes with β^+ decay

Chains are common: ${}^{20}_8O \rightarrow {}^{20}_9F \rightarrow {}^{20}_{10}Ne$

Basic Neutron-Nuclear, or *Neutron-Induced*, Reactions

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- ▶ Potential (Elastic) scattering
- ▶ Compound nucleus formation
 - ▶ Radiative capture
 - ▶ Fission
 - ▶ Particle emission (n,2n), (n,3n), (n,p), (n, α), ...
 - ▶ Inelastic scattering

Potential Scattering

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Potential scattering is an interaction in which the trajectory and energy of the incident neutron are altered by the potential of the nucleus. The lighter the nucleus, the greater a fraction of the neutron's kinetic energy can be transferred to it. 1H can stop a neutron in its tracks, while ^{235}U can absorb less than 1% of the neutron's kinetic energy.

Compound Nucleus Formation

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It takes an average neutron about 10^{-17} s to pass through a nucleus. Many reactions occur about 10^{-14} s after the neutron-nucleus interaction begins. This indicates formation of an excited *compound nucleus*:

The excited compound nucleus will take some time to figure out its place in the universe, then reduce its energy state through a process such as photon emission, fission, or ejection of one or more particles.

Compound Nucleus Decay

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Radiative capture: the nucleus de-excites by emitting one or more photons to drop between energy levels. The energy of the γ photon will be the difference between the levels. Multiple emissions are possible. This reaction is neutronically parasitic and hence undesirable for sustaining chain reactions.

Fission: the nucleus fractures into (typically) two *fission fragments*, some free neutrons, some photons, and a *lot* of energy distributed kinetically among the particles. More on fission in its own presentation.

Particle ejection: the nucleus ejects one or more simple particles, leaving behind a different nucleus in an energetically-stable state.

Inelastic scatter: the nucleus ejects a neutron traveling in a different direction with a different energy than that of the incident neutron. The nucleus typically remains in an excited state relieved through photon emission. This is a threshold reaction, important for slowing down high-energy neutrons.

Reaction Notation

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Typically we view a nuclear reaction as a two-body interaction between a moving light particle and an at-rest nucleus.

The usual output is a compound nucleus or a different two-body system subject to conservation of momentum, charge, mass-energy, and nucleon total.

The reaction is written

Nucleus(Particle, Product Particle)Product nucleus

and is referred to as a (Particle, Product Particle) reaction; e.g., an (n, α) reaction.

Reaction Notation Examples

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- ▶ ${}^9\text{Be}(\alpha, n) {}^{12}\text{C}$
- ▶ ${}^{16}\text{O}(n, p) {}^{16}\text{N}$
- ▶ ${}^{235}\text{U}(n, \gamma) {}^{236}\text{U}$
- ▶ ${}^{239}\text{Pu}(n, 2n) {}^{238}\text{Pu}$

Microscopic Cross Sections

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Consider a plane wave of monoenergetic neutrons with beam intensity I /nt/cm²/s. The wave is normally incident on a target one atomic layer thick (so that nuclei don't block each other's view of neutrons) with areal density N_A nuclei/cm²:

Microscopic Cross Sections

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The neutron-nucleus interaction rate density $R = \sigma \times I \times N_A$. The proportionality constant σ is called the *microscopic cross section* and characterizes the probability of a neutron-nucleus interaction.

Microscopic cross sections are on the order of 10^{-24} cm^2 , a unit called the *barn*.

The microscopic cross section is akin, but not identical, to the geometric cross section presented by the nucleus to the neutron. Quantum effects mean that reaction cross sections are often many orders of magnitude removed from the geometric cross section.

Most microscopic cross sections are functions only of the incident neutron energy.

Microscopic Cross Sections

LAP

Since microscopic cross sections represent a probability of reaction, they can be decomposed into additive terms representing the probability of mutually exclusive reactions:

$\sigma_t = \sigma_s + \sigma_a$, where σ_t is the *total* cross section representing the probability of any reaction, σ_s is the *scattering* cross section representing the probability of a scattering reaction, and σ_a is the *absorption* cross section representing the probability of an absorption reaction.

These too can be decomposed; *e.g.*, absorption includes fission, radiative capture, and particle ejection. This is shown on the next slide.

Microscopic Cross Sections

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The Differential Scattering Cross Section

LAP

The scattering cross section σ_s is unlike other cross sections. In scattering we are concerned not just with the probability that a scattering reaction occurs, but that a particular reaction that scatters a neutron from one specific angle into another specific angle. This is reflected by the *differential scattering cross section*.

If a neutron traveling in a direction Ω with energy E is scattered into a new direction Ω' with energy E' , the differential scattering cross section is written as

$$\sigma_s(\Omega \rightarrow \Omega', E \rightarrow E')$$

The differential scattering cross section must integrate over all destination directions and energies to the scattering cross section; that is,

$$\int_{\Omega}' \int_E' \sigma_s(\Omega \rightarrow \Omega', E \rightarrow E') dE' d\Omega' = \sigma_s(E)$$

Treatment of the differential scattering cross section is one of the more difficult problems in neutron transport.

