Neutron Diffusion

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1 Introduction

This analysis is concerned in the diffusion of neutrons in fissile material where collisions between free neutrons and nuclei results in a secondary release of these particles. As the fissile core increases in size the radioactive material will became critical and after this threshold there is an exponential runaway in the neutron density that leads to an intense explosion. The following calculations are performed to establish the size at which criticality occurs. At first it is presented an unphysical toy model made by a one-dimensional system of U^{235} atoms (or Pu^{239}) where we search for the critical length after which we obtain an uncontrolled runaway of neutrons. The second model is the three-dimensional version of the previous system describing thus a cubic volume of fissile material. Here we have a physically realizable situation and it is possible to calculate the mass of radioactive material necessary to build a nuclear bomb. These two models are extremely simplified by the choice of the boundary conditions of the problem, indeed we use here Dirichlet BCs, i.e. we limit the analysis on the specified region without allowing the escape of neutrons from the system. At the end we study a more realistic scenario considering a spherical volume from which the neutrons are able to escape, this concept is mathematically encoded inside the Neumann boundary conditions.

2 Nuclear Reaction - Mathematical description

Consider the diffusion of U^{235} (or Pu^{239}) neutrons with Dirichlet boundary conditions. The equation that governs this process is:

$$\frac{\partial n}{\partial t} = \mu \nabla^2 n + \eta n \tag{1}$$

where $n = n(t, \vec{x})$ represent the neutron density function. The two constants μ and η are called respectively the *diffusion constant* (with units $[m^2/s]$) and the *neutron rate of formation* ($[1/s]$). Both of them are positive $(\mu, \eta) > 0$.
This equation furnish a description of the phenomena of nuclear reaction in a volume Ω with boundary $\partial\Omega$, and to set the Dirichlet boundary conditions we have to impose:

$$n(t, x)|_{\partial\Omega} = 0$$

In each problem we impose also an initial condition that respect the boundary conditions of the form $n(0, \vec{x}) = f(\vec{x})$.

2.1 1D Cartesian coordinates - Dirichlet BCs

2.1.1 Theoretical considerations

We now consider the planar case, the equation (1) in 1D becomes:

$$\begin{gathered}\frac{\partial n}{\partial t} = \mu \frac{\partial^2 n}{\partial x^2} + \eta n, \quad n = n(t, x), \quad (\mu, \eta) > 0, \quad 0 > t >= \infty, \quad x \in \mathbb{R}; \\ BCs: \quad n(t, 0) = n(t, L_x) = 0; \\ IC: \quad n(0, x) = f(x)\end{gathered} \tag{2}$$

Now we can simply solve equation (2) by postulating a simple form of the solution that separates the time evolution and the spatial evolution:

$$n(t, x) = T(t)X(x) \tag{3}$$

substituting this into equation (2) we obtain the following equality:

$$\frac{1}{T}\frac{\partial T}{\partial t} - \eta = \mu \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\alpha \tag{4}$$

Since the evolution in time and in space is now divided the only way for these two to be equal is that both are equal to a single constant α that for mathematical reasons we write with the minus sign. Now we are able to separate the PDE into two different ODEs:

$$\frac{dT}{dt} = (\eta - \alpha)T, \quad and \quad -\mu \frac{d^2 X}{dx^2} = \alpha X \tag{5}$$

The solutions to these equations are well known from an analytical point of view, indeed they are:

$$T = A\exp([\eta - \alpha]t) \qquad and \qquad X = B\sin\left(\sqrt{\frac{\alpha}{\mu}}x\right) \tag{6}$$

where in the solution of the spatial equation has been used the fact that n has to be zero for x=0 and x=L to exclude the contribution of the $\cos\left(\sqrt{\frac{\alpha}{\mu}}x\right)$. Moreover, to satisfy the desired BC the argument of the sin function has to be equal to $p\pi x/L$ where $p \in \mathbb{Z}$. Using the *superposition principle* the total solution can be written as a series expansion:

$$n = \sum_{p=1}^{\infty} a_p \exp([\eta - \alpha]t) \sin\left(\frac{p\pi}{L}x\right) \tag{7}$$

