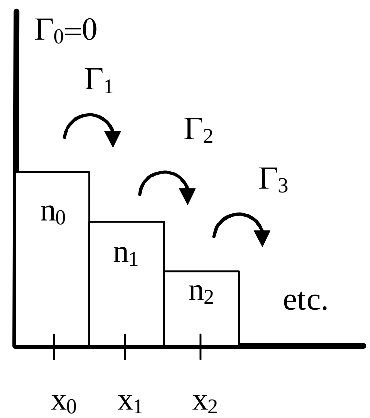
Diffusion with particle accounting



In steady-state plasmas the rate at which plasma is lost to the walls is equal to the rate at which it is created. If the plasma is collisional, the spatial profile of the number density n(x,t) may be found by solving the diffusion equation with a source term. In this exercise, we will find a solution to this equation for planar geometry. The continuity equation with a source term is

$$\frac{\partial n}{\partial t} + \vec{\nabla} \cdot \vec{\Gamma} = S$$

which in one dimension is $$\frac{\partial n}{\partial t} + \frac{\partial \Gamma}{\partial x} = S$$

where S is the source of particles (assumed to be independent of time and position), and Γ(x,t) is the particle flux toward the walls. Fick's law in one dimension is:

$$\Gamma = -D\frac{\partial n(x,t)}{\partial x}$$ where D is the diffusivity.

These equations will be solved in finite-difference form by iteration.
The continuity equation becomes:

$$\frac{n(x,t+\Delta t) - n(x,t)}{\Delta t} + \frac{\Gamma(x+\frac{1}{2}\Delta x,t) - \Gamma(x-\frac{1}{2}\Delta x,t)}{\Delta x} = S$$

where n(x,t) is defined on grid points x = x_m, and Γ is defined on "half grid" points x = $x_m+\Delta x/2$. The reason for half grid points is that it makes the derivative of Γ centered at the grid points x_m, which means that the derivative of Γ is correct to second order in Δx. Next we will write this equation with Γ(x,t) evaluated at grid points and n(x,t) evaluated at the half-grid points:

$$\frac{n(x+\frac{1}{2}\Delta x,t+\Delta t) - n(x+\frac{1}{2}\Delta x,t)}{\Delta t} + \frac{\Gamma(x+\Delta x,t) - \Gamma(x,t)}{\Delta x} = S$$ which gives:

$$n(x+\tfrac{1}{2}\Delta x,t+\Delta t) = n(x+\tfrac{1}{2}\Delta x,t) + S\ \Delta t + \left(\frac{\Delta t}{\Delta x}\right)\left[\Gamma(x+\Delta x,t) - \Gamma(x,t)\right]$$

The finite difference form of Fick's law is:

$$\Gamma(x,t) = -\frac{D}{\Delta x}\left[n(x+\tfrac{1}{2}\Delta x,t) - n(x-\tfrac{1}{2}\Delta x,t)\right]$$

This equation also has the number density evaluated at half grid points. The continuity equation and Fick's law may be combined to give the diffusion equation in one dimension:

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial n}{\partial x}\right) + S$$

In this exercise, we will solve simultaneously the continuity equation and Fick's law which is equivalent to solving the diffusion equation.

The x grid:

We will divide the x axis into cells with boundaries at multiples of Δx.
Γ_m is the flux of particles entering cell (m,m+1) at the left boundary (see the figure above).
Γ_{m+1} is the flux of particles leaving cell (m,m+1) at the right boundary and entering the next cell.
Cell number m is centered at $x_m + \Delta x/2$ and the number density n_m is the number density at the center of the cell.

$L := 5$ This is the distance from the midplane to the center of the last cell.

$mmax := 10$ mmax + 1 is the number of x grid points

$m := 0 .. mmax \quad x_m := L \cdot \frac{m + 0.5}{mmax + 0.5} \qquad \Delta x := x_1 - x_0 \quad \Delta x = 0.476$

These definitions put the center of the cells at half grid points and the cell boundaries at integer multiples of Δx. The center of the last cell, where the density is zero, is the plasma boundary.

