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The Transport Equation

Quantities of Interest Particle Balance Boundary Conditions Eigenvalue

Numerical Solution of the Transport

Discretizatio Solution

A Brief Introduction to Radiation Transport

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Outline

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The Transport Equation

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Particle interactions are incorporated through the concept of cross sections. Neutrons have a few interactions of interest in radiation transport: capture, fission, elastic, and inelastic scattering.

- Neutron Cross Sections:
 - Absorption:

$$\sigma_a(E) = \sigma_c(E) + \sigma_f(E) \tag{1}$$

Scattering (elastic and inelastic):

$$\sigma_s(E) = \sigma_n(E) + \sigma_{n'}(E) + \sum_{i=2}^{N} \sigma_{i,n}(E)$$
 (2)

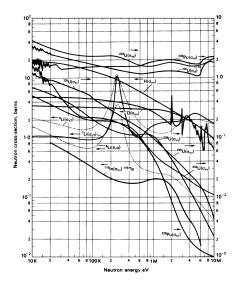
Nuclear Cross Sections Example of Neutron Cross Sections

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Cross Sections and Particle

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Nuclear Cross Sections Photon Cross Sections

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Photons have three interactions of interest in radiation transport: photoelectric, Compton scattering, pair production.

- Photon Cross Sections
 - Absorption:

$$\sigma_{\mathsf{a}}(\mathsf{E}) = \sigma_{\mathsf{pe}}(\mathsf{E}) \tag{3}$$

Scattering:

$$\sigma_s(E) = \sigma_{cs}(E) + \sigma_{pp}(E) \tag{4}$$

Nuclear Cross Sections Example of Photon Cross Section

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Cross Sections and Particle

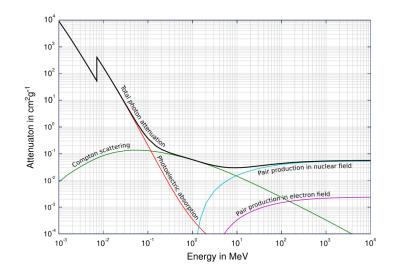
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Scattered Particle Distributions

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Express probability distribution laws governing scattered particle emission. The scattering cross section tells us the probability a scattered particle will be emitted in some specific direction with some specific energy:

$$\sigma_s(\vec{r}, E \to E', \hat{\Omega} \cdot \hat{\Omega}') dE' d\hat{\Omega}'$$
 (5)

Fission Neutron Distributions

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Discretizatio Solution Two quantities need to be defined in fission:

- $\nu(E) =$ mean number of fission neutrons produced in a fission caused by a neutron with energy E.
- $\chi(E)dE$ = probability that a fission neutron will have an energy dE about E.

$$\int_0^\infty \chi(E)dE = 1 \tag{6}$$

Particle Interactions

Assumptions

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Solution of the Transport Equation Discretization Solution Methods In the derivation of the TE, we assume the following:

- Particles are considered as points.
- Particles travel in straight lines between point collisions (neutral!).
- Particle-particle interactions can be neglected.
- Collisions are instantenous (some exceptions like delayed neutron emission).
- Material properties are assumed to be isotropic.
- Nuclei properties and material properties are assumed constant and known (can be relaxed).
- Only expected or mean particle density distribution is considered.

Definitions

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Angular Flux

Let the particle density distribution in a six-dimensional phase space (space, direction, energy, and time) be $N(\vec{r}, \hat{\Omega}, E, t)$, we define the neutron angular flux as

$$\psi(\vec{r}, \hat{\Omega}, E, t) = vN(\vec{r}, \hat{\Omega}, E, t)$$
(7)

which is convenient for the calculation of reaction rates. Usually reaction rates are independent of direction, so we define the scalar flux:

$$\phi(\vec{r}, \hat{\Omega}, E, t) = \int_{4\pi} \psi(\vec{r}, \hat{\Omega}, E, t). \tag{8}$$

The Transport Equation

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The TE is merely a balance equation (source - losses):

$$\frac{1}{\nu} \frac{\partial}{\partial t} \psi(\vec{r}, \hat{\Omega}, E, t) + \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, E, t) + \sigma(\vec{r}, E) \psi(\vec{r}, \hat{\Omega}, E, t) = q(\vec{r}, \hat{\Omega}, E, t), \quad (9)$$

where $q(\vec{r}, \hat{\Omega}, E, t)$ includes both the external and fission source.