Cross Section Resonances

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If the kinetic energy of the incoming neutron is such that the total energy of the compound nucleus is very near an excitation level then the probability of compound nucleus formation (the magnitude of the cross section) rises. Such a local increase is called a *resonance*.

At lower energies, resonances are discrete and widely spaced. At higher energies they begin to overlap and at still higher energies they are effectively continuous.

Treatment of resonance regions is one of the more difficult problems in neutron transport.

Macroscopic Cross Sections

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Now consider a plane wave of monoenergetic neutrons with initial beam intensity I_0 /nt/cm²/s normally incident on a thick target with density N nuclei/cm³:

Macroscopic Cross Sections

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The differential neutron-nucleus interaction rate density in a slice dx thick at x is

$$dR = \sigma \times I \times dN_A = \sigma \times I \times (Ndx),$$

so the change in intensity of unreacted neutrons is

$$dI = -dR = -I \times N\sigma \times dx.$$

This is the typical first-order attenuation problem with solution

$$I(x) = I_0 e^{-N\sigma x}.$$

The product of nuclear density N and microscopic cross section σ occurs frequently enough that we give it its own name, the *macroscopic cross section* and symbol, Σ .

Macroscopic Cross Sections

LAP

The macroscopic cross section represents the probability of a reaction with a nucleus per unit length traveled by a neutron. Units are inverse length.

Microscopic cross sections are intrinsic to a nucleus; macroscopic cross sections are extrinsic to the quantity of nuclei.

Microscopic cross sections are functions of energy and nuclear density is a function of space and time, so the macroscopic cross section is a function of space, time, and energy.

Macroscopic Cross Sections

LAP

Macroscopic cross sections can be decomposed by reaction the same way that microscopic cross sections can:

$$\Sigma_t = N\sigma_t = N(\sigma_s + \sigma_a) = N\sigma_s + N\sigma_a = \Sigma_s + \Sigma_a$$

Macroscopic cross sections for mixtures are additive as well. For a mix of nuclei x , y , and z ,

$$\Sigma = N_x\sigma^x + N_y\sigma^y + N_z\sigma^z = \Sigma^x + \Sigma^y + \Sigma^z$$

Mean Free Path, Collision Frequency, and Mean Lifetime

LAP

From the exponential solution for beam intensity we observe that the probability of a neutron traveling a distance x without undergoing a reaction is $e^{-\Sigma x}$.

The probability of a neutron undergoing its first reaction in dx after traveling a distance x is $p(x) = e^{-\Sigma x} \Sigma$.

The *mean free path* λ is the average distance traveled by a neutron between reactions: $\lambda = \int_0^\infty p(x) dx = \frac{1}{\Sigma}$.

If the neutrons are traveling with velocity v then $v\Sigma$ is the *collision frequency* and $\frac{1}{v\Sigma}$ is the *mean lifetime*, the average time between reactions.

Part II: Fission -n- Stuff

LAP

- ▶ What Is Fission?
- ▶ Fission Energy Distribution
- ▶ Fissile vs Fissionable
- ▶ Fission Products
- ▶ Fission Neutrons
- ▶ Chain Reactions
- ▶ Multiplication Factor k and Rate α

Part II: Fission -n- Stuff

LAP

(Binary) fission in a nuclear reaction in which an excited heavy nucleus reduces its total internal energy by breaking into several (usually two) lighter nuclei called *fission fragments*, accompanied by the release of a handful of fundamental particles, esp. neutrons.

Fission can occur spontaneously but is usually induced by bombarding a nucleus with neutrons, protons, or gamma rays to create an excited/compound nucleus.

Stages in Fission

LAP

Fission Reaction Products

LAP

Fission Energetics

LAP

The energy released by fission depends on the fissioning isotope and incident neutron energy but is generally around 200 MeV. About 5% is carried away by neutrinos and another 5% released by the radioactive decay of long half-life fission products, so the effective energy release is considered to be 180 MeV/f.

Reaction product	Energy (% of 200 MeV)	Timing
Fission fragment KE	80	Instantaneous
Fast neutrons	3	Instantaneous
Fission γ s	4	Instantaneous
Fission fragment β decay	4	Delayed
Neutrino emission	5	Delayed
Capture nonfissions	4	Delayed

Fission 1 lb $^{235}\text{U} \approx 1$ kton coal ≈ 100 kgal gasoline

Fissile vs Fissionable

LAP

Isotopes which undergo fission are divided into two groups:

1. *Fissile* isotopes are capable of being fissioned by a neutron essentially at rest; that is, the additional binding energy of the compound nucleus is sufficient to cause fission. These isotopes typically have an odd mass number A (^{235}U).
2. *Fissionable* isotopes are capable of being fissioned by a neutron with enough kinetic energy to overcome a threshold of several MeV; that is, the additional binding energy of the compound nucleus is *not* sufficient to cause fission. These isotopes typically have an even mass number A (^{238}U).