$D := 1$ is the diffusivity.

$Dtime := \frac{2}{D}\left(\frac{2 \cdot L}{\pi}\right)^2$ This is the decay time from analytic theory.

$tmax := 2 \cdot Dtime$ We will follow the solution for two decay times.

The time step needed for stability is approximately the diffusion time across one grid cell:

$\Delta t := \frac{\Delta x^2}{2 \cdot D} \qquad \Delta t = 0.113$ Approximate number of time steps: $Tsteps := \frac{tmax}{\Delta t}$

$Tsteps = 357.461$ Make this a number divisible by four to make the final plot nicer:

$jmax := 4 \cdot ceil\left(\frac{Tsteps}{4}\right) \qquad jmax = 360 \qquad \Delta t := \frac{tmax}{jmax} \qquad \Delta t = 0.113 \qquad j := 0 .. jmax$

jmax is the number of time steps and Δt is the time step.

Using symmetry:
We assume that our problem is symmetric about the midplane, thus it will be sufficient to solve only the right half of the problem. The midplane will be the point m = 0. The density will be peaked at the center, to the left of grid point zero, thus we will use an initial profile that is a cosine. There is no flux across the midplane because the first derivative of of the density is zero (see Fick's law). The profile is a maximum at the origin and is zero at the center of the last cell.

The **initial conditions** are a half-cosine profile: $n_m := \cos\left(\frac{\pi x_m}{2 \cdot L}\right)$

Because there is no flux across the midplane, Γ_0 [which is shorthand notation for $\Gamma(x_0)$] is zero. The particles lost from the system are lost at the left side of the cell numbered mmax thus the losses from the system are Γ_{mmax} summed for each time step. The number of particles in the last cell is zero, because this is a boundary condition, even though particles enter the cell from the left. Thus the particles entering the last cell from the left are the particles that are lost.

Particle conservation:
The source term S is the number of particles created per unit distance per unit time. Thus the number of particles added to the system to the left of the last cell is S (mmax Δx) (jmax Δt). The number of particles lost per unit time is Γ_{mmax}. The sum of Γ_{mmax} Δt at each time step is the total number of particles lost. We have conserved particles if the final number of particles minus the initial number of particles is equal to the gain in particles minus the loss in particles.

$S := 0$ We will begin with no source of new particles.

This is the program loop:

$$
M(n,S) := \left|
\begin{array}{l}
M_{jmax,mmax} \leftarrow 0 \\
\Gamma_{mmax} \leftarrow 0 \\
\text{for } m \in 0..mmax \\
\quad M_{0,m} \leftarrow n_m \\
\text{for } j \in 1..jmax \\
\quad \left| \begin{array}{l}
\text{for } m \in 1..mmax \\
\quad \Gamma_m \leftarrow -\dfrac{D}{\Delta x}\cdot\left(M_{j-1,m} - M_{j-1,m-1}\right) \\
\text{for } m \in 0..mmax-1 \\
\quad M_{j,m} \leftarrow M_{j-1,m} + \dfrac{\Delta t}{\Delta x}\cdot\left(\Gamma_m - \Gamma_{m+1}\right) + S\cdot\Delta t
\end{array}\right. \\
M
\end{array}\right.
$$

Initialize Γ and the answer matrix M.

Redefine the first row of M.

Do the main loop jmax times:

Find the fluxes between cells from Fick's law.

