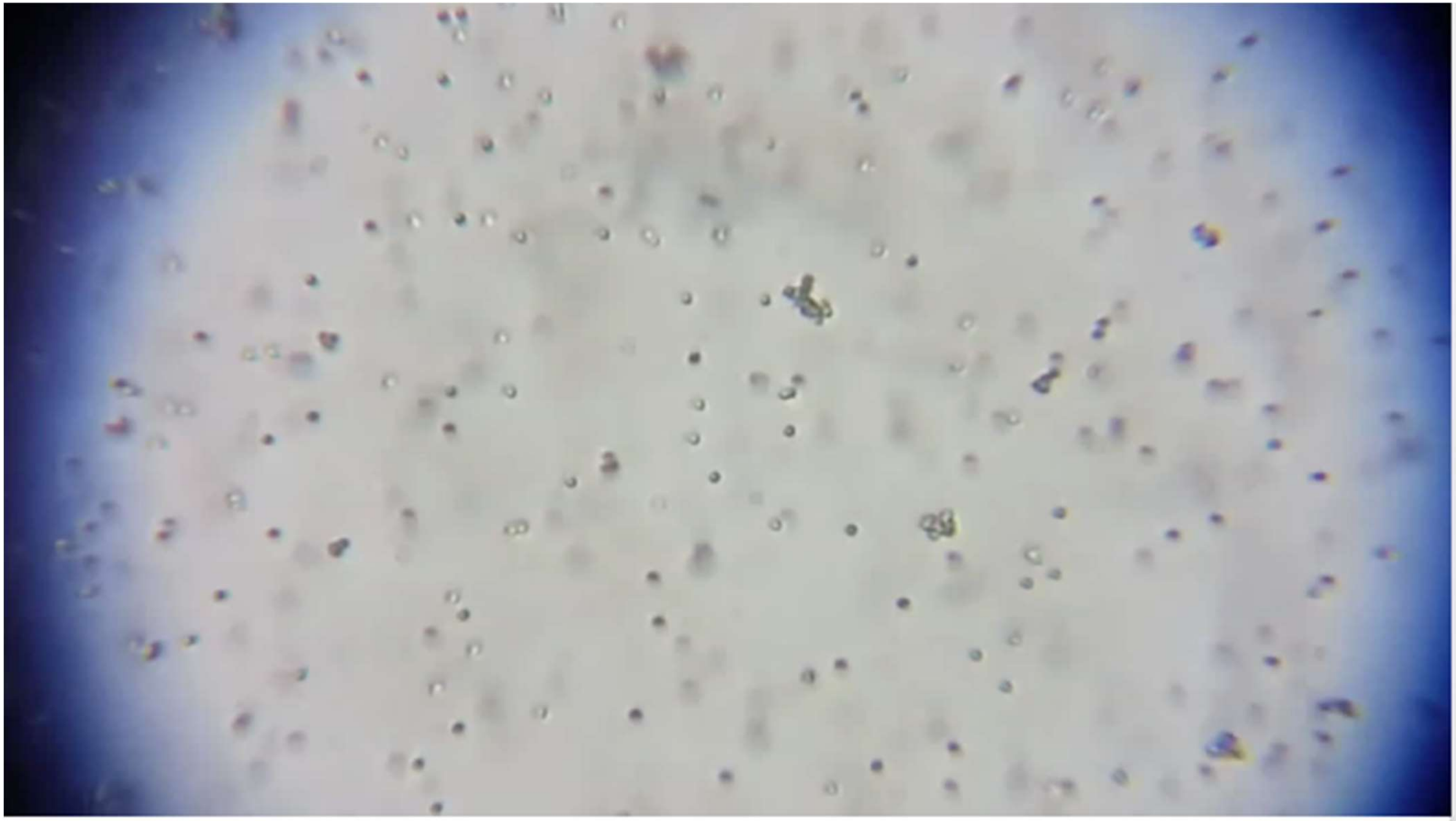
LS2102
Diffusion in Biology

LS2102 (Autumn 2020)