The word “fissile” is often used to describe any isotope that can be induced to fission, both the truly fissile and the merely fissionable. While a given isotope with mass number A is described as fissile or fissionable, it is actually the compound nucleus with mass number $A+1$ that fissions.

Fission Fragment Mass Distribution

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Fission fragment mass distribution is asymmetric in A and Z . Symmetric fission is less probable than a split roughly at a 3:2 mass ratio:

Mass ≈ 90

- Kr
- Br
- Sr
- Rb

Mass ≈ 140

- I
- Xe
- Cs
- Ba

Fission Product Decay

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Many fission product nuclei are themselves unstable and will quickly emit simple particles like γ , β , α , or neutrons, often in sequence, to lower their energy:

Fission Neutron Production

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Between 0 and 6-ish neutrons are released per fission, depending on the isotope and the energy of the incident neutron. The number roughly follows a Poissonian distribution around the average ($P(n) = e^{-\bar{\nu}} \frac{\bar{\nu}^n}{n!}$), with the average number of released neutrons $\bar{\nu}(E) = \nu_0 + aE$:

Fission Neutron Distribution

LAP

Fission neutrons are emitted isotropically with a continuous energy spectrum $\chi(E)$:

Fission spectrum for thermal fission in ^{235}U .

Fission Chain Reactions

LAP

Our ultimate goal is to produce self-sustaining chain reactions; that is, a process in which neutrons emitted by fission induce subsequent fissions. How neutron populations rise and fall is key to what we do and a solid understanding of the process and its terminology is essential.

Consider neutrons born into a particular generation. They might leak from the system, or be absorbed parasitically, or induce fissions:

Multiplication Factor k

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The ratio of populations in successive generations is the *multiplication factor*, typically written k .

If $k < 1$, the neutron population is falling from generation to generation and the system is said to be *subcritical*. If $k > 1$, the neutron population is rising from generation to generation and the system is said to be *supercritical*. If $k = 1$, the neutron population is constant from generation to generation and the system is said to be *critical*.

Multiplication Rate α

LAP

Let the average time between generations be l . Based on the definition of the multiplication factor, the neutron population growth rate is:

$$\frac{dn}{dt} = \frac{(k-1)n}{l} = \alpha n$$

The *multiplication rate* α governs the magnitude of the neutron population over time. Subcriticality means $\alpha < 0$ while supercriticality means $\alpha > 0$. The population follows simple first-order kinetics:

$$n(t) = n(t_0) e^{\alpha(t-t_0)}$$

If $\alpha(t - t_0) = 1$, the population increases by a factor of e . The time α^{-1} is called the *period* or the *e-folding time*.

Time-dependent α

LAP

We can rewrite

$$\alpha = \frac{1}{n} \frac{dn}{dt} = \frac{d \ln(n)}{dt},$$

that is, recognize the multiplication rate as the logarithmic derivative of the population. For time-varying system properties k and/or l we define a time-dependent multiplication rate as

$$\alpha(t) = \frac{d \ln(n(t))}{dt},$$

with solution

$$n(t) = n(t_0) e^{\int_{t_0}^t \alpha(\tau) d\tau}$$

Part III: Deriving the Neutron Transport Equation

LAP

Neutron transport is the study of neutron distribution within a system. If we know the neutron population then we can calculate criticality, reaction rates, radiation emission, and similar quantities.

The determination of the neutron distribution within a system is a challenging problem. This presentation includes

- ▶ A derivation of the transport equation
- ▶ Reduction to homogeneous/eigenvalue form

The Neutron Flux

LAP

Define the *neutron density* at any point $\hat{r}$ in a system as $n(\hat{r}, t)d\hat{r}$ = the number of neutrons in the differential volume $d\hat{r}$ around $\hat{r}$ at time t .

Recall from Part I that $v\Sigma_r$ is the frequency at which reactions of type r occur. The reaction rate density for type r reactions is therefore

$$R_r(\hat{r}, t)d\hat{r} = n(\hat{r}, t)v\Sigma_r d\hat{r}$$

The quantity nv occurs frequently enough that it is given its own name, the *neutron flux*, and symbol, ϕ . Note that unlike the entire world, nuclear engineers use the term “flux” for a scalar, not vector, quantity.

Neutron Flux Definitions

LAP

The preceding definition is easily extended to include a dependence on the incident neutron energy E and direction $\hat{\Omega}$: $n(\hat{r}, \hat{\Omega}, E, t)d\hat{r}d\hat{\Omega}dE$ = the expected number of neutrons in $d\hat{r}$ traveling in $d\hat{\Omega}$ and dE at t .

Define the *angular neutron flux* as

$$\varphi(\hat{r}, \hat{\Omega}, E, t) = n(\hat{r}, \hat{\Omega}, E, t)v(E)$$

and the *angular current density* as

$$\hat{j}(\hat{r}, \hat{\Omega}, E, t) = \hat{\Omega}\varphi(\hat{r}, \hat{\Omega}, E, t)$$

Since $\hat{\Omega}$ is a unit vector, the angular neutron flux is the magnitude of the vector quantity angular current density.