We need to impose boundary and initial conditions!

Equation

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Numerical Solution of the Transport Equation Discretization ■ We can impose an incoming angular flux. If no angular flux is imposed, the boundary condition is called vacuum.

$$\psi(\vec{r}, \hat{\Omega}, E, t) = \tilde{\psi}(\vec{r}, \hat{\Omega}, E, t), \quad \hat{\Omega} \cdot \hat{n} < 0, \vec{r} \in \Gamma$$
 (10)

Albedo (reflective) boundary condition:

$$\psi(\vec{r}, \hat{\Omega}, E, t) = \alpha(E)\psi(\vec{r}, \hat{\Omega}', E, t), \quad \hat{\Omega} \cdot \hat{n} < 0, \vec{r} \in \Gamma$$
 (11)

These are usually the two boundary conditions of interest in applications.

Eigenvalue Problems in Radiation Transport The Criticality Condition

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Numerical Solution of the Transport Equation Discretization

- A problem of special interest is the criticality condition.
- Criticality is defined as a system capable of sustaining a chain reaction without an external source indefinitely.
 That is, there is a time-independent solution to the problem.
- In most circumstances, a problem under consideration is not exactly critical (no time-independent solution exists). We must reformulate the TE into an eigenvalue problem to determine how subcritical or supercritical the problem really is.
- Reformulation of the TE into an eigenvalue problem is not a unique process (that is, we can create an eigenvalue problem any way we want to).

Eigenvalue Problems in Radiation Transport The Time-Independent Transport Equation

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Solution of the Transport Equation

Discretization Solution Methods No guarantee non-trivial solution exists for the following problem:

$$\left[\hat{\Omega} \cdot \nabla + \sigma(\vec{r}, E)\right] \psi(\vec{r}, \hat{\Omega}, E) =
\int dE' \int d\hat{\Omega}' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}') +
\chi(E) \int dE' \nu \sigma_f(\vec{r}, E') \int d\hat{\Omega}' \psi(\vec{r}, E', \hat{\Omega}'). \quad (12)$$

We "force" a solution to exist. We consider two formulations: the time-absorption and multiplication eigenvalues.

Eigenvalue Problems in Radiation Transport The α Eigenvalue

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Solution of the Transport Equation Assume an asymptotic solution to the previous equation in the form

$$\psi(\vec{r}, E, \hat{\Omega}, t) = \psi_{\alpha}(\vec{r}, E, \hat{\Omega}) e^{\alpha t}.$$
 (13)

In general there will be a spectrum of eigenvalues for which there are solutions. At long times only nonnegative solutions will predominate, so we can define criticality as

Re
$$\alpha_0$$
 $\begin{cases} > & 0 \quad supercritical, \\ = & 0 \quad critical, \\ < & 0 \quad subcritical. \end{cases}$ (14)

Eigenvalue Problems in Radiation Transport The Multiplication Eigenvalue

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Assume you can adjust ν , the average number of neutrons emitted in fission, to obtain a time-independent solution. Our fission source term becomes:

$$\frac{\chi(E)}{k} \int dE' \nu \sigma_f(\vec{r}, E') \int d\hat{\Omega}' \psi(\vec{r}, E', \hat{\Omega}'). \tag{15}$$

We can define critcality as

$$k \begin{cases} > & 1 \quad supercritical, \\ = & 1 \quad critical, \\ < & 1 \quad subcritical. \end{cases}$$
 (16)

Discretizing the Transport Equation in Energy Energy, Space, and Angle

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Energy Discretization

We divide energy into groups and define a corresponding angular flux in each group,

$$\psi_{g}(\vec{r},\hat{\Omega}) = \int_{g} dE \psi(\vec{r},\hat{\Omega},E), \quad \int_{g} dE = \int_{E_{g}}^{E_{g-1}} dE$$
 (17)

such that

$$\int_0^\infty dE' = \sum_{g'=1}^G \int_{g'} dE'.$$
 (18)

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Spatial Discretization

Derivatives are expressed using either the finite difference or finite element method.