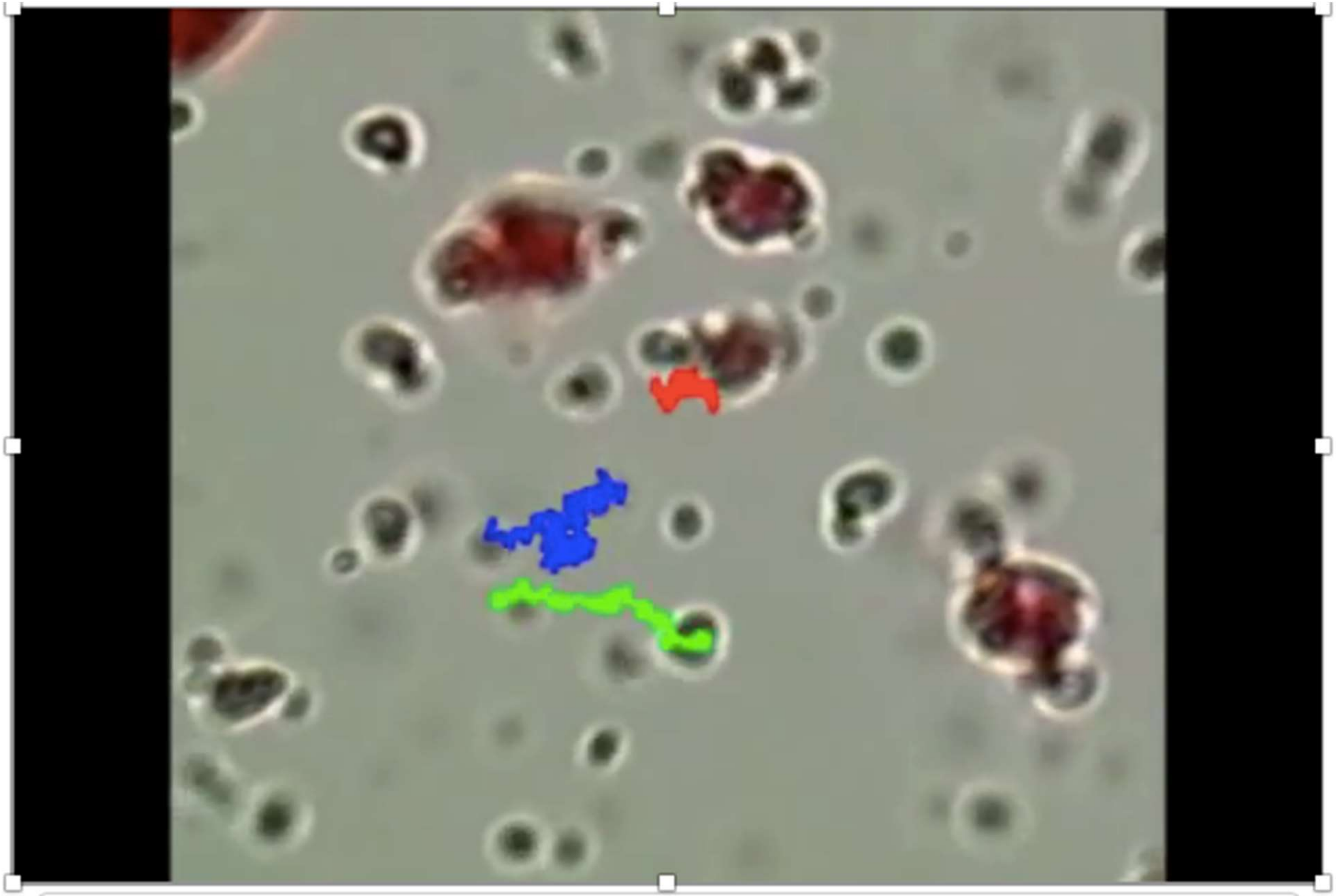
IISER Kolkata

13-11-2020

Very small plastic particles in water:



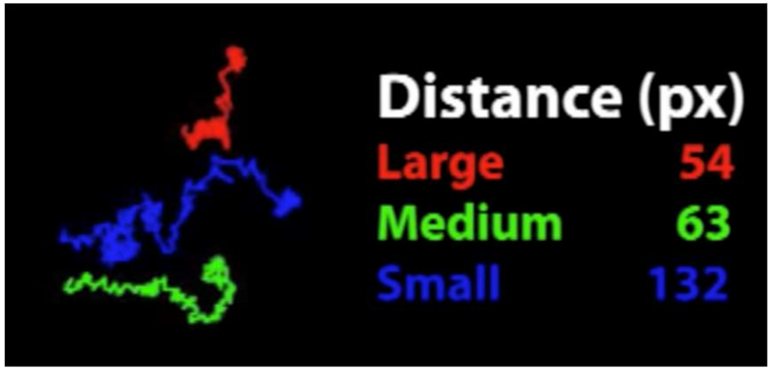
Pond water under the microscope:



Ink droplet in cold, normal and hot water:

Density (ink) > Density (water)