The quantity $\hat{j}(\hat{r}, \hat{\Omega}, E, t) \cdot d\hat{A}d\hat{\Omega}dE$ = the number of neutrons with energy in dE traveling in $d\hat{\Omega}$ passing through the differential area $d\hat{A}$ at t :

Derivation

LAP

Consider the traditional control volume with volume V and surface area A :

The number of neutrons with energy in dE traveling in direction $d\hat{\Omega}$ within the control volume at some time t is given by

$$\left(\int_V n(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE$$

The rate of change of this quantity is equal to the difference in production and loss of neutrons, so we identify all mechanisms of production and loss within the control volume and write a balance equation.

Mechanisms for gain

- ▶ (1) Neutron sources within V , such as fissioning nuclei
- ▶ (2) Neutrons streaming into V through the boundary A
- ▶ (3) Neutrons in $(\hat{\Omega}', E')$ scattering within V into $(\hat{\Omega}, E)$

Mechanisms for loss

- ▶ (4) Neutrons streaming out of V through the boundary A
- ▶ (5) Neutrons within V undergoing neutron-nucleus collisions removing them from $(\hat{\Omega}, E)$

We now derive expressions for each of these terms.

(1) Source Gains

LAP

Define the source density $s(\hat{r}, \hat{\Omega}, E, t) d\hat{r} d\hat{\Omega} dE dt$ as the rate at which neutrons appear in $d\hat{r}$ around $\hat{r}$ traveling in direction $d\hat{\Omega}$ around $\hat{\Omega}$ within dE around E at time t then the source gain of term (1) is

$$\left(\int_V s(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE$$

(5) Collision Losses

LAP

Recall that the reaction rate density for collisions at $\hat{r}$ of neutrons of energy E traveling in direction $\hat{\Omega}$ at t is

$$R(\hat{r}, \hat{\Omega}, E, t) = \Sigma_t(\hat{r}, E, t) \varphi(\hat{r}, \hat{\Omega}, E, t)$$

so the collision loss term (5) is

$$\left(\int_V \Sigma_t(\hat{r}, E, t) \varphi(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE$$

(3) Scattering gains

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From the definition of the differential scattering cross section, the rate at which neutrons arrive in $(\hat{\Omega}, E)$ from $(\hat{\Omega}', E')$ is

$$\Sigma_s(\hat{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E, t) \varphi(\hat{r}, \hat{\Omega}', E', t)$$

so the total rate at which neutrons arrive in $(\hat{\Omega}, E)$ is

$$\int_0^\infty \int_{4\pi} \Sigma_s(\hat{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E, t) \varphi(\hat{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE'$$

and the total rate at which neutrons *inscatter* is

$$\left(\int_V \int_0^\infty \int_{4\pi} \Sigma_s(\hat{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E, t) \varphi(\hat{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' d\hat{r} \right) d\hat{\Omega} dE$$

(2),(4) Streaming Gains and Losses

LAP

Using the definition of the angular current density, the rate at which neutrons of energy E traveling in direction $\hat{\Omega}$ at t stream through the differential area $d\hat{A}$ on the control volume's surface is $\hat{j}(\hat{r}, \hat{\Omega}, E, t) \cdot d\hat{A}d\hat{\Omega}dE$. The total leakage through the surface (4)-(2) is therefore

$$\int_A \hat{j}(\hat{r}, \hat{\Omega}, E, t) \cdot d\hat{A}d\hat{\Omega}dE$$

The Green-Gauss theorem allows us to rewrite this area integral as the volume integral of the divergence of the integrand:

$$\left(\int_V \nabla \cdot \hat{j}(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega}dE$$

$$\left(\int_V \hat{\Omega} \cdot \nabla \varphi(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega}dE$$

Putting it all back together, we have

$$\frac{\partial}{\partial t} \left(\int_V n(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE = (1) + (3) - ((4) - (2)) - (5)$$

Since the control volume is independent of time,

$$\left(\int_V \frac{\partial}{\partial t} n(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE = (1) + (3) - ((4) - (2)) - (5)$$

or using the definition of scalar flux,

$$\left(\int_V \frac{1}{v} \frac{\partial}{\partial t} \varphi(\hat{r}, \hat{\Omega}, E, t) d\hat{r} \right) d\hat{\Omega} dE - (1) - (3) + ((4) - (2)) + (5) = 0$$

The control volume is arbitrary, so the integrand=0:

$$\frac{1}{v} \frac{\partial}{\partial t} \varphi(\hat{r}, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \varphi(\hat{r}, \hat{\Omega}, E, t) + \Sigma_t(\hat{r}, E, t) \varphi(\hat{r}, \hat{\Omega}, E, t) = \int_0^\infty \int_{4\pi} \Sigma_s(\hat{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E, t) \varphi(\hat{r}, \hat{\Omega}', E', t) d\hat{\Omega}' dE' + s(\hat{r}, \hat{\Omega}, E, t)$$

The initial condition is some predefined distribution:

$$\varphi(\hat{r}, \hat{\Omega}, E, t_0) = \varphi_0(\hat{r}, \hat{\Omega}, E)$$

The boundary condition typically takes advantage of non-reentrance, so

$$\varphi(\hat{r}_A, \hat{\Omega}, E, t) = 0$$

for $\hat{r}_A$ on the boundary and $\hat{\Omega} \cdot \hat{n} < 0$.

