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Nuclear Reactor Physics : Neutronics

Chapter 2: The Boltzmann equation

2.1. Introduction

Well, we meet again. I must tell you that I am happy to see you back, as I was a little worried that the first chapter would kill your enthusiasm. Definitions are no fun when you don't know why you're defining. This chapter will aim at showing you what exactly it is that we care about and look for.

2.1.1. So, what is this equation?

This is quite a good question. *Thank you.* We've seen in chapter I that the neutron population we consider is very large. As a consequence, it can be treated as a whole by comparing its behavior to a fluid, hence applying the techniques of fluid mechanics. in order to do this, we will use an equation formulated by Ludwig Boltzmann (this pretty smart bloke lived from 1844 to 1906. And look at this beard!) as he was working on statistical mechanics in 1879. To put stuff into perspective here, that's more than half a century before the discovery of the neutron! The study and numerical processing of the Boltzmann equation for neutrons is one of the main challenges faced by neutron physicists.

Ludwig Eduard Boltzmann
(1844-1906)

I'm not going to lie, it's not very good looking, even if I guess it's all a matter of opinion. I will however try to break it down so that it makes sense.

2.1.2. What does this equation do exactly?

Fair enough, I'll show you. But first, let's set up some context here. A reactor is described in terms of its geometry, composition, and cross-sections. Once your reactor has been described, the purpose of a neutron physics calculation is to compute the reaction rates and therefore the neutron density or flux. That's where the Boltzmann equation comes in.
Let me try and illustrate that by a simplified problem.

2.2. A first approximation of the Boltzmann equation

The flux is the product of sources that are given in certain problems; they are usually sources of neutron-induced fission. They are, therefore, proportional to the flux and are also unknown. In other words, the flux depends on the sources, and the sources depend on the flux. As with the chicken and its egg, there is no easy starting point. The idea of evolution then sets in to answer this question in a practical way. It's basically all about mutation, and deciding of the appropriate threshold above which a chicken is a chicken and a chicken egg is a chicken egg.
Well, the story is similar here. The main objectives of numerical calculations of the Boltzmann equation will thus be:

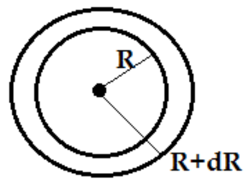
- We set one of the unknown arbitrarily
  - we decide what our starting “chicken” characteristics are.
- This will set a value for the second unknown
  - knowing the starting “chicken”, we know what kind of eggs it lays.
- From that value, we will be able to improve the first one,
  - basically introducing “mutation”
- which will again give a new second unknown,
  - our second generation “chicken” !
- et caetera.
- At some point, the solutions will converge
  - the differences between each generations of “chicken” will be negligible as per our criteria.

Anyhow, our present goal is to introduce this problem using a simple example before presenting the more general case. The example we will consider lies upon three important simplifying assumptions:

1. The neutrons are monokinetic, with speed v,
2. The sources and the neutron population are stationary in time.
3. The sources are isotropic

2.2.1. Case description

As said, we consider a simple case: a point source placed in a vacuum. This source emits S neutrons per unit time.



We'll need to estimate the density. In order to do that, knowing the volume considered is pretty damn useful. So let us say that the unit volume is delimited by two spheres of radius R and $\mathrm{R} + \mathrm{dR}$.
A simple equation tells us that neutrons take an amount of time:

$$\mathrm{dt} = \mathrm{dR}/\mathrm{v}$$

to pass through this volume. Consequently, we continuously observe the number of neutrons that have been emitted during this time, i.e. $\mathrm{S.dt} = \mathrm{S}.\frac{\mathrm{dR}}{\mathrm{v}}$.
The density is thus obtained by dividing this number by the volume $V = 4\pi.R^2.dR$, and the flux is obtained by multiplying by v :

$$n = \frac{S}{4\pi.R^2 v}$$

$$\varphi = \frac{S}{4\pi.R^2}$$

2.2.2. Absorption

Let's say now that we place this point source in an absorbent material. This means that the neutrons present between the radii R and R+dR will be the ones that have passed through this material without interaction over the distance R, between the source and the volume considered. You'll recall (maybe) that the probability of that happening is $e^{-\Sigma R}$

