22.211 Lecture 11

Transport Theory

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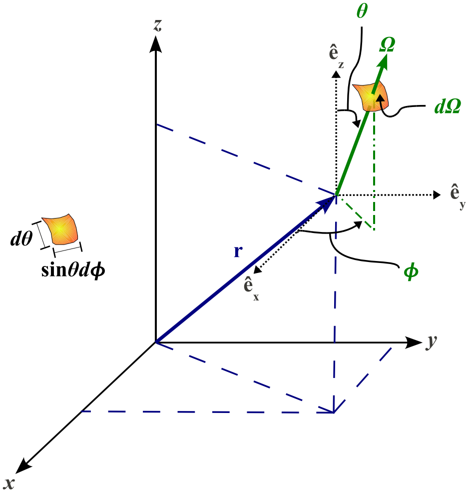
Outline

1. Transport Equation
2. Boundary and Initial Conditions
3. Multigroup
4. Integral Form

Outline

Phase Space



Transport Equation

- For a constant volume, $(\partial/\partial t)\int_V d^3r\, n = \int_V d^3r\,(\partial n/\partial t)$

$$\overbrace{\left(\int_V d^3r\,\frac{\partial}{\partial t}n(\mathbf{r},\mathbf{v},t)\right)}^{\text{total rate of change of } n \text{ in } V} = -\overbrace{\int_V d^3r\,\mathbf{v}\cdot\nabla n(\mathbf{r},\mathbf{v},t)}^{\text{streaming rate}} + \overbrace{\int_V d^3r\left(\frac{\partial n}{\partial t}\right)_{\text{coll}}}^{\text{collision rate}}$$

$$+\underbrace{\int_V d^3r\, s(\mathbf{r},\mathbf{v},t)}_{\text{source emission rate}}\;.$$

Collision Term in Reactor Physics

- The collision term is expressed by balancing the reaction rates in the arbitrary volume
- Loss term:

$$\Sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, \mathbf{\Omega}, E, t)$$

- Gains via scattering into E and Ω from all other directions and velocities

$$\int d\Omega' \int dE' \Sigma_s(\mathbf{r}, E' \to E, \Omega' \to \Omega)\psi(\mathbf{r}, \mathbf{\Omega}', E', t)$$

Collision Term in Reactor Physics

- Gains via fission into E and Ω from all fissions

$$\int d\Omega' \int dE' \nu\Sigma_f(\mathbf{r}, E' \to E, \Omega' \to \Omega)\psi(\mathbf{r}, \mathbf{\Omega}', E', t)$$

- assume that fission is isotopic and outgoing energy distribution is $\chi(E)$

$$\frac{\chi(E)}{4\pi} \int dE' \nu\Sigma_f(\mathbf{r}, E')\phi(\mathbf{r}, E', t)$$

- Other neutron producing reactions can be expressed in a similar fashion

$$\int d\Omega' \int dE' \nu_x\Sigma_x(\mathbf{r}, E' \to E, \Omega' \to \Omega)\psi(\mathbf{r}, \mathbf{\Omega}', E', t)$$

- Combined with the scattering kernel to account for energy and angular distributions or treated as negative absorption

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Neutron Transport Equation

- The collision term is expressed by balancing the reaction rates in the arbitrary volume

$$
\begin{aligned}
\frac{1}{v}\frac{\partial \psi}{\partial t} + \hat{\Omega}\cdot\nabla\psi + \Sigma_t(\mathbf{r},E)\psi(\mathbf{r},\boldsymbol{\Omega},E,t) = \\
&+ \int_0^\infty dE' \int_{4\pi} d\Omega' \nu_s \Sigma_s(\mathbf{r},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}',E'\rightarrow E)\psi(\mathbf{r},\boldsymbol{\Omega}',E',t) \\
&+ \frac{\chi(E)}{4\pi}\int_0^\infty dE' \nu\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',t) \\
&+ s(\mathbf{r},\boldsymbol{\Omega},E,t)\,.
\end{aligned}
$$

Linear vs Non-Linear

- If the x.s. are known and independent of the flux, the equation is linear.
- In gas dynamics, the equation is non-linear because we are solving for the gas particle distribution which also impacts the density, hence the x.s.
- In photon transport, the x.s. are strongly dependent on temperature
  - With high energy gamma's, the energy deposition will impact the material significantly which leads to a highly non-linear equation
  - For low energy gamma's, the deposited energy is low enough that we can assume a linear process
- In neutron transport, we usually state that the equation is linear, but temperature changes will affect x.s..