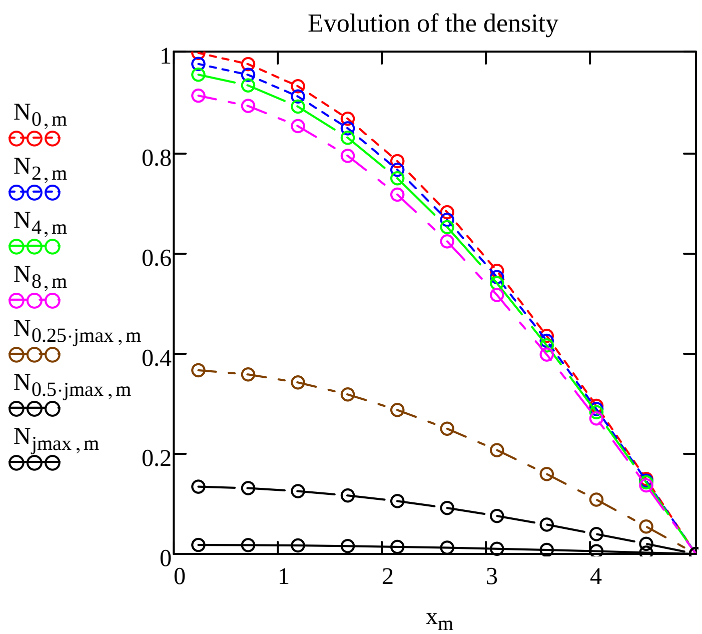
Find the changes in the density due to the fluxes.

The loop does not change $M_{j,mmax}$, thus the boundary condition at L is preserved at zero.

M(n, S) =

	0	1	2	3	4	5	6	7	8	9	10
0	1	0.97	0.93	0.87	0.78	0.68	0.56	0.43	0.29	0.15	0
1	0.99	0.96	0.92	0.86	0.77	0.67	0.56	0.43	0.29	0.15	0
2	0.98	0.95	0.91	0.85	0.76	0.67	0.55	0.42	0.29	0.15	0
3	0.96	0.94	0.9	0.84	0.76	0.66	0.54	0.42	0.29	0.14	0
4	0.95	0.93	0.89	0.83	0.75	0.65	0.54	0.41	0.28	0.14	0
5	0.94	0.92	0.88	0.82	0.74	0.64	0.53	0.41	0.28	0.14	0
6	0.93	0.91	0.87	0.81	0.73	0.64	0.53	0.41	0.28	0.14	0
7	0.92	0.9	0.86	0.8	0.72	0.63	0.52	0.4	0.27	0.14	0
8	0.91	0.89	0.85	0.79	0.72	0.62	0.52	0.4	0.27	0.14	0
9	0.9	0.88	0.84	0.78	0.71	0.62	0.51	0.39	0.27	0.13	0
10	0.89	0.87	0.83	0.77	0.7	0.61	0.5	0.39	0.26	0.13	0
11	0.88	0.86	0.82	0.77	0.69	0.6	0.5	0.38	0.26	0.13	...

$N := M(n, S)$ M(g,S) was made a function so that we could change g or S without typing again the program loop. If we convert M from a function to a fixed matrix N, the regions below compute faster.



Question:
Is the central density e^{-2} of the starting density after the two decay times?

Demonstration of particle conservation:

$$\Gamma mmax(j) := -\frac{D}{\Delta x} \cdot \left(N_{j,mmax} - N_{j,mmax-1}\right)$$

This is the loss flux at the left side of the last cell (mmax-1, mmax).

$$Loss := \sum_{j=0}^{jmax-1} (\Gamma mmax(j) \cdot \Delta t) \qquad Loss = 3.12$$

This is the sum over times j of the losses at the right boundary. The loss per unit time is multiplied by Δt.

$$Initial := \sum_{m=0}^{mmax} \left(N_{0,m} \cdot \Delta x\right) \qquad Initial = 3.177$$

The initial number of particles is found by summing the particles in each cell at the time step j = 0.

$$Final := \sum_{m=0}^{mmax} \left(N_{jmax,m} \cdot \Delta x\right) \qquad Final = 0.057$$

The final number of particles is found by summing the particles in each cell at the time step j = jmax.

$$Gain := S \cdot (mmax \cdot \Delta x) \cdot (jmax \cdot \Delta t) \qquad Gain = 0$$

This is the number of particles added to the left of the last cell.

$Final - Initial = -3.12$ Note that the change in the number of particles, (Final-Initial), is very near to the gain in particles minus the loss of particles (Gain-Loss).

