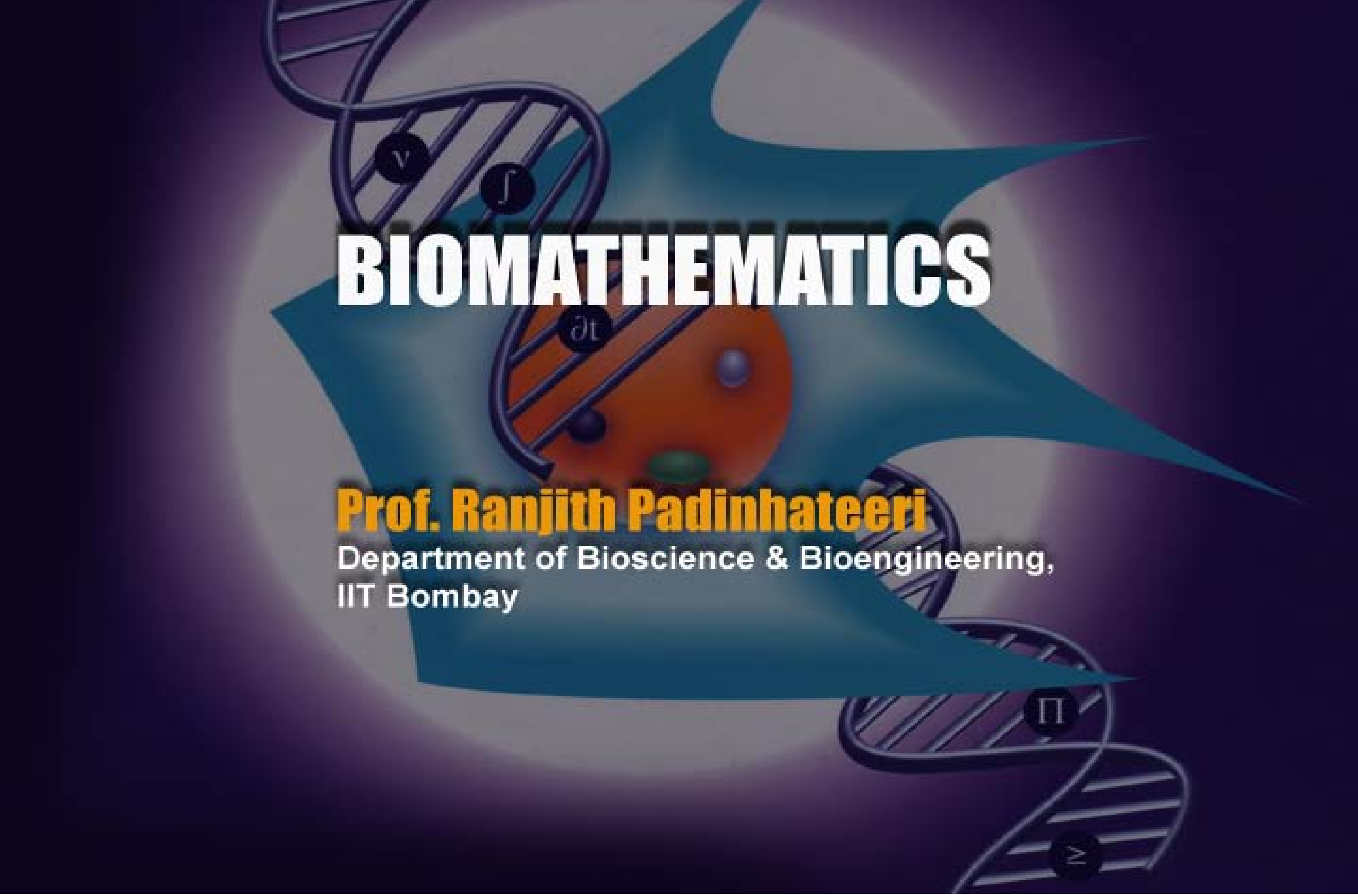