Introduction to Transport Solution Methods

LAP

There are two ways of solving the transport equation computationally:

- ▶ probabilistic (Monte Carlo)
- ▶ deterministic (discretized linear system)

Probabilistic methods solve the transport equation as derived, but include a statistical uncertainty that can require tremendous computational effort to reduce.

Deterministic methods discretize/approximate the transport equation to produce a linear system of equations. Tremendous computational effort can be required here to reduce the “order error” of the discretizations.

Part IV: The Monte Carlo Method

LAP

Covered by others.

Part V: Deterministic Methods

LAP

- ▶ Introduction
- ▶ Deterministic Methods
- ▶ Reduction to Multigroup
- ▶ Finite Elements
- ▶ Harmonic Expansion
- ▶ Discrete Ordinates

A Quick Description of Deterministic Methods

LAP

Using numerical approximations for the functions that appear in the transport equation allows reduction of the equation to a linear system of equations that can be solved with your matrix solver of choice. These approximations are called *deterministic methods*.

The independent variables of the transport equation are treated with approximations relevant to their type. In order, we'll discuss energy, space, angle, and time treatments.

Multigroup Energy Treatment

LAP

In nearly every deterministic approach we begin by subdividing the energy spectrum into groups within which nuclear properties and fluxes are piecewise constant. This is the so-called *multigroup* formulation. In general group boundaries are selected uniformly in lethargy (the negative logarithm of energy) as that approach best captures neutron behavior in a purely-scattering medium. Boundaries can be further refined to resolve phenomena of interest.

The groups are numbered sequentially from group 1 containing the highest-energy neutrons to group G containing the lowest-energy neutrons.

Define a group-average flux $\varphi_g = \int_{E_g}^{E_{g-1}} \varphi(E) dE$ (ignoring other variables for momentary simplicity).

The group-averaged cross section for reactions of type r is defined as:

$$\Sigma_{rg} = \frac{\int_{E_g}^{E_{g-1}} \Sigma_r(E) \varphi(E) dE}{\varphi_g}$$

These definitions preserve reaction rates within an energy group.

Since group constants preserve reaction rates, it is possible to perform “group collapsing” to reduce the problem size. For example, collapsing groups g and $g-1$ to group g' would be done as

$$\begin{aligned} \varphi_{g'} &= \varphi_g + \varphi_{g-1} \\ \Sigma_{rg'} &= \frac{\Sigma_{rg} \varphi_g + \Sigma_{r,g-1} \varphi_{g-1}}{\varphi_{g'}} \end{aligned}$$

By integrating from E_g to E_{g-1} , the single transport equation in seven independent variables becomes a set of G equations in six independent variables coupled through fission source and scattering terms:

$$\begin{aligned} \frac{1}{v_g} \frac{\partial}{\partial t} \varphi_g(\hat{r}, \hat{\Omega}, t) + \hat{\Omega} \cdot \nabla \varphi_g(\hat{r}, \hat{\Omega}, t) + \Sigma_{t_g}(\hat{r}, t) \varphi_g(\hat{r}, \hat{\Omega}, t) = \\ \sum_{g'=1}^G \int_{4\pi} \Sigma_{sg'g}(\hat{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, t) \varphi_{g'}(\hat{r}, \hat{\Omega}', t) d\hat{\Omega}' + \\ \frac{\chi_g}{4\pi} \sum_{g'=1}^G \int_{4\pi} \bar{\nu}_{g'} \Sigma_{fg'}(\hat{r}, t) \varphi_{g'}(\hat{r}, \hat{\Omega}', t) d\hat{\Omega}' + S_g(\hat{r}, \hat{\Omega}, t) \end{aligned}$$

for $1 \leq g \leq G$, subject to

$$\varphi_g(\hat{r}, \hat{\Omega}, t_0) = \varphi_{g_0}(\hat{r}, \hat{\Omega})$$

and

$$\varphi_g(\hat{r}_A, \hat{\Omega}, t) = 0, \hat{r}_A \text{ on the surface and } \hat{\Omega} \cdot \hat{n} < 0.$$

Isolating the scattering, fission, and inhomogeneous sources we have

$$\frac{1}{v_g} \frac{\partial}{\partial t} \varphi_g(\hat{r}, \hat{\Omega}, t) + \hat{\Omega} \cdot \nabla \varphi_g(\hat{r}, \hat{\Omega}, t) + \Sigma_{tg}(\hat{r}, t) \varphi_g(\hat{r}, \hat{\Omega}, t) = S_{sg} + S_{fg} + S_g$$

Each of these sources will be handled in an appropriate manner.