The flux then becomes:

$$\varphi = \frac{S.e^{-\Sigma R}}{4\pi.R^2}$$

2.2.3. Sources

Adding hypotheses, let us now suppose that we don't have only one source, but a set of sources distributed at $\mathrm{S}(\mathrm{r}').d^3r'$ in the volume element d^3r'.
Here, we have $R = |\vec{r}' - \vec{r}|$

If we have several sources, the flux Φ is obtained by just adding every fluxes φ from each source. This can be written with an integral:

$$\Phi(\vec{r}) = \int \frac{e^{-\Sigma R}}{4\pi . R^2} S(\vec{r}'). d^3r'$$

I hope you're still following. If I stop a little to sum up what happened…

We started from a single point source giving S neutrons per unit time (the number of neutrons we see in the volume of interest only depends on how many were created in the considered time).

We have put this source in an absorbent medium (not all neutrons created by the source reach the volume we're looking at)

We have multiplied the number of sources giving away neutrons, distributed over a volume d^3r' (more realistic source)

Let's get on the next step now, shall we?

What if all the sources we had were fissions? After all, we're talking of a nuclear reactor here, so that'll be our main source, right? We have thus to express $S(\vec{r}')$ accordingly. Well, we obtain:

$$S(\vec{r}') = \nu . \Sigma_f \Phi(\vec{r}'),$$

where ν is the number of neutrons emitted per fission.

Therefore, we can write:

$$\Phi(\vec{r}) = \int \frac{e^{-\Sigma R}}{4\pi . R^2} . \nu . \Sigma_f \Phi(\vec{r}'). d^3r'$$

2.2.4. Scattering

Earlier, we have basically said that every neutrons interacting with matter were lost by absorption. In fact, as chapter 1 taught us, they might be scattered and thus re-emitted. What is the difference between an emission (by the sources, i.e. fissions here) and a re-emission (by scattering)? Well, for us in neutron physics, none. Of course, the mechanisms are very different. But we're just looking at the results. In both cases, a neutron "appears", and we'll say that scattering does not impact the speed and re-emits isotropically. This implies that we ought to add the scattering sources to the "real" sources we had defined. How do we account for the scattering sources? Well, easy, isn't it ? That'd be the scattering reaction rate, $\Sigma_s . \Phi$.

$$\Phi(\vec{r}) = \int \frac{e^{-\Sigma R}}{4\pi . R^2} . [\nu . \Sigma_f \Phi(\vec{r}') + \Sigma_s . \Phi(\vec{r}')]. d^3r'$$

2.2.5. *Heterogeneous material*

Now, and that's the last step of this "simple" example, we can consider that the medium is not made of only one material. Indeed, it can be heterogeneous. In this case, we can "combine" the probabilities, each material having a specific cross-section.

Thus, we can write:

$$\kappa = \int_{\vec{r}}^{\vec{r}\prime} \Sigma\,(\vec{r}').\,d^3r'$$

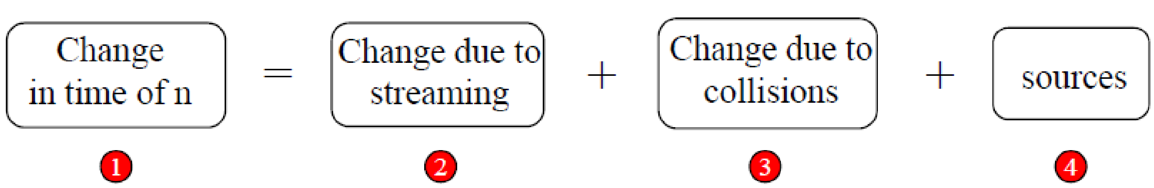
This represents the combination of all the cross-sections (hence different atoms) the neutrons can encounter on their way "out".
We finally obtain:

$$\Phi(\vec{r}) = \int \frac{e^{-\kappa}}{4\pi.R^2}.[\nu.\Sigma_f(\vec{r}')\Phi(\vec{r}') + \Sigma_s(\vec{r}').\Phi(\vec{r}')].d^3r'$$

2.3. The Boltzmann equation

The Boltzmann equation is an equation that represents in our case the neutron balance. By "simply" balancing the loss and gain of neutrons mechanism in a delimited arbitrary "volume" (phase volume) which have a specific velocity, we will derive the equation. Something essential was introduced in the latter sentence – "specific velocity". Indeed, we do not only want to consider the mere number of neutrons in the volume, we also want the neutrons among those that have the velocity we consider! This here is very important.

