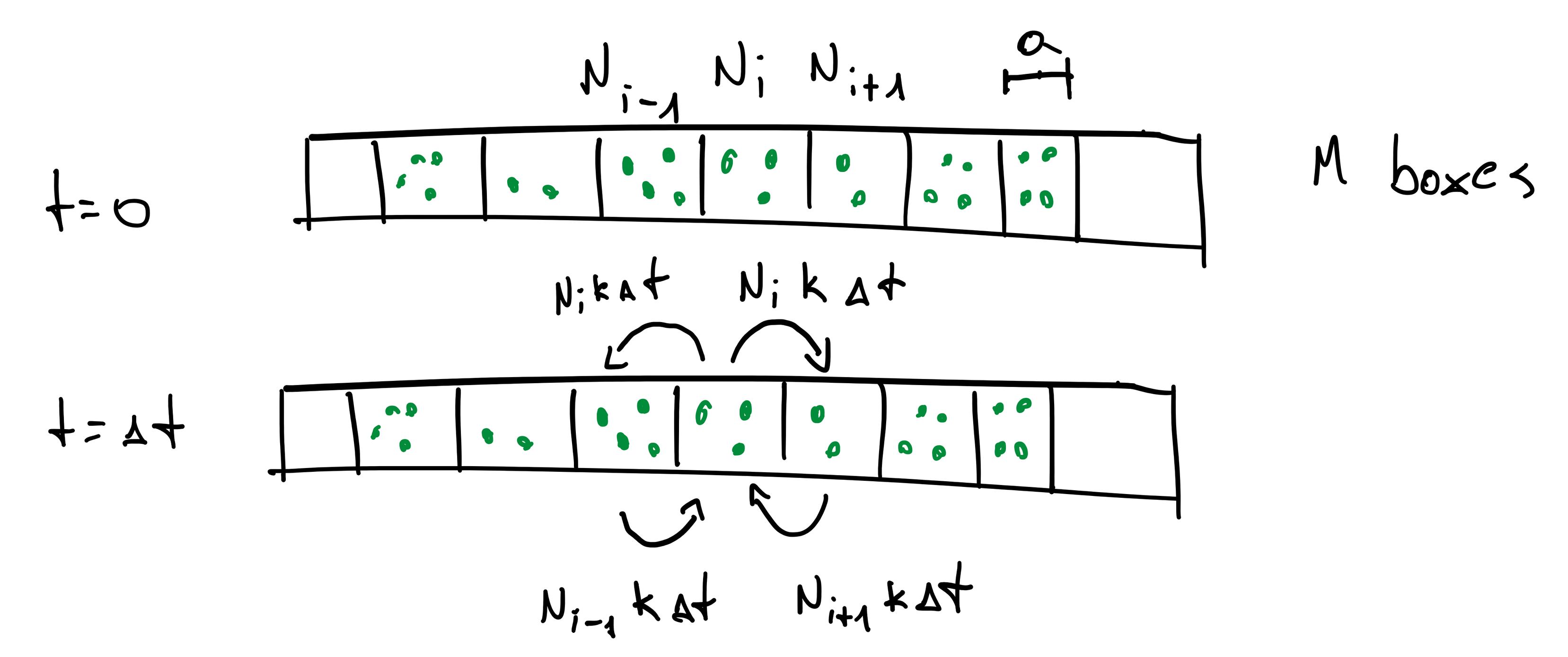
We want to solve the concentration profile dynamics due to diffusion

Simple model of diffusion:



$$N(i,t+\Delta t) = N(i,t) + \underbrace{N(i-1,t)k\Delta t}_{i-1\to i} + \underbrace{N(i+1,t)k\Delta t}_{i+1\to i}$$
$$- \underbrace{N(i,t)k\Delta t}_{i\to i-1} - \underbrace{N(i,t)k\Delta t}_{i\to i+1}$$