At the end, from the previous considerations regarding boundary conditions it is possible to extract the value of the critical length, indeed from the condition that the solution has to be zero at the boundaries we can find that:

$$L_{crit} = \pi\sqrt{\frac{\mu}{\eta}} \tag{8}$$

2.1.2 Numerical analysis

From the numerical point of view the first step is to solve the two differential equations. We start from the spatial one:

$$-\mu\frac{d^2}{dx^2}X = \alpha X \tag{9}$$

The latter can be disctretized on the space interval $x \in [0, L]$ and transformed in an Eigenvalue problem

$$D_{ij}X_j = \alpha_i X_i \tag{10}$$

where the matrix D_{ij} is the discrtization, using the finite difference calculus, of the second derivative times $-\mu$:

$$-\frac{\mu}{h^2}\begin{pmatrix} -2 & 1 & \cdots & \cdots & & 0 \\ 1 & -2 & 1 & \cdots & & \vdots \\ \vdots & & & \ddots & & \\ 0 & \cdots & \cdots & & 1 & -2 \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \end{pmatrix} = \alpha_i \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \end{pmatrix} \tag{11}$$

Numerically at the beginning and at the end of each eigenvector X_i are inserted by hand two zeros to enforce the boundary conditions and to avoid an exponential growth in these points.
Regarding the time ODE from the initial condition $n(0, x) = f(x)$ we can extract the information about the initial condition related to $T(t)$, indeed the latter is true if $T(0) = 1$ or equal to some constant that can be included inside the initial condition. To solve this equation we used the Python method **odeint** included in the library **scipy.integrate**.
At this point it is possible to find the critical length from pure numerical analysis. From the solution of the first ODE we can extract the value of α that we can use to solve the time ODE. The criticality happens when the exponential solution diverges, so it is sufficient to analyze the change in the slope of this function to find the critical value:

$$L_{th} = 11.050\ cm \qquad\qquad L_{num} = 11.048\ cm \tag{12}$$

in accordance with [Gri15] .
At the end we have to calculate the coefficients a_p of the series expansion. These constants are given by the integral:

$$a_p = \frac{2}{L}\int_0^L \exp\left(\frac{-4\lambda(x - \frac{L}{2})^2}{L^2}\right) X_p \ \ dx \tag{13}$$

where X_p represent the p-th eigenvector and the exponent is the initial function $f(x)$ where $\lambda = 100$.

The first 30 resulting coefficients are reported in the following table:

p	a_p
1	0.1762
3	0.1679
5	-0.1519
7	-0.1310
9	-0.1086
11	0.0853
13	0.0625
15	-0.0443
17	-0.0298
19	0.0191
21	0.0117
23	0.0068
25	0.0038
27	-0.0020
29	-0.0010

Table 1: Non zero coefficients of the series expansion calculated at L=12.00 cm.

These coefficients up to the sign are in perfect accordance with [Gri15]. The differences in signs are due to the fact that in [Gri15] instead of X_p in the previous integral there was the analytical sin function, and during the resolution of the Eigenvalue problem some solutions have a 180° phase with respect to these functions. The coefficients appear with the right sign to correct this phase problem.
Now, we have all of the ingredients to visualize the solution to this one-dimensional problem:

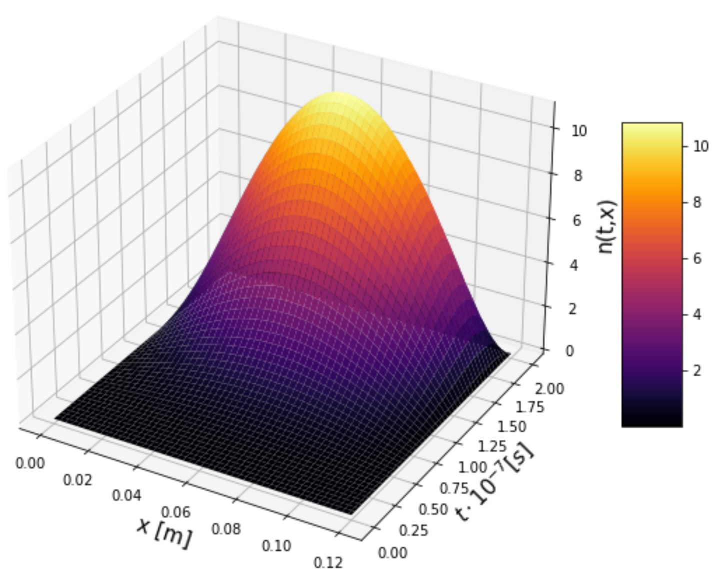

Figure 1: Neutron density evolution in time $t \in [0, 0.2]\mu s$ for a sovracritical length L=12.00 cm

Here we can see the runaway of neutrons also in this one dimensional toy model. We are considering a slightly larger length L with respect to the critical one and after a time $t = 0.2\mu s$ we can see a strong growth. This fact can be better appreciated if we wait some more:

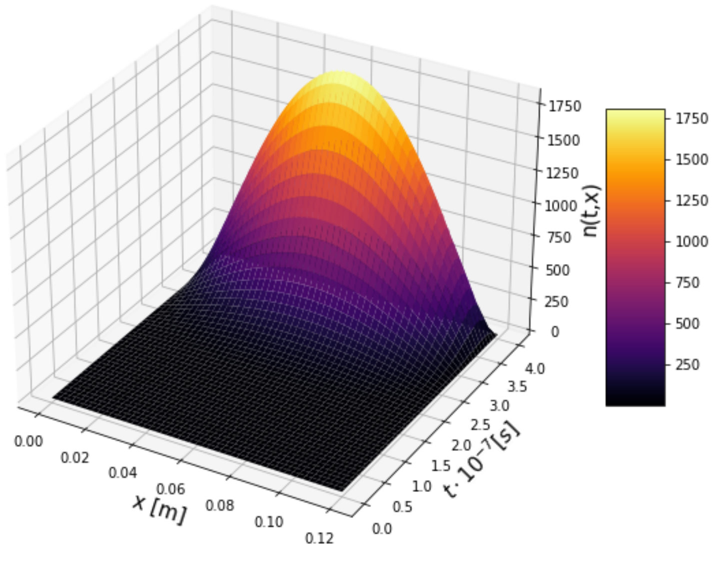

Figure 2: Neutron density evolution in time $t \in [0, 0.4]\mu s$ for a overcritical length L=12.00 cm

After less than one microsecond the divergence is evident: the neutron density increases unbounded.

2.2 3D Cartesian coordinates - Dirichlet BCs

2.2.1 Theoretical considerations

The three dimensional case is the straight generalization of the previous one dimensional system. Here we consider a cubic volume of fissile material, and the equation (1) becomes:

$$\frac{\partial n}{\partial t} = \mu\left(\frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2}\right) + \eta n, \quad n = n(t, x, y, z), \quad (\mu, \eta) > 0, \quad 0 > t >= \infty, \quad (x, y, z) \in \mathbb{R}; \tag{14}$$

Where now the boundary conditions set to zero the neutron density in all of the faces of the cube and the initial condition is a function of $\mathbb{R}$: $n(0, x, y, z) = f(x, y, z)$.
The solution is the analogous of (7) but in three dimensions:

$$n = \sum_{p,q,r}^{\infty} a_{p,q,r} \exp([\eta - \alpha]t) \sin\left(\frac{p\pi}{L}x\right) \sin\left(\frac{q\pi}{L}y\right) \sin\left(\frac{r\pi}{L}z\right) \tag{15}$$

Also this time it is possible to find a theoretical value of the critical length, from which using the density of the fissile material can be extracted the volume and the mass needed to create a nuclear explosion.

$$L = \pi\sqrt{\frac{3\mu}{\eta}} \tag{16}$$

2.2.2 Numerical analysis

The resolution of the spatial ODEs is completelly equal to the simple 1D case but this time we have three separated equations for all of the spatial coordinates:

$$-\mu\frac{d^2}{dx^2}X = \alpha_x X \qquad -\mu\frac{d^2}{dy^2}Y = \alpha_y Y \qquad -\mu\frac{d^2}{dz^2}Z = \alpha_z Z \tag{17}$$

Solving the eigenvalue problems we are able to find the solutions to these equations. The solution of the temporal ODE is found using the solver **scipy.integrate.odeint**, the only difference is that $\alpha = \alpha_x + \alpha_y + \alpha_z$.

Performing the same analysis on the slope of the time solution we are able to find the critical length:

$$L_{th} = 19.136\ cm \qquad\qquad L_{num} = 19.138\ cm \tag{18}$$

in accordance with the result reported in [Gri15].
We are able to compute the coefficients of the series expansion of our solution using an initial condition which respects the boundary conditions. This time we have to deal with multi-indices coefficients:

$$a_{p,q,r} = \left(\frac{8}{L^3}\right)^2 \int_0^L \int_0^L \int_0^L xyz \left(1-\frac{x}{L}\right)\left(1-\frac{y}{L}\right)\left(1-\frac{z}{L}\right)\ X_p\ Y_q\ Z_r\ dx\ dy\ dz \tag{19}$$

This time a vast number of coefficients is equal to zero due to the great number of odd combinations of sin function that are computed numerically and encoded inside $X_p\ Y_q\ Z_r$. Here we report only the coefficients among the first 64 that are different from zero:

p	**q**	**r**	$a_{p,q,r}$
1	1	1	1.3741E-01
1	1	3	-5.0962E-03
1	3	1	-5.0962E-03
1	3	3	1.8893E-04
3	1	1	-5.0962E-03
3	1	3	1.8893E-04
3	3	1	1.8893E-04
3	3	3	-7.0048E-06

Table 2: First non-zero coefficients of the series expansion for L=19.14cm.