Note that the multigroup formulation of the continuous problem is only “correct” if we

- ▶ already know the continuous solution
- ▶ know the continuous solution for a similar problem, or
- ▶ iterate over fluxes and cross sections to some convergence

Finite Elements

LAP

In the finite element method, the problem domain is decomposed into a number of elements with nodes at their vertices, within which the flux is expressed as a (usually linear) combination of nodal values. A weighted residual or discontinuous Galerkin method is employed to produce a set of equations for the nodal values.

A shortcoming of the finite element method is that it imposes an averaging over the problem domain, allowing nonphysical solutions to exist locally while still satisfying the transport equation globally. This may not be acceptable.

Orthogonal Function Expansion

LAP

The orthogonal function expansion technique expands the neutron flux and source terms into a set of basis functions (typically spherical harmonics in the angular variables). Orthogonality conditions are applied to derive sets of equations for the expansion coefficients. This is the so-called P_n approximation. The simplest case uses Cartesian coordinates to describe position and spherical coordinates to describe direction:

LAP

The streaming operator is

$$\boldsymbol{\Omega} \cdot \nabla \varphi = \mu \frac{\partial \varphi}{\partial x} + \eta \frac{\partial \varphi}{\partial y} + \xi \frac{\partial \varphi}{\partial z}$$

where the direction cosines are

$$\begin{aligned}\mu &= \cos \phi \\ \eta &= \sqrt{1 - \mu^2} \cos \omega \\ \xi &= \sqrt{1 - \mu^2} \sin \omega\end{aligned}$$

and

$$d\boldsymbol{\Omega} = d\mu d\omega$$

The differential scattering cross section's angular dependence is generally a function of the angle between incoming and outgoing direction vectors; that is, a function of $\mu_0 = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}'$. Write the differential scattering cross section in a Legendre expansion as

$$\Sigma_{g'g}(\hat{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, t) = \Sigma_{g'g}(\hat{r}, \mu_0, t) = \sum_{l=0}^L \frac{(2l+1)}{4\pi} \Sigma_{g'g}^l(\hat{r}, t) P_l(\mu_0),$$

where

$$\Sigma_{g'g}^l(\hat{r}, t) = 2\pi \int_{-1}^1 \Sigma_{g'g}(\hat{r}, \mu_0, t) P_l(\mu_0) d\mu_0$$

The truncation index L should be large enough to provide an accurate representation of the differential scattering cross section.

Write μ_0 in terms of the polar variables:

$$\mu_0 = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}' = \mu\mu' + \sqrt{1 - \mu^2} \sqrt{1 - \mu'^2} \cos(\omega - \omega')$$

and write the Legendre polynomial $P_l(\mu_0)$ as

$$P_l(\mu_0) = \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}^*(\mu', \omega') Y_{lm}(\mu, \omega),$$

where the Y_{lm} are spherical harmonic functions.

The truncation index L should be large enough to provide an accurate representation of the differential scattering cross section.

The flux and source terms are also written with spherical harmonic expansions in the angular variables, *e.g.*:

$$\varphi_g(\hat{r}, \boldsymbol{\Omega}, t) = \sum_{l=0}^L \sum_{m=-l}^l \varphi_{gl}^{(m)}(\hat{r}, t) Y_{lm}(\mu, \omega),$$

where

$$\varphi_{gl}^{(m)}(\hat{r}, t) = \int_{-1}^1 \varphi_g(\hat{r}, \boldsymbol{\Omega}, t) Y_{lm}^*(\mu, \omega) d\omega d\mu$$

The truncation index L should be large enough to provide an accurate representation of the differential scattering cross section.

Combining all this into the scattering source term and taking advantage of orthogonality, we get

$$S_{sg} = \sum_{g'=1}^G \sum_{l=0}^L \Sigma_{g'g}^l(\hat{r}, t) \sum_{m=-l}^l \varphi_{g'l}^{(m)}(\hat{r}, t) Y_{lm}(\mu, \omega)$$

We can rewrite the entire transport equation in terms of the harmonic expansion functions $Y_{lm}(\Omega)$. The next step in the orthogonal function solution technique is to multiply the equation by a different function $Y_{l'm'}^*(\Omega)$ and integrate over $d\Omega$, this “sifting” out a set of equations for the expansion coefficients.

If we do this, however, the presence of Ω in the streaming term leads to

$$\sum_{l=0}^L \sum m = -l^l \int Y_{l'm'}^*(\Omega) Y_{l'm'}^*(\Omega) \Omega \cdot \nabla \varphi_{gl}^{(m)}(\hat{r}),$$

which does not readily simplify. Additive relationships between the spherical harmonics allow this term to be written as a set of coupled flux moments (7 in 3D, 3 in 1D) but this coupling makes computational solution impractical.

The resolution of differential scattering via expansion has value even without a full expansion treatment. If we renumber the harmonics we can write

$$S_{sg}(\hat{r}, \boldsymbol{\Omega}, t) = \sum_{g'=1}^G \sum_{n=1}^{NM} (2l+1) \Sigma_{g'g}^l(\hat{r}, t) R_n(\mu, \omega) \varphi_{g'n}(\hat{r}),$$

where NM is the total number of moments, R_n is the spherical harmonic function corresponding to the simple index n , and $\varphi_{g'n}$ is the n^{th} flux moment in group g' .