Quantitative Explanation



Robert Brown

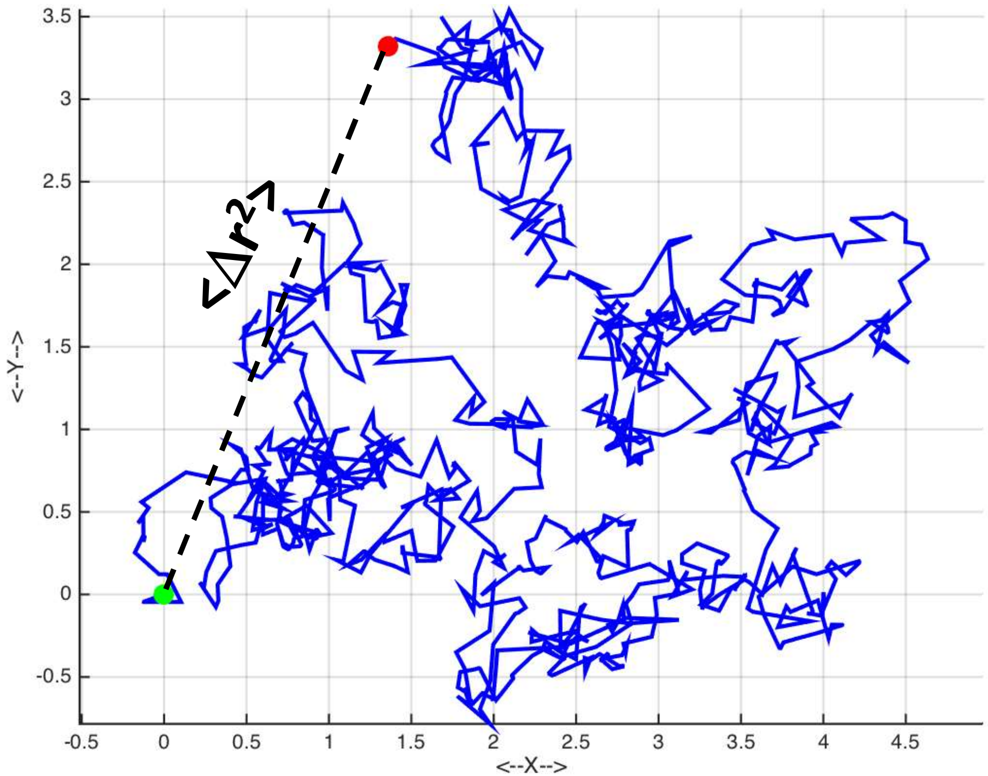
Brownian motion was discovered by **Robert Brown** in **1827**

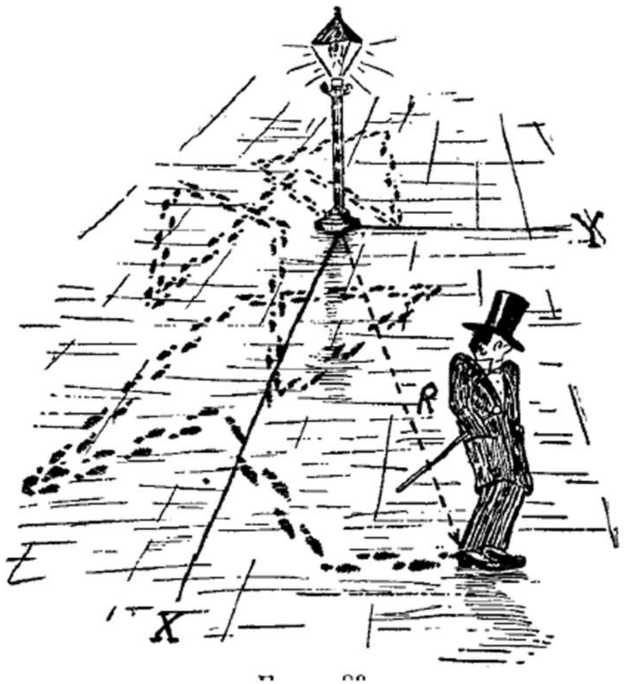
5. Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen;
von A. Einstein.

The explanation was formulated by **A. Einstein** in **1905**

(before the Laws of Thermodynamics were put forward)