These are the same coefficients founded in [Gri15] except for the sign for the same reason reported previously. In the following we report the plots of the initial condition at time $t = 0$ and its evolution on a slice z=L/2 for a time $t = 8 \cdot 10^{-7} s$ and for a overcritical length $L = 25.00\ cm$.

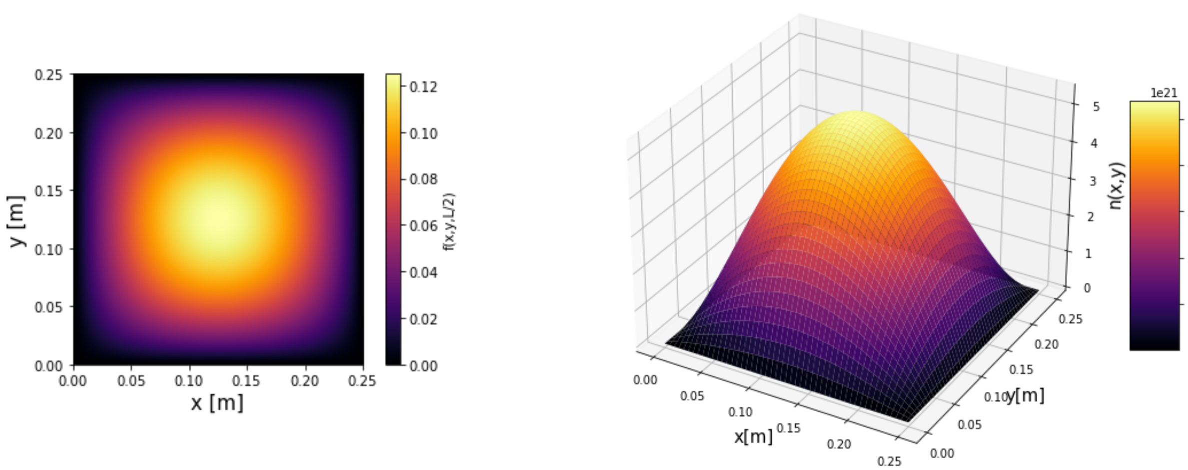

Figure 3: On the left the 2D projection of the initial condition at t=0. On the right its evoution in time respresented as the embedded solution at a slice z=L/2

Also in this case it is possible to notice the fast divergence of the neutron density of the system. Indeed in this example we see that in less than a microsecond the density increases of tens orders of magnitude.

2.3 3D Spherical coordinates - Neumann BCs

2.3.1 Theoretical considerations

We consider now neutron diffusion in a 3D symmetrical core. We analyze the situation of a spherical volume of fissile material with the more realistic Neumann boundary conditions that allow for the escape of some neutrons from the system. The equation (1) in spherical coordinates becomes:

$$\begin{gathered} \frac{\partial n}{\partial t} = \mu \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) n + \eta n, \quad n = n(t,r), \quad (\mu, \eta) > 0, \quad 0 > t >= \infty, \quad r \in \mathbb{R}; \\ BCs: \frac{dn(t,r_1)}{dr} = -\frac{3}{2}\frac{n(t,r_1)}{\lambda_t} \qquad ICs: n(0,r) = f(r) \end{gathered} \tag{20}$$

Where r represents the radial distance from the centre of the ball, r_1 the ball radius, λ_t represents transport free path and other symbols are as previously defined.
We use the same approach as (3) postulating a solution of the form:

$$n(t,r) = T(t)R(r) \tag{21}$$

Obtaining thus two separated Odes:

$$\frac{dT}{dt} = -\alpha T; \quad \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + k^2 R = 0; \tag{22}$$

where $k = \sqrt{\dfrac{\eta + \alpha}{\mu}}$.
The solution to the first equation of (22) is:

$$T = A \exp(-\alpha t) \tag{23}$$

and for a bounded solution we need $\alpha > 0$. The solution to the second of eqns. (22) combined with the fact that we require a finite value at $r = 0$ is:

$$R = \frac{B}{r} \sin(kr) \tag{24}$$

Imporsing analytically the condition deriving from the BCs we are able to find the connection between k and α:

$$\frac{dR}{dr} = -\frac{3}{2}\frac{R}{\lambda_t} \Longrightarrow -1 + kr \cot kr + \frac{3}{2}\frac{r}{\lambda_t} = 0 \tag{25}$$

The latter equation has to be solved numerically and if we let $\alpha = 0$ this will create the criticality condition from which we find $r_{crit} = 8.369cm$. At the end the full solution will be of the form:

$$n(t,r) = A \exp(-\alpha t) \frac{\sin(kr)}{r} \tag{26}$$

The constant A can be fixed for specifying the desired value of n at the surface at t=0. In any case the precise shape of the initial condition $f(r)$ is not important, because for $r > r_{crit}$ any value will cause $n(r,0)$ to increase exponentially with time.