Assumptions

- Neutron density is large (treat as an average)
- Neutrons can be treated as point particles (no QM effects)
- Collisions are well-defined 2 body events which occur instantaneously
- Neutrons stream with constant velocity between collisions
- No neutron-neutron collisions
- Neutron interaction do not alter medium
- Neutrons have no memory
- Neutrons do not decay

Particle Clustering

The assumption of large neutron density allows us to avoid the issue of particle clustering that appears in Monte Carlo simulations. Monte Carlo simulations do not readily solve the continuous differential operator but approximate by sampling a discrete number of particles. If the number of discrete particles is too small (i.e. under-sampling), this leads to particle clustering.

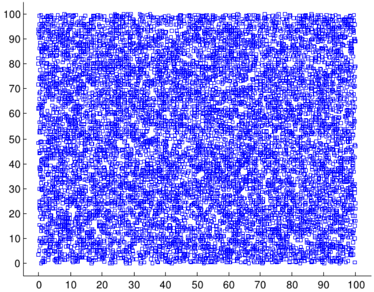

Figure: Particle Clustering - Initial State

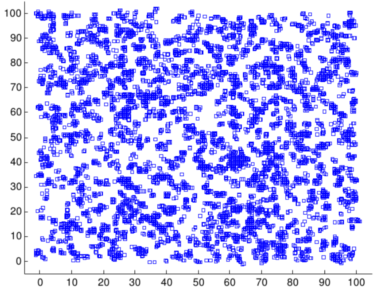

Figure: Particle Clustering - Final State

Particle Clustering - More particles

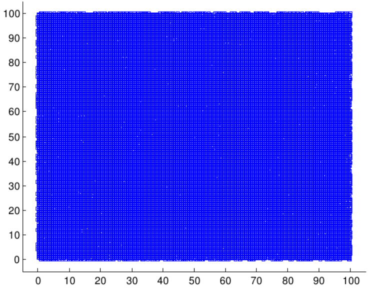

Figure: Particle Clustering - Initial State

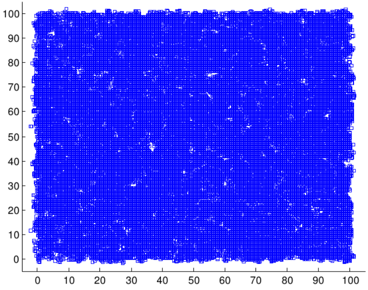

Figure: Particle Clustering - Final State

Another way to derive the transport equation

- We can consider directly the material derivative

$$
\begin{aligned}
\frac{Dn}{Dt} &\equiv \frac{\partial n}{\partial t} + \frac{\partial x}{\partial t}\frac{\partial n}{\partial x} + \frac{\partial y}{\partial t}\frac{\partial n}{\partial y} + \frac{\partial z}{\partial t}\frac{\partial n}{\partial z} + \frac{\partial v_x}{\partial t}\frac{\partial n}{\partial v_x} + \frac{\partial v_y}{\partial t}\frac{\partial n}{\partial v_y} + \frac{\partial v_z}{\partial t}\frac{\partial n}{\partial v_z} \\
&= \frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + \mathbf{a} \cdot \nabla_{\mathbf{v}} n \\
&= \frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} n \,,
\end{aligned}
$$

Adding collisions and sources

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} n = \left(\frac{\partial n}{\partial t}\right)_{\text{coll}} + s \,.$$

Outline

Initial Conditions

- Relatively straightforward, just define an initial function in the phase space at $t = t_0$

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, t)|_{t=t_0} = f(\mathbf{r}, \mathbf{\Omega}, E),$$

- Time dependent problems are in general stiff, due to the various time scales at play.
- In this class we will focus mainly on steady-state problems.

Vacuum BC

- No neutrons can re-enter a volume

$$\psi(\mathbf{r}, \mathbf{\Omega}, E, t) = 0\,, \quad \hat{\mathbf{n}} \cdot \mathbf{\Omega} < 0\,,$$

- Also called Void or Free Surface
- Be careful of re-entrant geometries!

Specified BC

- A known incident flux is applied at the boundary

$$\psi(\mathbf{r}_s, \mathbf{\Omega}, E, t) = f(\mathbf{r}_s, \mathbf{\Omega}, E, t) \,.$$

- Can be useful to represent sources.
- This is an inhomogeneous BC.