Diffusion: movement of particles in unbiased random walks in any dimension

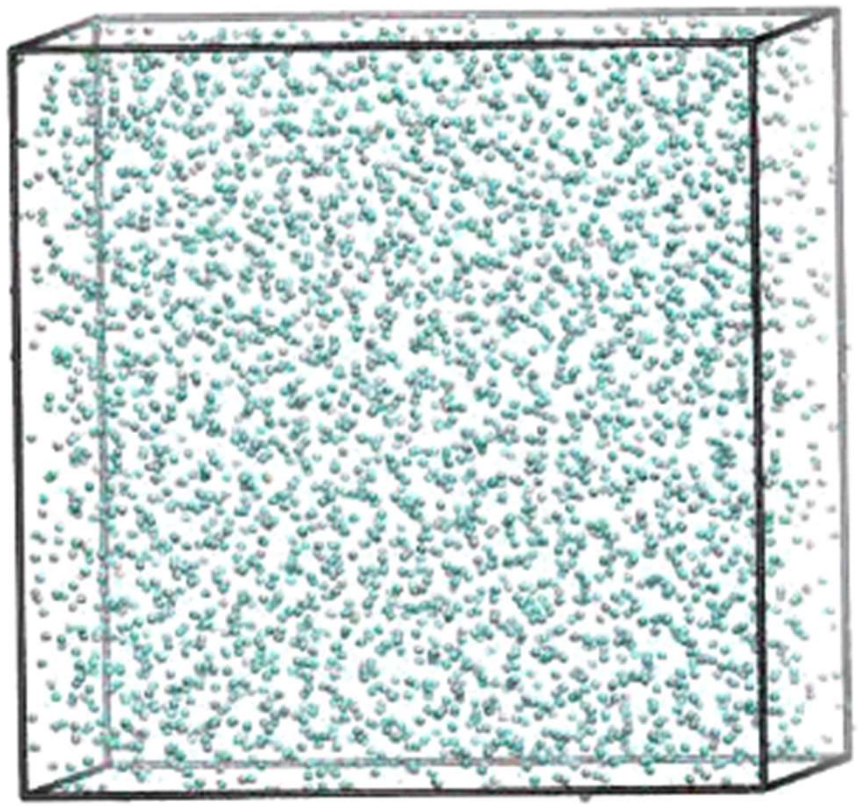




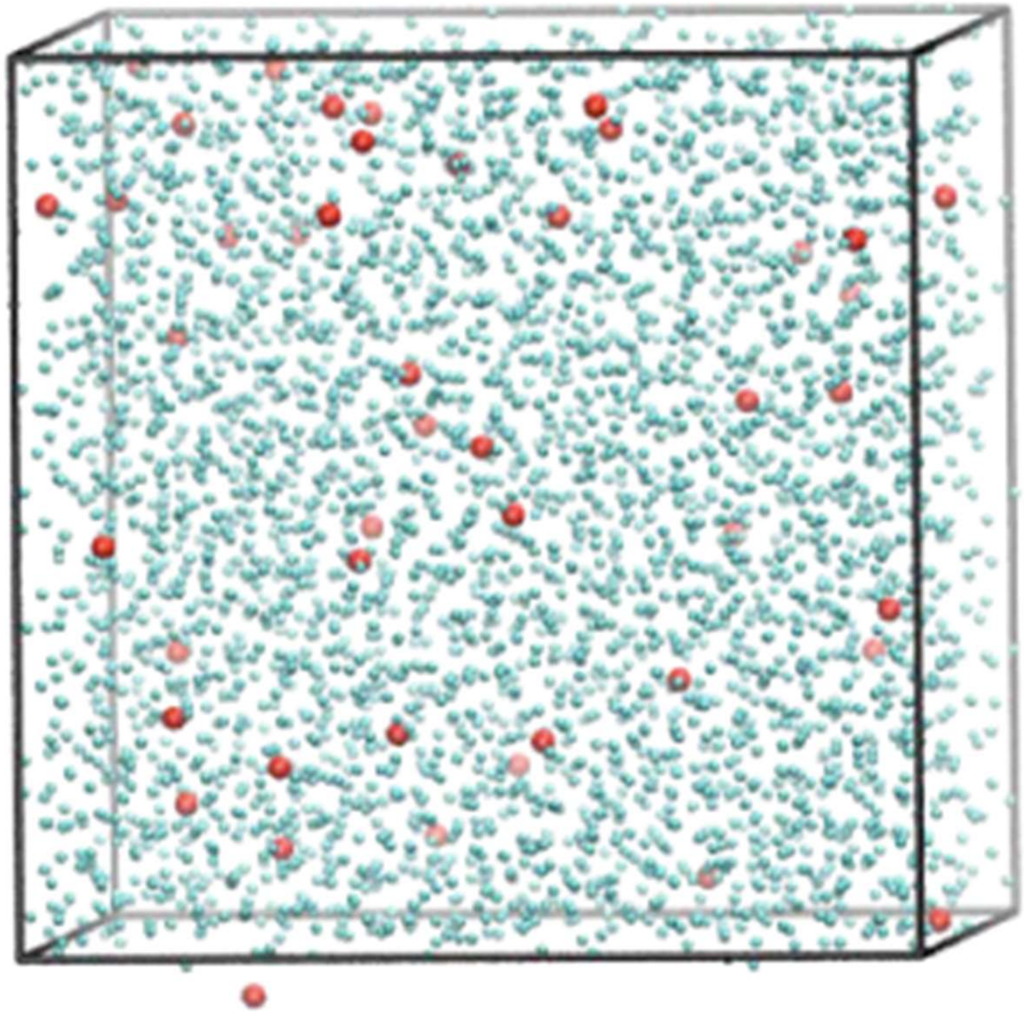
General Relationship:

$$\boxed{<r_N^2> = (2d)DT}$$

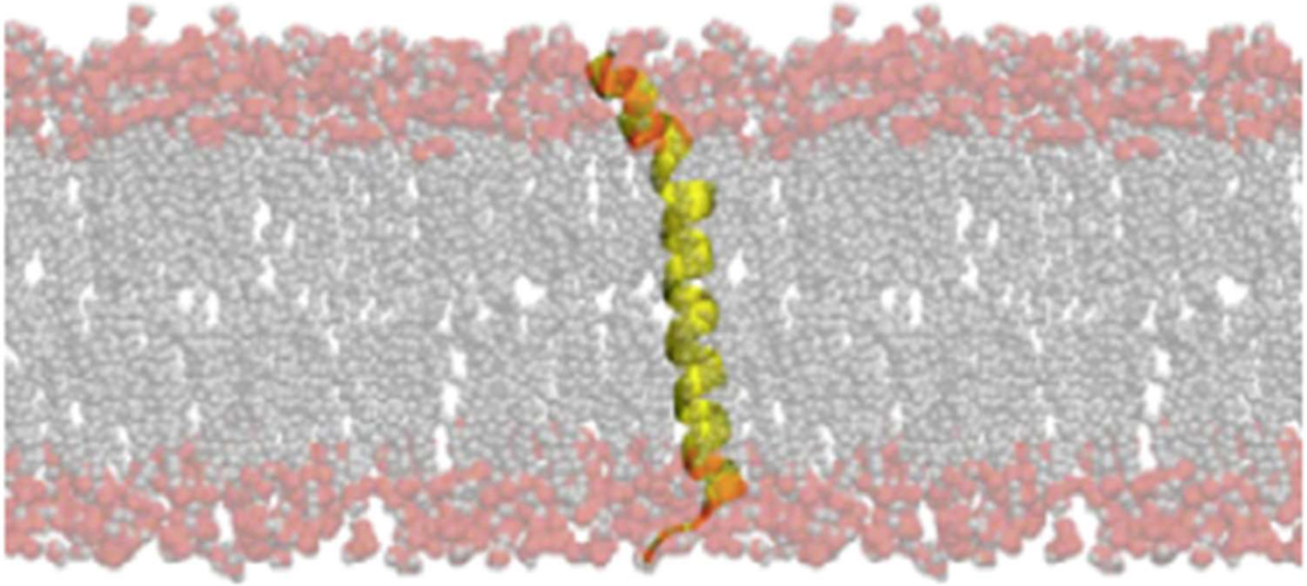
1A. Bulk Liquid - pure
(Computer Simulation data)



1B. Bulk Liquid – mixture (Computer Simulation data)