Let's bring up the concentration: $\dfrac{N(i,t)}{V_{box}} = c(i,t)$

Let's bring in the x coordinate: $i \to x$
$i+1 \to x+a$

$$c(x,t+\Delta t) = c(x,t) + c(x-a,t)k\Delta t + c(x+a,t)k\Delta t$$
$$- c(x,t)k\Delta t - c(x,t)k\Delta t$$

Move $c(x,t)$ and divide by Δt:

$$\underbrace{\frac{c(x,t+\Delta t) - c(x,t)}{\Delta t}}_{\frac{\partial c}{\partial t}} = c(x-a,t)k + c(x+a,t)k - c(x,t)k - c(x,t)k$$

$$k\left[c(x+a,t) - c(x,t)\right]\cdot\frac{a}{a}$$
$$= ka\,\frac{c(x+a,t)-c(x,t)}{a} = ka\,\frac{\partial c}{\partial x}\left(x+\frac{a}{2},t\right)$$

$$= -ka\,\frac{\partial c}{\partial x}\left(x-\frac{a}{2},t\right)$$

$$\frac{\partial c}{\partial t} = ka\left[\frac{\partial c}{\partial x}\left(x+\frac{a}{2},t\right) - \frac{\partial c}{\partial x}\left(x-\frac{a}{2},t\right)\right]\frac{a}{a}$$

$$= ka^2\,\frac{\frac{\partial c}{\partial x}\left(x+\frac{a}{2},t\right) - \frac{\partial c}{\partial x}\left(x-\frac{a}{2},t\right)}{a} = ka^2\frac{\partial^2 c}{\partial x^2}$$

$$\Downarrow$$

$$\frac{\partial c}{\partial t} = \underbrace{ka^2}_{\frac{1}{T}L^2}\frac{\partial^2 c}{\partial x^2} \implies \boxed{\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}}$$ diffusion equation

$$D = ka^2$$

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D=10;        #Diffusion constant in um^2/s
L=2;         #Size of our cell in um
Ntotal=100;  #Number of molecules

#Now, we need the simulation parameters. We need our time and space
#intervals to be smaller than any other quantity in the process.
dx=0.01;     #Size of our boxes in um
k=D/dx^2;    #D=k*dx^2
dt=1/k/10;   #Temporal interval in s, has be smaller than 1/k
TotalTime=0.01; #Total simulation time in s.
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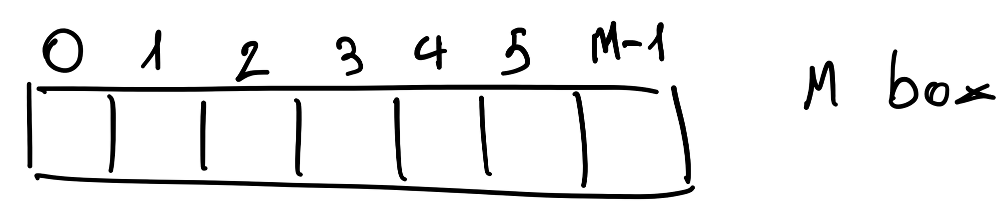
Initial conditions

$N[100, 0] = N_{total}$

middle box   t=0

Now we're ready to write our simulation.



For boxes 1 through 5:

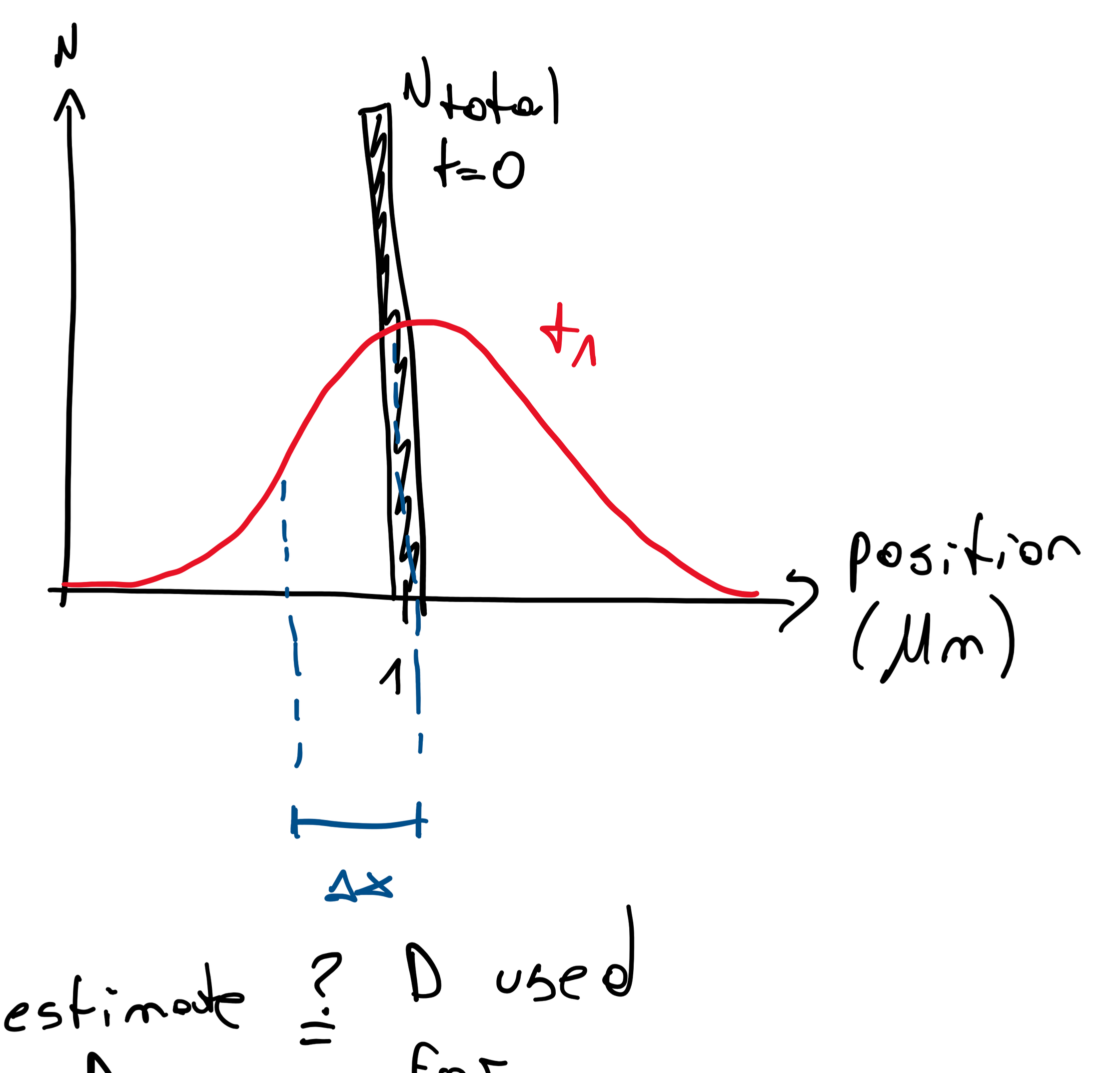
$$N(i,t+\Delta t) = N(i,t) + \underbrace{N(i-1,t)k\Delta t}_{i-1\to i} + \underbrace{N(i+1,t)k\Delta t}_{i+1\to i}$$
$$- \underbrace{N(i,t)k\Delta t}_{i\to i-1} - \underbrace{N(i,t)k\Delta t}_{i\to i+1}$$

For box 0:

$$N(0,t+\Delta t) = N(0,t) + N(1,t)k\Delta t - N(i,t)k\Delta t$$

For box M-1

$$N(M-1,t+\Delta t) = N(M-1,t) + N(M-2,t)k\Delta t - N(M-1,t)k\Delta t$$



$\dfrac{\Delta x^2}{t}$ = estimate $\overset{?}{=}$ D used for simulation