On a general note, here is how we can express those mechanisms. Not too bad, is it?



Translated into words, this gives something along the lines of:

"The change of the number of neutrons in the phase space considered during time is caused by:

- *the gains and losses of neutrons due to streaming, that is the neutrons that enter the volume from the outside or that leave the volume, during the time t.*
- *the gains and losses of neutrons due to collisions*

- *the gains of neutrons due to the source”*

Nothing groundbreaking here, we just translated the image into words without adding anything meaningful. Or did we? You see, the only pieces of information added with the literal translation are the words “gains“ and “losses”. The balance indeed likes upon the neutrons gained and lost, and that will be what we’ll used to compute the final equation. For each processus (streaming, collisions, sources), we must count the gains and the losses, in time and in the phase space (velocity, position) that was introduced in the first chapter.

2.3.1. Time change term (1)

The change of time in time is written:

$$\frac{\partial}{\partial t}\int_{V} n(\vec{r},\vec{v},t).d^3r.d^3v$$

Indeed, $\frac{\partial}{\partial t}$ represents the passage of time, it literally translates into a “variation of the value (here the integral) per time variation”.
Inside the integral, we have the neutron density of course, it is after all the number of neutrons per unit “volume” (by volume here, one has to understand space and velocity).
Why the integral then? Well, because we want a number of neutrons, not a number of neutrons per “volume”.
We thus have written the neutron population changes within the volume considered (space,d^3r) and within the “velocity volume” considered (velocity,d^3v).

2.3.2. Streaming term (2)

This term is already more complicated. First we should identify that the losses are the outgoing neutrons and the gains are the… incoming neutrons. Well, that could have been worse. The streaming term only consider the neutrons going in or out the space volume.
It boils down to the currents, which we defined in the previous chapter.

The leakage into or from the space volume can of course be combined. It relates to the surface of the volume (forming entry or exit points). If we use the definition of the angular current density defined in chapter 1,

$$\vec{J}(\vec{r},\vec{v},t) = -\int_{\delta V} d^2S\,.\vec{j}(\vec{r},\vec{v},t).\widehat{n_s}.d^3v$$

We can use the divergence theorem on this equation. It is to note that the minus sign depends on the definition of the unitary vector $\widehat{n_s}$. In our case, it is the outgoing normal.

This gives:

$$\vec{J}(\vec{r},\vec{v},t) = \int_V \overrightarrow{\nabla.J}(\vec{r},\vec{v},t).d^3r.d^3v$$

Since velocity and space are independent variables, one can finally write the change due to streaming:

$$\int_V \vec{v}.\vec{\nabla}.n(\vec{r},\vec{v},t).d^3r.d^3v$$

2.3.3. Collision term 3

This term acts within the phase space $(\vec{r},\vec{v})$. So, what are the losses and gains mechanisms in the phase space?

Well, one cause of losses is the neutrons that disappear because they are absorbed within the volume. That's pretty straightforward. The second one is not that difficult to grasp but I feel like it's not a common logic, indeed, you don't often think in terms of velocity volume. So, the second cause of losses is the neutrons that are scattered and whose velocity (speed and direction) is changed! Therefore, they leave our population of interest. Every scattering collision changes the velocity of the neutron.

As for the gains, it is also unexpected. At least, that's my take on it: obvious when you know, unexpected when you don't. If every neutrons of interest that collides is lost for us (absorbed or out of the velocity we consider), then what can be gained? Well, the neutrons that had a velocity outside our velocity volume and which, by scattering, got that modified to the "good" velocity, therefore "appearing" in our phase space.

How do we write that in mathematical form?