Reflective BC

- Also called specular or mirror

$$\psi(\mathbf{r}_s, \mathbf{\Omega}, E, t) = \psi(\mathbf{r}_s, \mathbf{\Omega}_R, E, t)\,, \quad \hat{\mathbf{n}} \cdot \mathbf{\Omega} < 0\,,$$

- Used to define repeated geometries or to reduce size of symmetric problem
- An albedo BC is defined as a mix between vacuum and reflective

Periodic BC

- Repeated geometries with a specific pattern are better represented with the periodic BC.

$$\psi(\mathbf{r}_1, \mathbf{\Omega}, E, t) = \psi(\mathbf{r}_2, \mathbf{\Omega}, E, t)\,,$$

White BC

- Neutrons incident on a boundary are reflected isotropically

$$\psi(\mathbf{r}_s, \boldsymbol{\Omega}, E, t) = \frac{\int_{\hat{\mathbf{n}}\cdot\boldsymbol{\Omega}'>0} \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}' \psi(\mathbf{r}, \boldsymbol{\Omega}', E, t) d\Omega'}{\int_{\hat{\mathbf{n}}\cdot\boldsymbol{\Omega}'<0} \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}' d\Omega'}$$

$$= \frac{J_+(\mathbf{r}_s, E, t)}{\int_{\hat{\mathbf{n}}\cdot\boldsymbol{\Omega}'<0} \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}' d\Omega'}, \quad \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}' < 0 .$$

Wigner-Seitz

- White BC became useful when square pin cells were rounded off for computational efficiency

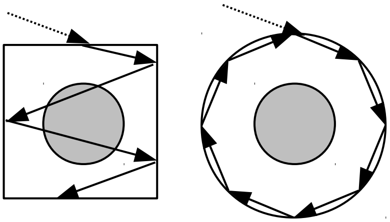

Figure: Square pin cell and equivalent Wigner-Seitz cell. Same incident direction and location.

Recap

- Neutron transport equation is linear only if we neglect thermal feedback
- Many justifiable assumptions are made when deriving the equation
- Typical homogeneous BCs are vacuum, reflective, periodic, white ...
- Inhomogeneous BCs can be used to represent a plane source

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Outline

Multigroup Approximation

Define the group flux

$$\psi_g(\mathbf{r}, \mathbf{\Omega}) = \int_{E_g}^{E_{g-1}} \psi(\mathbf{r}, \mathbf{\Omega}, E)dE$$

And group constant that preserve reaction rates

$$\Sigma_{tg}(\mathbf{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\mathbf{r}, E)\phi(\mathbf{r}, E)dE}{\int_{E_g}^{E_{g-1}} \phi(\mathbf{r}, E)dE}$$

We usually use ϕ instead of ψ to avoid having directional dependent group constants.

Multigroup Approximation

$$\Sigma_{sg'\to g}(\mathbf{r}) = \frac{\int_{E_g}^{E_{g-1}} \int_{E'_g}^{E_{g'-1}} \Sigma_s(\mathbf{r}, E' \to E)\phi(\mathbf{r}, E')dE'dE}{\int_{E'_g}^{E_{g'-1}} \phi(\mathbf{r}, E')dE'}$$

$$\chi_g = \int_{E_g}^{E_{g-1}} \chi(E)dE$$

The fission spectrum must also be weighted by isotopic fission rates since each isotope has a different spectrum.

Multigroup Equation

$$\hat{\Omega} \cdot \nabla \psi_g(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_{tg} \psi_g(\mathbf{r}, \boldsymbol{\Omega}) = + \int_{4\pi} d\Omega' \sum_{g'=1}^{G} \Sigma_{s,g' \to g}(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \psi_{g'}(\mathbf{r}, \boldsymbol{\Omega}') + \frac{\chi_g}{4\pi k} \sum_{g'=1}^{G} \nu \Sigma_{fg'}(\mathbf{r}) \phi_{g'}(\mathbf{r})$$

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Forms of the TE

- So far, the TE was only presented in its integro-differential form
- An integral form also exists, but a full differential form cannot exist
  - In a collision, energy and angle change discontinuously. As a consequence, these terms must always include an integral over E' and Ω'.
- Integro-Differential form: Particle change in a volume element
- Integral form: Particle change along a given path

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Other forms of TE

- Even/Odd parity
- Slowing down kernel
- Multiple collision
- Invariant embedding
- Singular integral
- Green's function
- Pseudo flux

For more details on these, you can look at a book by Prof. Barry Ganapol: "Analytical Benchmarks for Nuclear Engineering Applications: Case Studies in Neutron Transport Theory"

Method of Characteristic

- Define the emission density

$$Q_g(\mathbf{r},\boldsymbol{\Omega}) = \int_{4\pi} d\Omega' \sum_{g'=1}^{G} \Sigma_{sg'\to g}(\mathbf{r},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\psi_{g'}(\mathbf{r},\boldsymbol{\Omega}')$$

$$+ \frac{\chi_g}{4\pi}\sum_{g'=1}^{G} \nu\Sigma_{fg'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + S_g(\mathbf{r},\boldsymbol{\Omega})$$