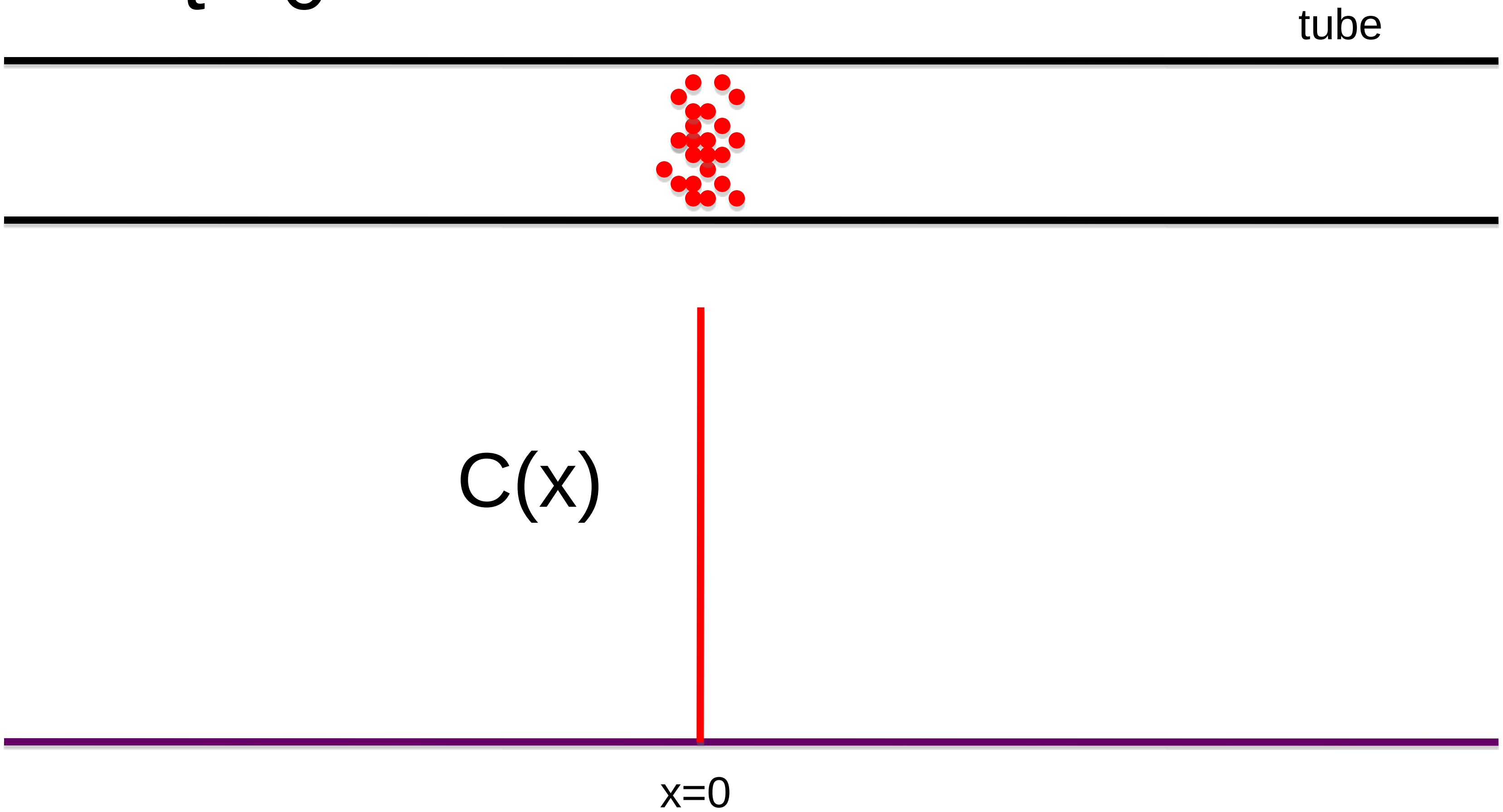