Well, the losses term is written:

$$-\int_V v\Sigma(\vec{r},v).n(\vec{r},\vec{v},t).d^3r.d^3v$$

The gains term is written:

$$\int_V \int d^3v'.v'\Sigma_s(\vec{r},\vec{v}' \rightarrow \vec{v}).n(\vec{r},\vec{v}',t).d^3r.d^3v$$

2.3.4. Source term 4

That's an easy one. We consider that we have an infinity of point sources in the phase volume (space and velocity) considered. We just have to sum them up to have to global source term:

$$\int_V s(\vec{r},\vec{v},t).d^3r.d^3v$$

2.3.5. The Boltzmann equation

Putting everything together, we obtain:

$$\int_V d^3r.\left[\frac{\partial n}{\partial t} + \vec{v}.\vec{\nabla}.n + v\Sigma.n - \int d^3v'.v'\Sigma_s(\vec{v}' \rightarrow \vec{v}).n(\vec{v}') - s\right] = 0$$

Since the volume V is arbitrary, we can write:

$$\frac{\partial n}{\partial t} + \vec{v}.\vec{\nabla}.n + v\Sigma(\vec{r},v).n(\vec{r},\vec{v},t) = \int d^3v'.v'\Sigma_s(\vec{r},\vec{v}' \rightarrow \vec{v}).n(\vec{r},\vec{v}',t) + s\,(\vec{r},\vec{v},t)$$

Congratulations! We just wrote the Boltzmann equation, also known in neutron physics as the transport equation.

I swear that we are almost done. We have the transport equation that gives us the neutron density, and that is expressed using the velocity. Hidden behind this velocity are two variables, as introduced in chapter 1: the kinetic energy (E) and the direction ($\hat{\Omega}$). Moreover, rather than the neutron density, the angular flux is more interesting. We are now going to write the transport equation for the angular flux.

For that, we need to recall from the previous chapter that the angular flux is:

$$\Psi = n.v,$$

Thus, $\Psi/v = n$.

We can thus obtain:

$$\frac{1}{v}\frac{\partial \Psi}{\partial t} + \hat{\Omega}.\vec{\nabla}\Psi + \Sigma(\vec{r},E).\Psi(\vec{r},\mathrm{E},\hat{\Omega},t) = \int_0^\infty dE' \int_{4\pi} d^2\hat{\Omega}'.\Sigma_s(\vec{r},E' \rightarrow \mathrm{E},\hat{\Omega}'.\hat{\Omega}).\Psi(\vec{r},\mathrm{E}',\widehat{\Omega'},t) + s(\vec{r},\mathrm{E},\hat{\Omega},t)$$

Question n°1 : ✪

Can you explain how you obtain the transport equation for the angular flux ?

$\hat{\Omega}'.\hat{\Omega}$ is the scattering angle (isotropic medium)

This equation is:

- integro-differential: differential in time and space, integral in angle and energy. This means that the flux will be continuous in space and time but not necessarily in angle and energy
- linear, if the cross-sections are independent of the flux. This implies that if in a given geometry, $\Psi_1$is solution for a source S_1, and Ψ_2 for a source S_2, then the solution for a source $S_1 + S_2$ is $\Psi_1 + \Psi_2$.

This equation also exhibits boundary layers. Indeed, being differential in space and time, this equation requires initial and boundary conditions.

2.4. Criticality problems

We will very often consider, as we want to compute the neutron flux inside a nuclear reactor, that the source term contains a fission term. In that case, the source term is proportional to the flux.

The fission rate at $\vec{r}$ for an isotope i is:

$$\tau_f^i(\vec{r}) = \int_0^\infty dE'.\Sigma_f^i(\vec{r},E')\int_{4\pi} d^2\,\Omega.\Psi(\vec{r},E',\widehat{\Omega}')$$

The number ν of fission neutrons depends on the isotope and on the energy of the incident neutron. We aso have an energy spectrum, χ, that depends on the isotope and (weakly) on the energy of the incident neutron. The angular distribution of fission neutrons is isotropic, we can therefore write the fission source term:

$$\sum_i \frac{\chi^i(E)}{4\pi}\int_0^\infty dE'.\nu^i(E').\Sigma_f^i(\vec{r},E')\,\Phi(\vec{r},E')$$