- Introduce integrating factor

$$IF = e^{\int_{-\infty}^{s} \Sigma_{tg}(\mathbf{r}+s'\boldsymbol{\Omega})ds'}$$

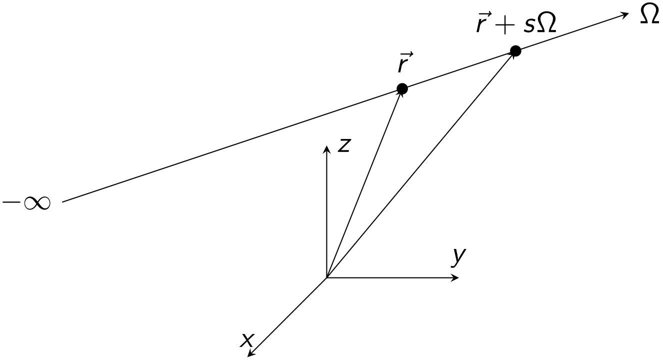
Forward Characteristic

- Integrate between $-\infty$ and s

$$\psi_g(\mathbf{r}+s\boldsymbol{\Omega},\boldsymbol{\Omega}) = e^{-\int_{-\infty}^{s}\Sigma_{tg}(\mathbf{r}+s'\boldsymbol{\Omega})ds'} \int_{-\infty}^{s} e^{\int_{-\infty}^{s'}\Sigma_{tg}(\mathbf{r}+s''\boldsymbol{\Omega})ds''} Q_g(\mathbf{r}+s'\boldsymbol{\Omega},\boldsymbol{\Omega})ds'$$

- Simplify to yield

$$\psi_g(\mathbf{r}+s\boldsymbol{\Omega},\boldsymbol{\Omega}) = \int_{-\infty}^{s} e^{-\int_{s}^{s'}\Sigma_{tg}(\mathbf{r}+s''\boldsymbol{\Omega})ds''} Q_g(\mathbf{r}+s'\boldsymbol{\Omega},\boldsymbol{\Omega})ds'$$


Ω
$\vec{r} + s\Omega$
$\vec{r}$
z
$-\infty$
y
x

Backward Characteristic

If we reverse the direction of travel and set $s = 0$

$$\psi_g(\mathbf{r}, \mathbf{\Omega}) = \int_0^{\infty} e^{-\int_0^{s'} \Sigma_{tg}(\mathbf{r}-s''\mathbf{\Omega})ds''} Q_g(\mathbf{r} - s'\mathbf{\Omega}, \mathbf{\Omega})ds'$$

If we had a more meaningful boundary condition in a finite system

$$\psi_g(\mathbf{r}, \mathbf{\Omega}) = \int_0^{s_{BC}} e^{-\int_0^{s'} \Sigma_{tg}(\mathbf{r}-s''\mathbf{\Omega})ds''} Q_g(\mathbf{r} - s'\mathbf{\Omega}, \mathbf{\Omega})ds' + \psi_g(\mathbf{r} - s_{BC}\mathbf{\Omega}, \mathbf{\Omega})e^{-\int_0^{s_{BC}} \Sigma_{tg}(\mathbf{r}-s'\mathbf{\Omega})ds'}$$

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Notes on MOC

- Characteristic curved in neutron transport are straight lines
- For a given set of discrete angles (i.e. tracks), one can solve the angular flux along each angle throughout a geometry
- Using an iterative process, angular fluxes from a given iteration can be used to provide the source and calculate the next iteration of angular fluxes
- This equation will be the basis for lectures 5-7 where we will develop the MOC solution technique.

Optical Path Length

$$\tau_g(\mathbf{r}, \mathbf{r} - s'\boldsymbol{\Omega}) = \int_0^{s'} \Sigma_{tg}(\mathbf{r} - s''\boldsymbol{\Omega})ds'' = \tau_g(\mathbf{r}, \mathbf{r}')$$

$e^{\tau_g(\mathbf{r},\mathbf{r}')}$ is the probability of not making a collision between $\mathbf{r}$ and $\mathbf{r}'$ in group g

Peierls Equation

Assuming isotropic source and scattering, and integrating over all angles:

$$\phi_g(\mathbf{r}) = \int_{V'} \frac{Q_g(\mathbf{r}')e^{-\tau_g(\mathbf{r},\mathbf{r}')}dV'}{4\pi|\mathbf{r}-\mathbf{r}'|^2} .$$

Recap

- Transport equation can take many forms
- Integral form follows particle along a characteristic line
- Nothing more than a source of neutrons attenuated along the path of interest

Resources

- Chapter 5 of handbook