This approximation proves to be computationally well-behaved as well as easily programmed. As a result, the harmonic expansion of differential scattering is typically used even when applying a different overall technique like discrete ordinates.

A key advantage of spherical harmonic expansion is its immunity to the so-called “ray effects” found in the less-costly discrete ordinates methods. If ray effect minimization is needed, a pure P_n expansion technique may justify the higher computational cost.

Discrete Ordinates

LAP

In the discrete ordinates method, the angular variable Ω is allowed to take on only certain discrete values. Angular integration is done via weighted sums. The choice of ordinates and weights is made to satisfy

- ▶ physical symmetries
- ▶ accurate representation of differential scattering, and
- ▶ simple representation of derivatives w/r/t angle

The angular variable Ω is allowed to take on certain discrete values Ω_p , each associated with a weight w_p defined as

$$w_p = \int_{\Omega_p} d\Omega$$

Put another way, the direction Ω_p is equivalent to a point on a unit sphere with associated surface area w_p .

The transport equation for a given energy group is

$$\boldsymbol{\Omega} \cdot \nabla \varphi(\hat{r}, \boldsymbol{\Omega}) + \Sigma_t(\hat{r}) \varphi(\hat{r}, \boldsymbol{\Omega}) = S_s(\hat{r}, \boldsymbol{\Omega}) + S_f(\hat{r}) + S(\hat{r}, \boldsymbol{\Omega}),$$

where the three RHS terms represent scattering, isotropic fission, and inhomogeneous sources.

If we integrate this equation over $\boldsymbol{\Omega}_p$ and define a stream average flux as

$$\varphi_p(\hat{r}) = w_p^{-1} \int_{\boldsymbol{\Omega}_p} \varphi(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega},$$

then

the transport equation for a given energy group is

$$\int_{\Omega_p} \boldsymbol{\Omega} \cdot \nabla \varphi(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega} + w_p \Sigma_t(\hat{r}) \varphi_p(\hat{r}) = \int_{\Omega_p} S_s(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega} + w_p S_f(\hat{r}) + \int_{\Omega_p} S(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega}$$

where the three RHS terms represent scattering, isotropic fission, and inhomogeneous sources.

Two terms are of particular interest: the streaming quantity $\int_{\Omega_p} \boldsymbol{\Omega} \cdot \nabla \varphi(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega}$ and the scattering source $\int_{\Omega_p} S_s(\hat{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega}$. (Take the angular dependence of an inhomogeneous source as given.)

Discrete Streaming

LAP

Integration of the transport equation over a spherical area (versus direct evaluation at a given direction) permits the conservation of streamed neutrons and provides a more accurate numerical solution. Accordingly, we need to express the streaming operator in its conservative form.

Cartesian

LAP

Let μ, η, ξ be the direction cosines of Ω relative to the Cartesian axes x, y, z :

The streaming operator $\Omega \cdot \varphi$ is

$$\mu \frac{\partial \varphi}{\partial x} + \eta \frac{\partial \varphi}{\partial y} + \xi \frac{\partial \varphi}{\partial z}$$

Cylindrical

LAP

Let μ, η, ξ be the direction cosines of Ω relative to the cylindrical axes r, θ, z . Let ω be the angle between the radial direction and the projection of Ω into the r, θ plane:

The direction cosines are $\mu = \sqrt{1 - \xi^2} \cos \omega$ and $\eta = \sqrt{1 - \xi^2} \sin \omega$. The streaming operator $\Omega \cdot \varphi$ is

$$\frac{\mu}{r} \frac{\partial(r\varphi)}{\partial r} + \frac{\eta}{r} \frac{\partial\varphi}{\partial \theta} + \xi \frac{\partial\varphi}{\partial z} - \frac{1}{r} \frac{\partial(\eta\varphi)}{\partial \omega}$$

The peculiar fourth term is a consequence of a phenomenon called *angular redistribution*. As the figure shows, a streaming particle is constantly changing its angular position as it changes its radial position. Angular redistribution preserves the total number of streaming neutrons in curvilinear geometries.

Spherical

LAP

Let μ, η, ξ be the direction cosines of Ω relative to the spherical axes r, θ, ϕ . The direction vector Ω is characterized by the polar angle (relative to the radial direction) ψ and azimuthal angle ω :

The direction cosines are $\mu = \cos \psi$, $\eta = \sqrt{1 - \mu^2} \cos \omega$, $\xi = \sqrt{1 - \mu^2} \sin \omega$.
The streaming operator $\Omega \cdot \varphi$ is

$$\frac{\mu}{r^2} \frac{\partial(r^2 \varphi)}{\partial r} + \frac{\eta}{r \sin \theta} \frac{\partial(\sin \theta \varphi)}{\partial \theta} + \frac{\xi}{r \sin \theta} \frac{\partial \varphi}{\partial \phi} + \frac{1}{r} \frac{\partial((1 - \mu^2) \varphi)}{\partial \mu} - \frac{\cot \theta}{r} \frac{\partial(\xi \varphi)}{\partial \omega}$$

with the final two terms accounting for angular redistribution.