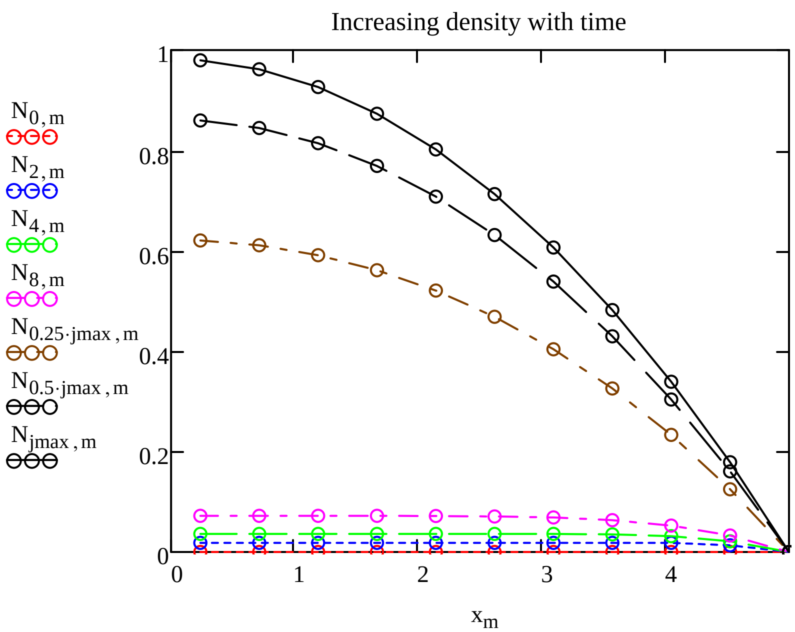
$Gain - Loss = -3.12$

$(Final - Initial) - (Gain - Loss) = -1.332 \times 10^{-15}$ Particle number is conserved vey well.

Diffusion with a source term:

The number of particles created between the midplane and x is Sx per unit time. The diffusive flux -D (dn/dx) must remove these particles, so dn/dx = -Sx/D and the number density must be $n(x) = N [1-(x/L)^2]$ with $N = SL^2 /2D$. For a number density of 1.0, we need a source rate of $2D/L^2$. Now we will repeat the above example with the value of S that gives unity density after a steady state is reached. We will use a starting density that is zero everywhere:

$n_m := 0$ $\quad S := \frac{2 \cdot D}{L^2}$ $\quad$ Find the new solution: $\quad N := M(n, S)$



Question: Why is the solid line (for t = tmax) located at the top of this graph and at the bottom of the previous one?

$N_{jmax, 0} = 0.979$ $\quad$ This is the density nearest the origin.

Try it: Increase the maximum time tmax by a factor of 4, so that it is:
Does the density approach unity at the center of the graph? $\quad tmax := \frac{8}{D} \left(\frac{2 \cdot L}{\pi} \right)^2$

Question: Are the half grid points x_m used anywhere (except in the plots)?

Demonstration of particle conservation with the source term above:

The loss flux at the wall: $\Gamma mmax(j) := -\frac{D}{\Delta x}\cdot\left(N_{j,mmax} - N_{j,mmax-1}\right)$

$$Loss := \sum_{j=0}^{jmax-1} (\Gamma mmax(j)\cdot\Delta t) \qquad Loss = 12.173$$

$$Initial := \sum_{m=0}^{mmax} \left(N_{0,m}\cdot\Delta x\right) \qquad Initial = 0$$

$$Final := \sum_{m=0}^{mmax} \left(N_{jmax,m}\cdot\Delta x\right) \qquad Final = 3.267$$

$$Gain := S\cdot(mmax\cdot\Delta x)\cdot(jmax\cdot\Delta t) \qquad Gain = 15.439$$

$$Final - Initial = 3.267$$

$$Gain - Loss = 3.267$$

$$(Final - Initial) - (Gain - Loss) = 1.776 \times 10^{-14}$$

Note that the change in the number of particles is very near to the gain in particles minus the losses of particles. Particle number is conserved very well. Mathcad keeps 15 decimal places, so an error of order 10^{-15} is round off error, and is probably not systematic error.