BIOMATHEMATICS
Prof. Ranjith Padinhateeri
Department of Bioscience & Bioengineering,
IIT Bombay

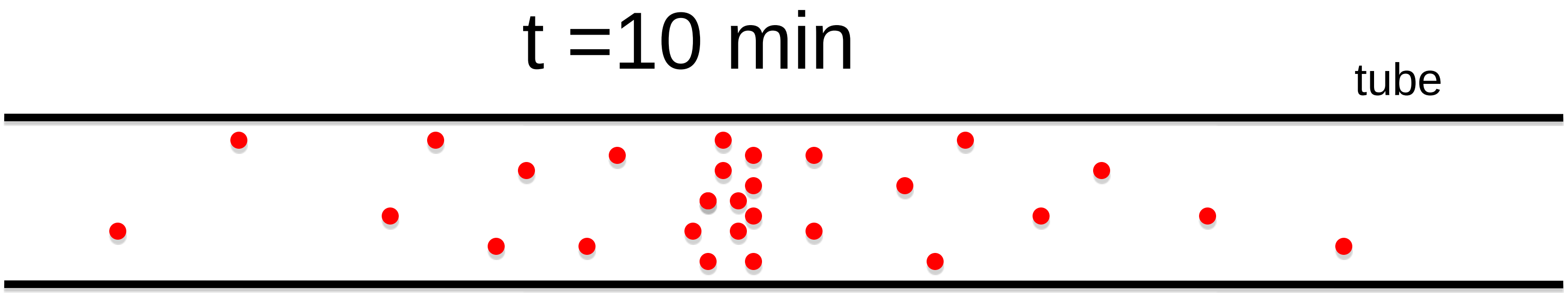
Lecture 19

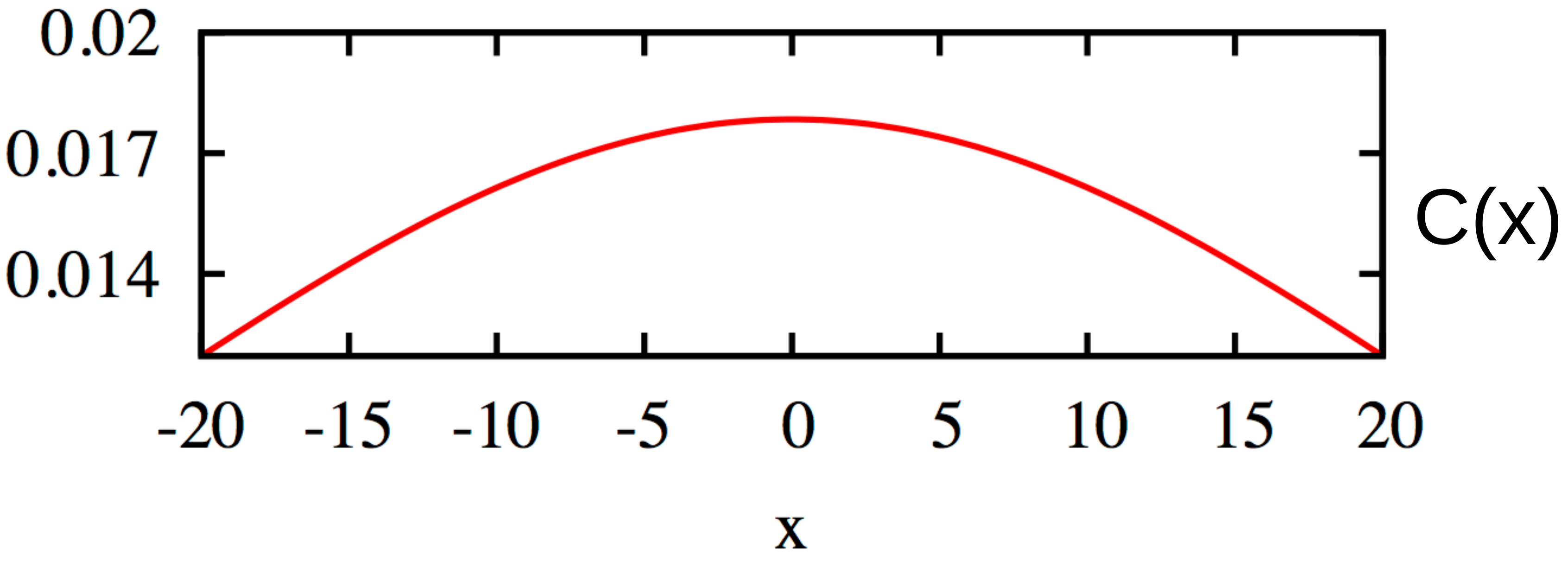
Applications of calculus and vector algebra in biology