For the differential scattering term, retain the spherical harmonics expansion and evaluate the flux moment via quadrature:

$$\begin{aligned}
 \int_{\Omega_p} S_s d\Omega &= \int_{\Omega_p} \sum_{g'=1}^G \sum_{l=0}^L \Sigma_{g'g} \sum_{m=-l}^l Y_{lm}(\Omega) \varphi_{g'l}^{(m)} \\
 &= w_p \sum_{g'=1}^G \sum_{l=0}^L \Sigma_{g'g} \sum_{m=-l}^l Y_{lm}(\Omega_p) \varphi_{g'l}^{(m)} \\
 \varphi_{g'l}^{(m)} &= \sum_p w_p Y_{lm}^*(\Omega_p) \varphi_{g'}(\hat{r}, \Omega)
 \end{aligned}$$

LAP

Having obtained expressions for the streaming and scattering terms, we now seek to determine the sets of directions (the discrete ordinates) and weights which maximize computational accuracy.

The direction cosines for a given direction Ω_p are μ_p, η_p, ξ_p . They satisfy the relation $\mu_p^2 + \eta_p^2 + \xi_p^2 = 1$. The most common *quadrature set* is the level symmetric set, in which the same positive values of direction cosine are used for each of the three directions:

Level symmetric quadratures are examples of S_n quadratures. Originally the S_n method was a one-dimensional quadrature with n ordinates assuming a linear angular dependence.

Multidimensional S_n methods have $n(n+2)/8$ ordinates per spherical octant.

Symmetry constraints and rotational invariance impose constraints on the weights. Leaving out the math, we get:

Level	n	μ_n	w_n^b
S_4	1	0.3500212	0.3333333
	2	0.8688903	
S_6	1	0.2666355	0.1761263
	2	0.6815076	0.1572071
S_8	3	0.9261808	
	1	0.2182179	0.1209877
	2	0.5773503	0.0907407
	3	0.7867958	0.0925926
	4	0.9511897	
*Data from Ref. 5.			
*See Fig. 4-3 for ordinate directions corresponding to weight w_n .			
Level	n	μ_n	w_n^b
S_{12}	1	0.1672126	0.0707626
	2	0.4595476	0.0558811
	3	0.6280191	0.0373377
	4	0.7600210	0.0502819
	5	0.8722706	0.0258513
	6	0.9716377	
S_{16}	1	0.1389568	0.0489872
	2	0.3922893	0.0413296
	3	0.5370966	0.0212326
	4	0.6504264	0.0256207
	5	0.7467506	0.0360486
	6	0.8319966	0.0144589
	7	0.9092855	0.0344958
	8	0.9805009	0.0085179

LAP

In certain circumstances, reduced symmetry constraints may be desirable, leading to greater freedom in the selection of weights. Likewise, selection of a different underlying coordinate system might allow alternative sets. For example, hexagonal cells are common in reactor analysis and are better served by quadratures such as these:

Level	ξ_n^b	$\tilde{\omega}_n^c$	w_n^d
S_2	0.5773503	$\pi/6$	1.000000
S_4	0.3399810	$\pi/12, \pi/4$	0.3260726
	0.8611363	$\pi/6$	0.3478548
	0.2386192	$\pi/18, \pi/6, 5\pi/18$	0.1559713
	0.6612094	$\pi/12, \pi/4$	0.1803808
	0.9324695	$\pi/6$	0.1713245
S_8	0.1834346	$\pi/24, \pi/8, 5\pi/24, 7\pi/24$	0.0906709
	0.5255324	$\pi/18, \pi/6, 5\pi/18$	0.1045689
	0.7966665	$\pi/12, \pi/4$	0.1111905
	0.9602899	$\pi/6$	0.1012285

^aData from ref. 10.

^bDirection cosine with respect to z axis.

^cAzimuthal angle with respect to z axis $0 < \tilde{\omega} < \pi/3$.

^dWeights sum to one over a 30° sector.

LAP

One consequence of discrete ordinates methods is the bias of angular flux in the allowed directions – the “ray effects”. The angular flux estimates maximize in the allowed directions and minimize between them. An S_{16} (r, z) calculation of the isotropic flux through a spherical shell surrounding a point source demonstrates the phenomenon:

Spatial and Temporal Derivatives

LAP

However the angular variables are resolved, the transport equation still includes derivatives with respect to space and time.

Spatial derivatives are frequently handled by superimposing a regular grid over the problem domain and differencing between grid points. Second-order accurate schemes are common.

For unstructured grids, least-squares estimates of gradients are employed.

Spatial and Temporal Derivatives, cont'd

LAP

The time derivative is almost always handled as a simple first-order difference. Backward (implicit) differencing is possible but more likely is forward (explicit) differencing with a stability criterion met by limiting the size of the timestep:

$$\begin{aligned}\frac{\partial f}{\partial t} &= H(t) \\ f(t_{i+1}) &= f(t_i) + (t_{i+1} - t_i) \times H(t_i)\end{aligned}$$