2.3.2 Numerical analysis

The first step in this numerical analysis was to solve the equation relating r to α using the analytical form (25), to solve this relation we used the numerical algoritm present in the library scipy of Python **scipy.optimize.fsolve**. The critical value for the radius was found to be:

$$r_{crit} = 8.363\ cm$$

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Using the same relation and increasing the value of r sligthly above the critical one we computed the corresponding k to be used to solve the two ODEs. For a value $r = 9.0\ cm$ we obtained $k = 26.88\ m$ (correspondig to $\alpha = -2.0E + 7$).
Using this value it is possible to solve the two differential equations. The resolution of the temporal equation is equal to the one described in the previous cases using **scipy.integrate.odeint**. The radial equation is more difficult due to the boundary conditions. The resolution required the use of another algorithm present in the library scipy of Python, more precisely **scipy.integrate.solve_bvp** that solves differential equations with non trivial boundary conditions.
At the border of the sphere we imposed the Neumann condition (20) while at r=0 is set equal to the value of the limit $\lim_{r\to 0} \sin(kr)/r$ thus k. The resulting solution, that correspond to the value of the neutron density at exactly the critical length (and thus in a static situation), is the following:

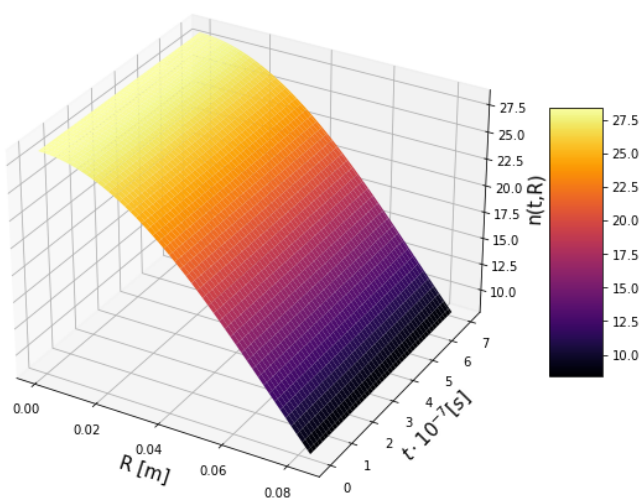

Figure 4: Neutron density at t=0 for a radius $r = 9.0cm$

If we combine the solutions of the two differential equation we have the exponential growth of the function, for a time $t = 7.0E - 7$ the neutron density looks like:

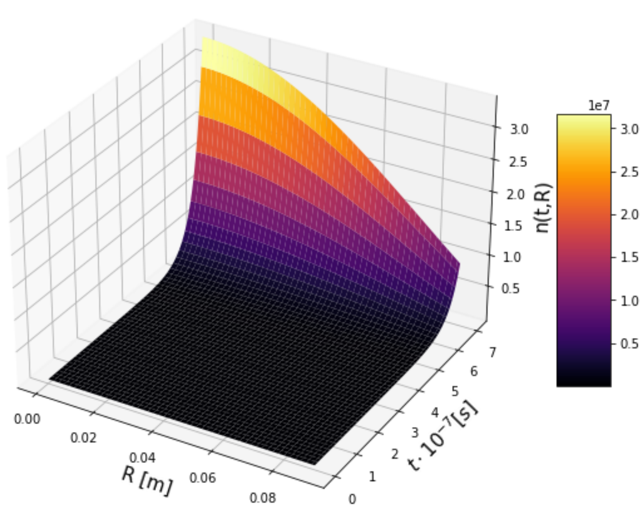

Figure 5: Neutron density at $t = 7.0E - 07$ for a radius $r = 9.0cm$

Note that also the value of $n(r = 0.09, t)$ increases with time with Neumann boundary conditions, unlike the case with Dirichlet BC.

References

[Gri15] Graham W. Griffiths. Neutron diffusion. 2015.