Taking in this new term for the sources, we can rewrite the transport equation.

$$\frac{1}{v}\frac{\partial\Psi}{\partial t} + L\Psi = H\Psi + F\Psi + s$$

In which:

$$L\Psi = \hat{\Omega}.\vec{\nabla}\Psi + \Sigma(\vec{r},E).\Psi\big(\vec{r},\mathrm{E},\hat{\Omega},t\big)$$

$$H\Psi = \int_0^\infty dE' \int_{4\pi} d^2\hat{\Omega}'.\Sigma_s\big(\vec{r},E' \to \mathrm{E},\hat{\Omega}'.\hat{\Omega}\big).\Psi\big(\vec{r},\mathrm{E}',\widehat{\Omega'},t\big)$$

$$F\Psi = \sum_i \frac{\chi^i(E)}{4\pi}\int_0^\infty dE'.\nu^i(E').\Sigma_f^i(\vec{r},E')\,\Phi(\vec{r},E')$$

One could recognize here, but do not worry, that's definitely okay if you didn't, an initial value problem (or the Cauchy problem). This states that a solution exists and that it is unique. Isn't that convenient?

In a nuclear reactor, we look for a stationary solution without external sources. Stationary means that it doesn't change with time, therefore the derivative over time of the flux equals 0. No external sources means that the term s in the above equation also disappears.

This yields:

$$L\Psi = H\Psi + F\Psi$$

It is to note that a stationary solution does not always exit!

Inorder to solve that equation, one will want to modify it a bit. The number of fission neutrons ν becomes $\frac{\nu}{k_{eff}}$, where k_{eff} is the value by which we need to divide the productions in order to have a stationary solution. One could have recognized there the effective neutron multiplication factor. We thus obtain:

$$L\Psi = H\Psi + \frac{1}{k_{eff}} F\Psi$$

The goal is now to seek a solution to this eigenvalue problem, called criticality calculation. We can always find a couple (k_{eff}, Ψ) which satisfies the critical equation.

This is a difficult problem to solve, of course. Wouldn't be fun otherwise, would it? Basically, the way to solve this equation is to use the power iteration method.

$$L\Psi^n = H\Psi^n + \frac{1}{k^{n-1}} F\Psi^{n-1}$$
$$k^n = \frac{F\Psi^n}{F\Psi^{n-1}/k^{n-1}}$$

We could show that:

$$k^n \xrightarrow{n\to\infty} k_{eff} \text{ and } \Psi^n \xrightarrow{n\to\infty} \Psi$$