Discretizing the Transport Equation in Energy Energy, Space, and Angle

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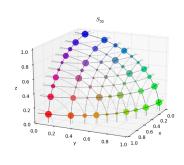
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Angular Discretization

The Discrete Ordinate Method is used to discretize angle. The TE equation is solved along specific directions and a quadrature formula is used to reconstruct the angular flux.



The Transport Sweep Algorithm The TE in Matrix Form

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Solution Methods We can rewrite the discretized TE equation into matrix form:

$$\mathbf{H}\psi = \chi \mathbf{f}^{\mathsf{T}} \int d\mathbf{\hat{\Omega}}\psi + \mathbf{q}^{\mathsf{e}} \tag{19}$$

and recast it into the multiplication eigenvalue formulation:

$$\mathbf{H}\psi = \frac{1}{k}\chi \mathbf{f}^{T} \int d\hat{\mathbf{\Omega}}\psi + \mathbf{q}^{e}. \tag{20}$$

We define a spatial fission neutron distribution source (scalar):

$$F(\vec{r}) = \mathbf{f}(\vec{r})^T \int d\hat{\mathbf{\Omega}} \psi(\vec{r}, \hat{\mathbf{\Omega}}). \tag{21}$$

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Solution Methods We rewrite our problem in terms of this distribution and doing some manipulations we obtain

$$AF = kF \tag{22}$$

where define the scalar multigroup transport operator as

$$A \equiv \mathbf{f}^T \int d\mathbf{\hat{\Omega}} \mathbf{H}^{-1} \chi. \tag{23}$$

This is an eigenvalue problem that can be solved using the power method.

The Power Method

Updating the Eigenvector and Eigenvalue

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Solution Methods We determine the eigenvector and eigenvalue using the power method. Assume the problem has a largest eigenvalue, the eigenvalue is positive, and is real and unique, we can obtain the better approximation to the eigenpair using the relationships

$$F_{i+1} = \frac{1}{k_i} A F_i, \tag{24}$$

and

$$k_{i+1} = k_i \frac{\int dV \ wAF_i}{\int dV \ wF_i}.$$
 (25)

The Power Method Why Does This Method Work?

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Solution Methods Suppose there are distinct eigenvalue problem solutions:

$$AF^{\ell} = \kappa_{\ell}F^{\ell}, \quad \ell = 1, 2, \dots, \tag{26}$$

where

$$k = \kappa_1 > \kappa_2 > \kappa_3 \dots \tag{27}$$

Suppose we guess a linear combination of these solutions

$$F_0 = \sum_{\ell} \alpha_{\ell} F^{\ell}. \tag{28}$$

If we continue to apply on operator (algorithm) say n times, we obtain the following:

$$A^{n}F_{0} = \sum_{\ell} \alpha_{\ell} \kappa_{\ell}^{n} F^{\ell} = \alpha_{1} \kappa_{1}^{n} F^{1} + \sum_{\ell > 1} \alpha_{\ell} \kappa_{\ell}^{n} F^{\ell}. \tag{29}$$

The Power Method Why Does This Method Work?

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Solution Methods Factoring out κ_1^n (which is the value we are interested in) we see that

$$A^n F_0 \to \alpha_1 \kappa_1^n F^1, \quad n \to \infty.$$
 (30)

since $(\kappa_{\ell}/\kappa_1)^n$ goes to zero as n goes to zero due to the ordering of the eigenvalues.

Inverting **H**We Haven't Solved Anything Yet...

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Solution Methods Hidden in the math is the fact we need to invert **H**. How do we do this?

- Iteratively! Matrix too large and process too expensive to invert directly.
- Gauss-Seidel, Jacobi, many other methods!
- A lot of research in acceleration (preconditioning) of problems. (Me hopefully)

Comparisons to Monte Carlo Why Not Just Monte Carlo All the Time?

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Solution Methods

Advantages

- No random error. Error is caused by discretization and data only.
- Fast! Matrix iterative methods are well studied and are less expensive than random sampling.
- Give global solutions (solution defined at every point).
- No need for variance reduction. We are solving an equation and not simulating particles.

Disadvantage

- Difficult to represent complex geometries (requires mesh).
- Energy treatment is not continuous (multigroup approximation).
- Difficult to parallelize (can be done however).