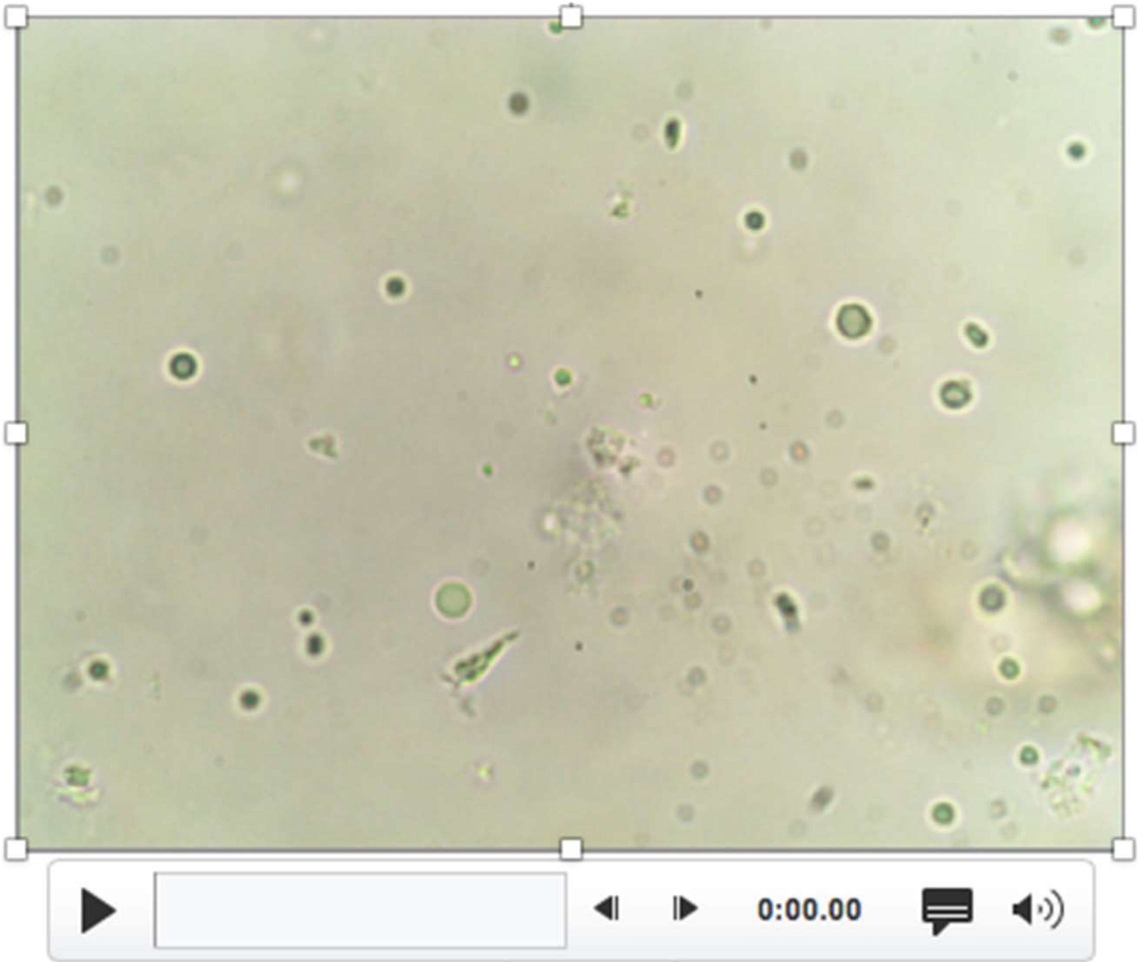


2. Protein fragment within a DPPC Bilayer (Computer simulation data)



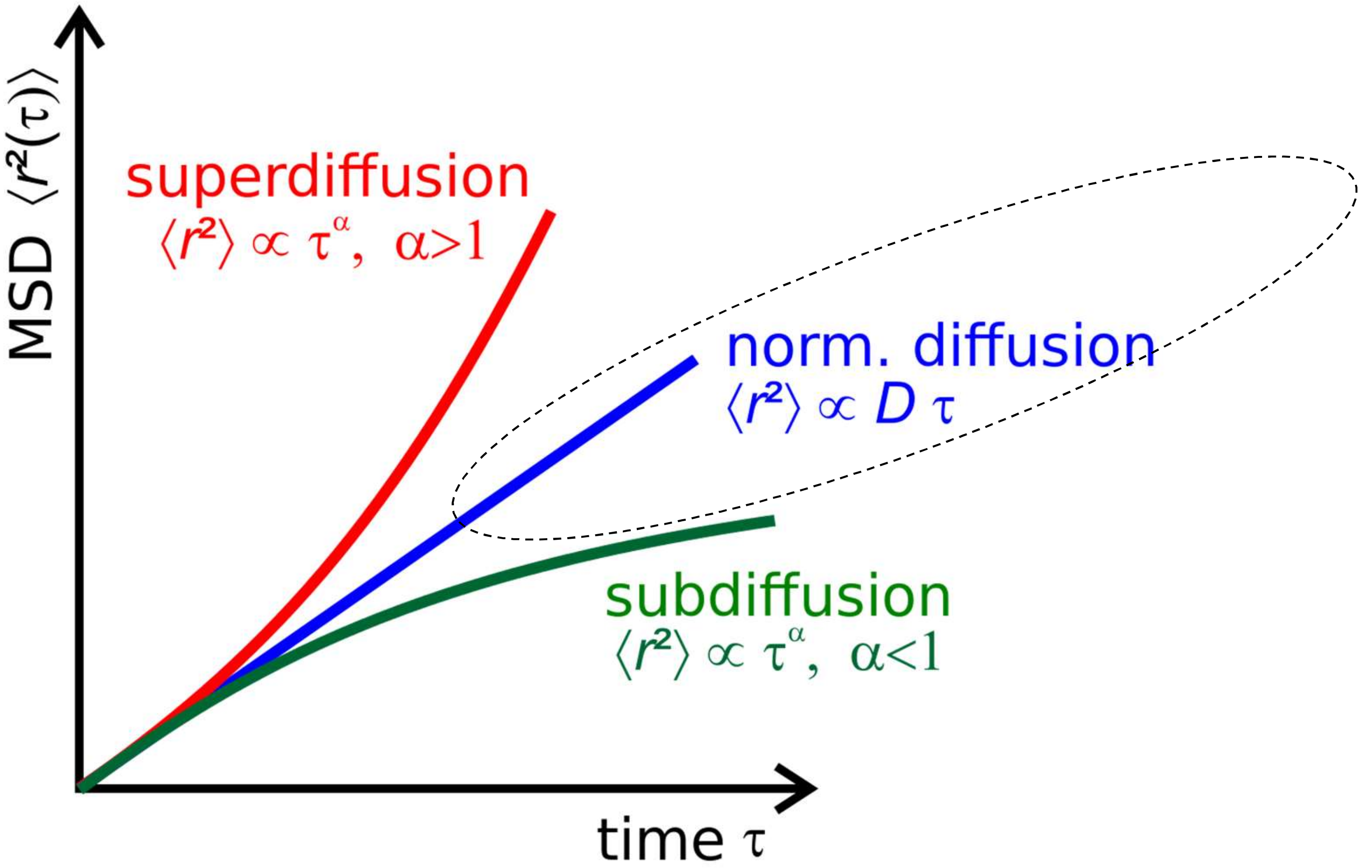
Frames spaced by Δt = 10 picoseonds

2. Pollen grain in water
(Experimental data - Light microscopy)



Frames spaced by Δt = 0.1 seconds

Deviations from linearity:



Linear fits may still be done to extract and compare ‘D’

Deviations from linearity:

1. Poor statistics

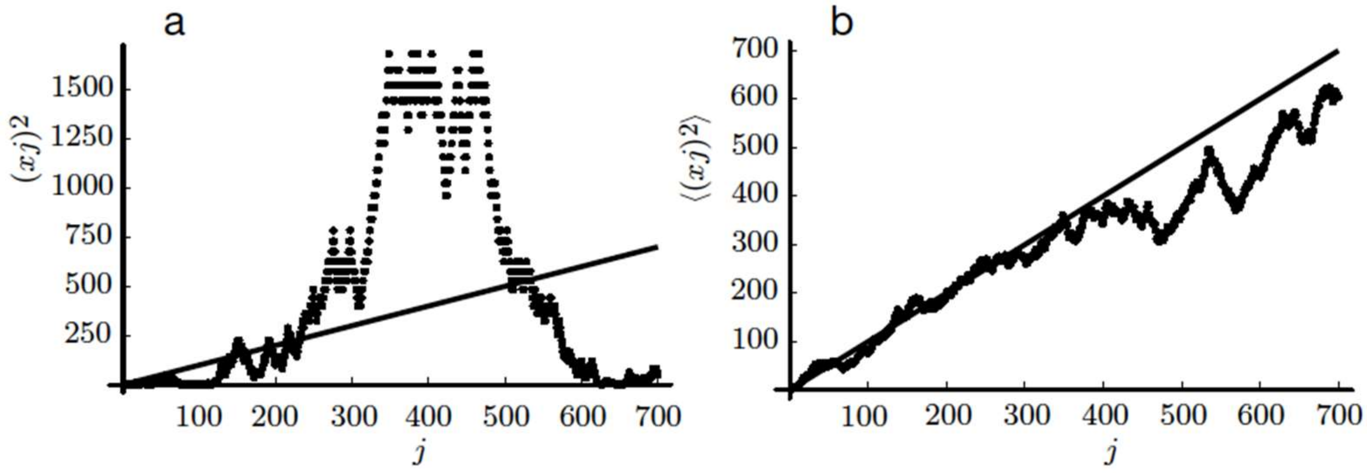


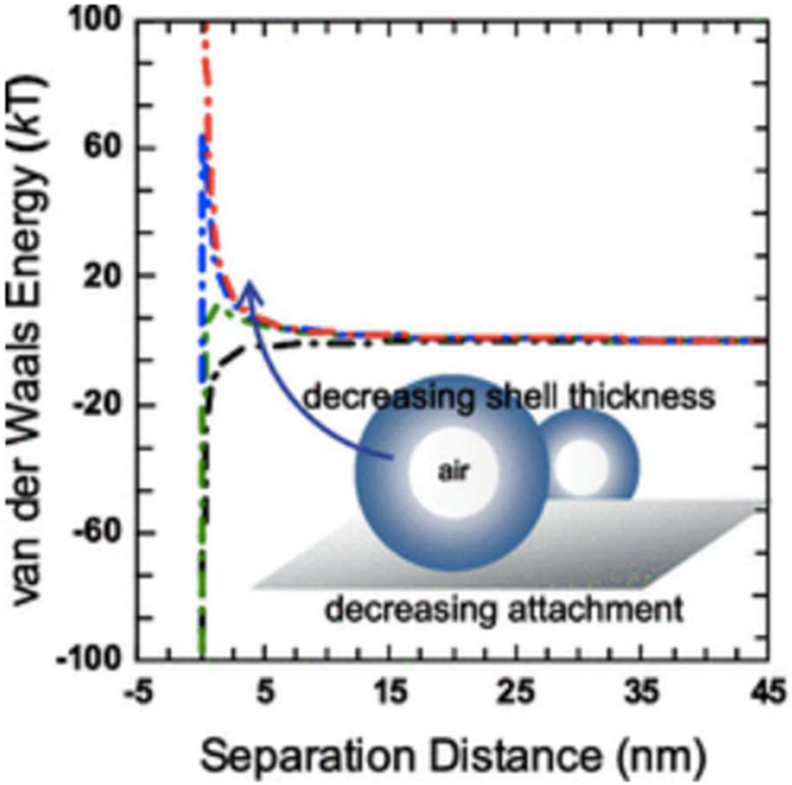
Figure 4.5: (Mathematical functions.) (**a**) Squared deviation $(x_j)^2$ for a single, one-dimensional random walk of 700 steps. Each step is one unit long. The solid line shows j itself; the graph shows that $(x_j)^2$ is not at all the same as j. (**b**) As (a), but this time the dots represent the *average* $\langle (x_j)^2 \rangle$ over thirty such walks. Again the solid line shows j. This time $\langle (x_j)^2 \rangle$ does resemble the idealized diffusion law (Equation 4.4).

Nelson, *Biological Physics*, Ch. 4

Deviations from linearity:

2. Particle-Particle Interaction

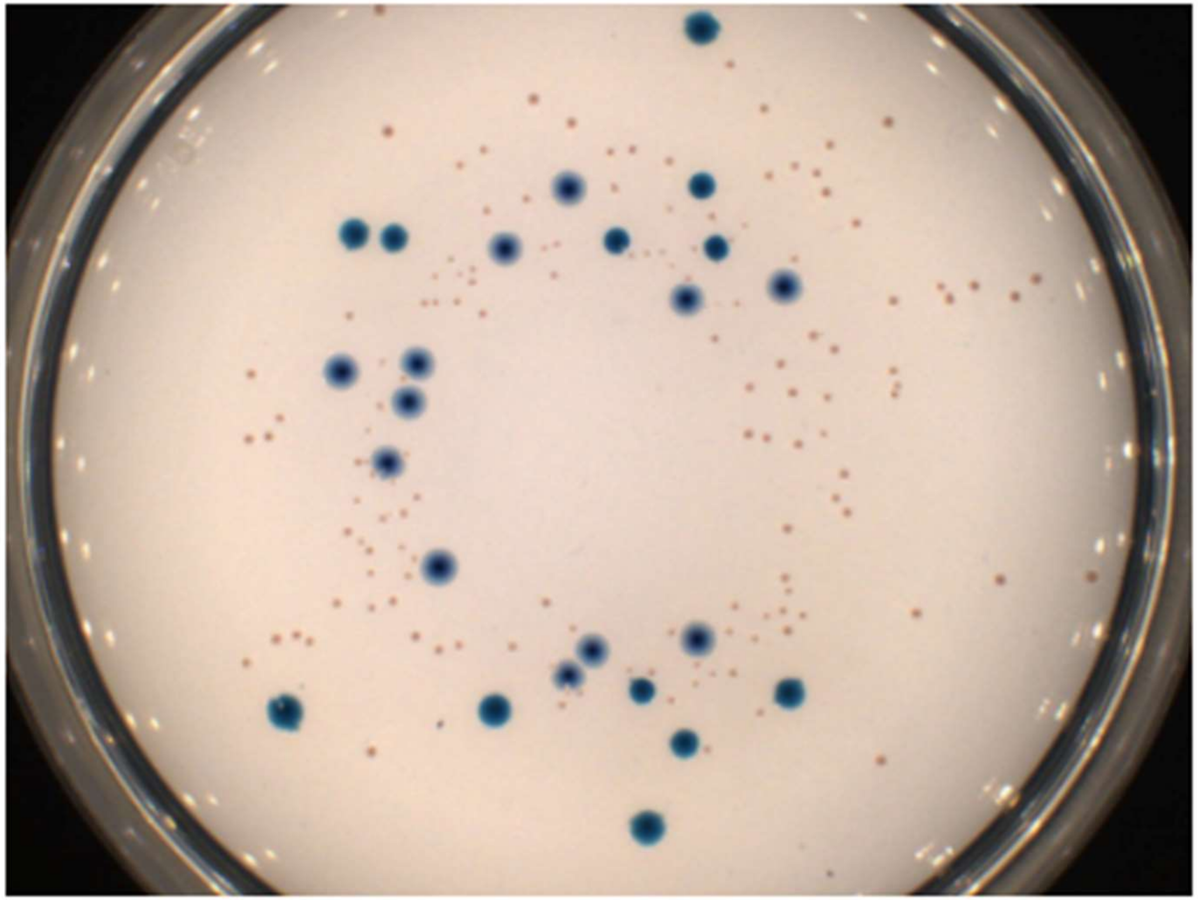
- Movement is not truly 'random'



Deviations from linearity:

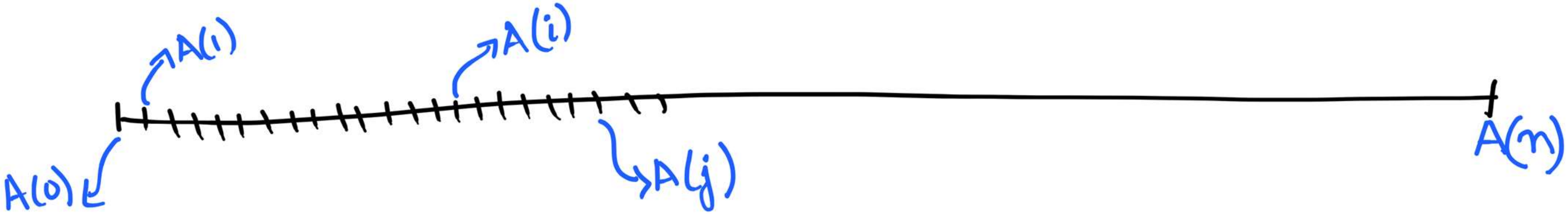
3. Finite Diffusion Volume

- Spatial restriction and interaction with boundaries (walls)



Time Correlation Formalism (TCF)

- Time Dependent Physical Quantity: **A(t)**
- Measurement or Computation at discrete time points



$$TCF(t) = \langle A(0) \otimes A(t) \rangle$$

Average:
over origin,
over systems

moving time origin

time 't' after origin

General Time Correlation Function (TCF) Formalism

Part I

- Initialize the correlation function
- Decide the correlation time.
- *General thumb rule: correlation time is (1/10)th of the data set*

Part II

- Move time origin over the data set
- Calculate correlation function over multiple time intervals
- Find total correlation for a given time difference (Δt)
- Collect the number of times TCF(Δt) is estimated

Part III

- Find the Average for each time difference (Δt)
- Rescale or Normalize so that TCF(0) $\equiv$ 1.0

Part IV

- Plot TCF
- **Extract physically meaningful quantities**

Assignment

- **Q1.** Identify Part I, II, III and IV from tcf_av.py
- Copy the relevant parts and provide your own comments.

- **Q2.** Identify and write down the mathematical function used in tcf_av.py