By iterations, we can work out Ψ and k_{eff}

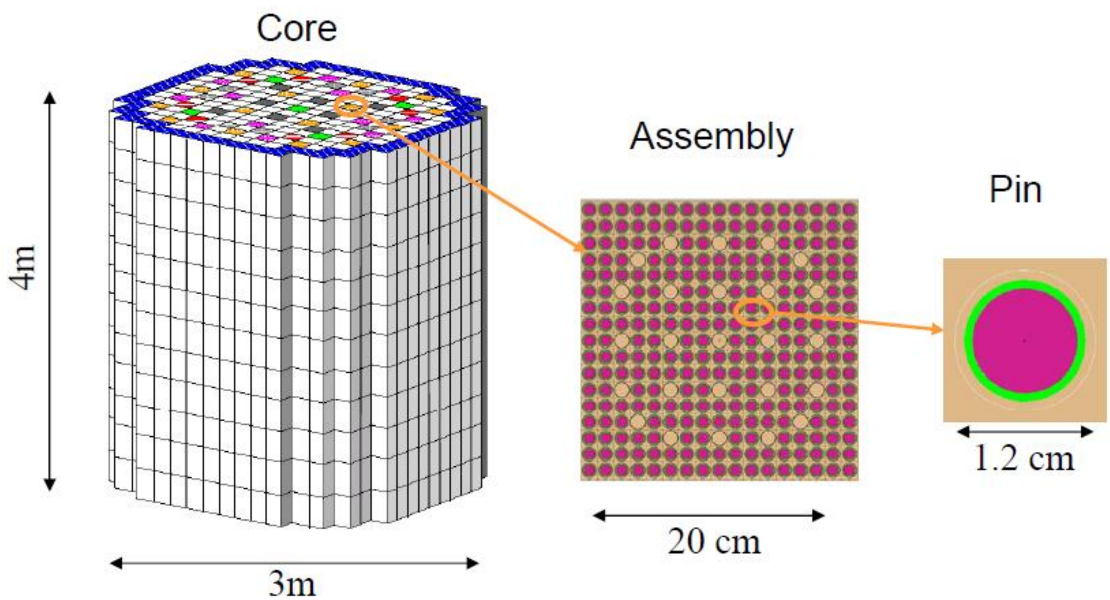
2.5. Calculation power limitations

We have the equations. Why then would it be difficult now, might you think? Aren't we capable of calculating a lot of things with today's calculation power throughout the world?

Well, we're getting there, but slowly. Let me show you the problems of trying to solve the exact transport equation as defined earlier.

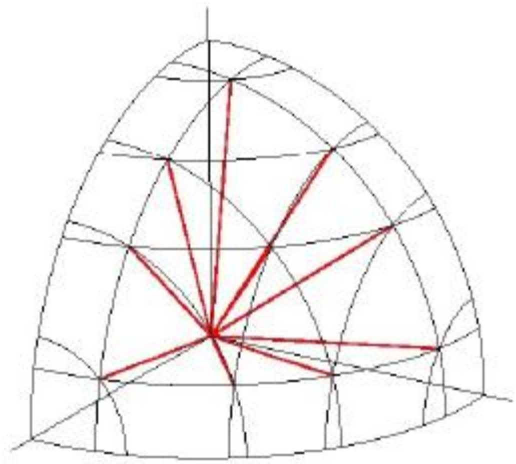
First, we need to partition the phase space $(\vec{r}, \mathrm{E}, \hat{\Omega})$ in pieces (meshes) where:
- The cross-sections Σ are constants
- The solution Ψ is linear

On the next figure, you can see the size of what we want to compute. Keep in mind that a mesh is one of the regions in a pin.



Roughly, this translates to 10^9 meshes *for space*!

Now, let's consider the angular meshes. We need to discretize the space for angles too (see the figure below). One can approximate the number of meshes needed for th eangular discretization to 10^3!



Finally, one needs to discretize the energy! Each isotopes must have around 10^5 "meshes" to be described properly, notably because of all the resonances (we'll talk about that later, next chapter!). Considering all the isotopes in our core, we're eventually talking about 10^7 energy "meshes"!

So, if we calculate the number of "meshes" needed to set up our problems and compute the resulting flux, that is:

$$10^9 * 10^3 * 10^7 = 10^{18} \text{ meshes!}$$

Curently, we can "only" solve for $\sim 10^9$ degrees of freedom. So, we can see that we are quite far from it, even if 50 years ago being able to do that was unthinkable. In the future, there is little doubt that our computational power will be enough to do that. In the meantime, we already have nuclear reactors, and we need to be able to compute the flux in those.

As an order of magnitude, the industry requires calculation times of:

- 1 minute for a steady state core calculation
- 1 hour for a cycle length calculation

This is not achievable with today's computational power. So, we need to make assumptions and to cut down on precision. For example, we homogenize the cross-section (average in space), we condense them (average in energy), we introduce simplified models (the diffusion equation, SPn calculations, etc). We will talk about that later on, in this class.

Well, this ends the second lecture. If you have any question, please let me know directly or post a thread in the dedicated subreddit. Do not forget, and I can't stress this enough: if you have a question, then someone else in the class is wondering the same thing, or should be. Therefore, asking it will help you and others.

The homework #2 will only contain the question asked in this lecture, for now. I will try to imagine a problem I might realistically ask, but it seems unlikely, considering the nature of the lecture.

There is another thing that I should repeat. If you do not understand something, do not feel like it's your fault, and do not give up. It merely means that my explanations were not good enough. I will gladly upgrade the class by taking into account your suggestions and remarks.