molecules diffusing in a volume $\rightarrow$ collide + react; "chemistry" $\rightarrow$ networks of chemical reactions

$\rightarrow$ add fuel (energy source) $\rightarrow$ living systems (organisms) $\rightarrow$ populations & evolution

link b/t levels: mathematics of stochastic (random) processes

Start: crowded "soup" of the cell

Question: two molecules diffusing inside, how long before they meet?

volume $V = L^3$

dynamics are complex + random
assume above some timescale \( t > \delta t \)

randomization occurs b/c interactions
of many of particle w/ surroundings

many physical aspects (temp., viscosity, density, boundaries) may influence this randomization

divide up volume into little boxes of size \( \alpha \)

1) state of particle \( \vec{n} = (i, j, k) \) = label of box where the particle resides

\[
\begin{align*}
i &= 1, \ldots, N = \frac{L}{\alpha} \\
j &= 1, \ldots, N \\
k &= 1, \ldots, N
\end{align*}
\]

physical position: \( \vec{r} = \alpha \vec{n} \)

2) define dynamics: focus on 1D description

at time \( t \) particle is at \( i \)
where is it at time \( t + \delta t \)?
\[\begin{align*}
i &\rightarrow i+1 : \text{probability} \quad wS_t \\
i &\rightarrow i-1 : \text{symmetry} \quad wS_t \\
i &\rightarrow i : 1-2wS_t \\
\text{large steps are unlikely b/c} \\
S_t \text{ is small enough}
\end{align*}\]

Whole dynamics described by one parameter:

\[w = \frac{\text{probability}}{\text{time}} = \text{probability rate} = \text{transition rate}\]

\[\Rightarrow \text{units: } [\text{time}]^{-1}\]

depends on all physical characteristics

(if constant in time \(\Rightarrow w \text{ constant})\)

Imagine running many experiments all starting with one molecule (for simplicity) at pos. \(i_0\) at \(t=0\)

\[
\begin{align*}
t=0 & \\
t=S_t & \\
t=2S_t &
\end{align*}
\]
$p_i(t) = \text{prob. of having pos. } i \text{ at time } t$

$= \frac{\# \text{ exper. w/ molec. at } i \text{ at time } t}{\text{total } \# \text{ exper. } = N_{\text{trials}}} \uparrow$

$t = 0$

$t = 5t$

$t = 25t$

$p_i(0)$

$p_i(5t)$

$p_i(25t)$

average pos:

$\langle i \rangle_t = \sum_{i=1}^{N} i \ p_i(t)$

average of any func. of $i$

$f(i) = i^2$

$\langle f(i) \rangle_t = \sum_{i=1}^{N} f(i) \ p_i(t)$

$\langle i^2 \rangle_t = \sum_{i=1}^{N} i^2 \ p_i(t)$

$2\text{nd moment of } p$

$\langle i^n \rangle_t = \text{n th moment of } p$
focus on one quantity: displacement

\[ f(i) = \Delta_i = a(i-i_0) = \text{how far has part. moved from } i_0? \]

mean squared displacement (MSD)

\[ \equiv \left\langle \Delta_i^2 \right\rangle_t \]

How to calculate? Two questions:

1) How does \( p_i(t) \) evolve in time?

2) How to calculate \( \left\langle \Delta_i^2 \right\rangle_t \) average?

\[
\left\langle \Delta_i^2 \right\rangle_t = \sum_{i=1}^{N} a^2(i-i_0)^2 p_i(t)
\]

\[
= \left\{ \sum_i i^2 p_i(t) - 2i_0 \sum_i i \, p_i(t)
+ i_0^2 \sum_i p_i(t) \right\} a^2
\]

\[
= \left[ \left\langle i^2 \right\rangle_t - 2i_0 \left\langle i \right\rangle_t + i_0^2 \right] a^2
\]

\( \implies \) How to calculate dynamics of moments?