Diffusion

t =0







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Diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\tilde{C}(x)\,dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2\tilde{C}(x)\,dx$$

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$$\frac{\partial \tilde{C}}{\partial t} = D \frac{\partial^2 \tilde{C}}{\partial x^2}$$

$$\frac{\partial}{\partial t} \int_{-\infty}^{+\infty} x^2 \tilde{C}(x) dx = D \int_{-\infty}^{+\infty} x^2 \frac{\partial^2 \tilde{C}(x)}{\partial x^2} dx$$

$$\frac{\partial}{\partial t}\langle x^2\rangle = Dx^2\frac{\partial\tilde{C}}{\partial x}\Bigg|_{-\infty}^{+\infty} - D\int_{-\infty}^{+\infty}\frac{\partial\tilde{C}}{\partial x}2x\,dx$$

$$\frac{\partial}{\partial t}\langle x^2\rangle = -2D\int_{-\infty}^{+\infty}\frac{\partial\tilde{C}}{\partial x}x\,dx$$

$$\frac{\partial}{\partial t}\langle x^2\rangle = -2D\left(x\tilde{C}\Big|_{-\infty}^{+\infty}\right) + 2D\int_{-\infty}^{+\infty}\tilde{C}\,dx$$

$$\frac{\partial}{\partial t}\langle x^2 \rangle = 2D\int_{-\infty}^{+\infty}\tilde{C}dx$$

$$\frac{\partial}{\partial t}\langle x^2 \rangle = 2D$$

$$\langle x^2 \rangle = 2Dt$$

Again,

$$\frac{\partial \tilde{C}}{\partial t} = D\frac{\partial^2 \tilde{C}}{\partial x^2}$$

Now,

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty} x\tilde{C}(x)dx = D\int_{-\infty}^{+\infty} x \ \frac{\partial^2 \tilde{C}(x)}{\partial x^2}dx$$

$$\frac{\partial}{\partial t}\langle x\rangle = Dx\frac{\partial \tilde{C}}{\partial x}\Bigg|_{-\infty}^{+\infty} - D\int_{-\infty}^{+\infty}\frac{\partial \tilde{C}}{\partial x}dx$$

$$\frac{\partial}{\partial t}\langle x\rangle = -D\int_{-\infty}^{+\infty}\frac{\partial \tilde{C}}{\partial x}dx$$

$$\frac{\partial}{\partial t}\langle x\rangle = 0$$

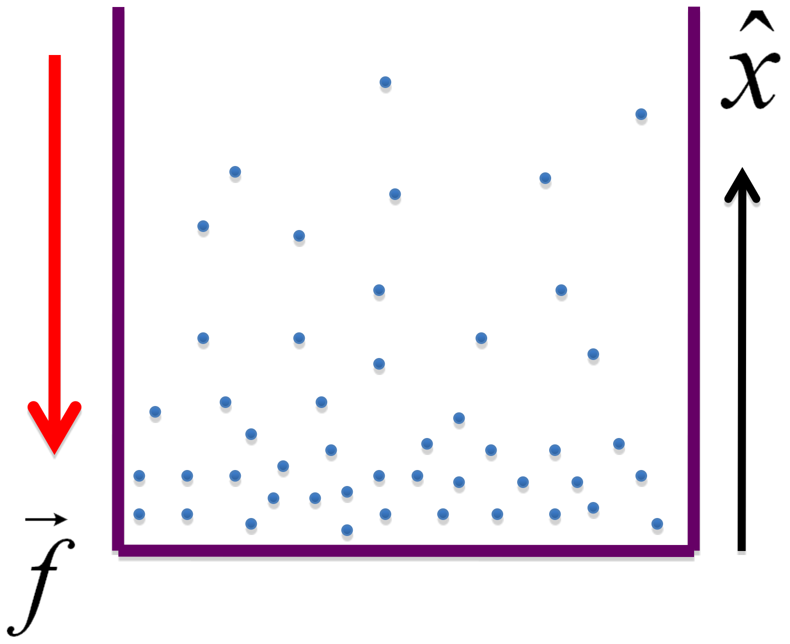
Einstein’s Relation

Einstein 1905

Particles under an external field

$$\vec{f} = -g\hat{x}$$

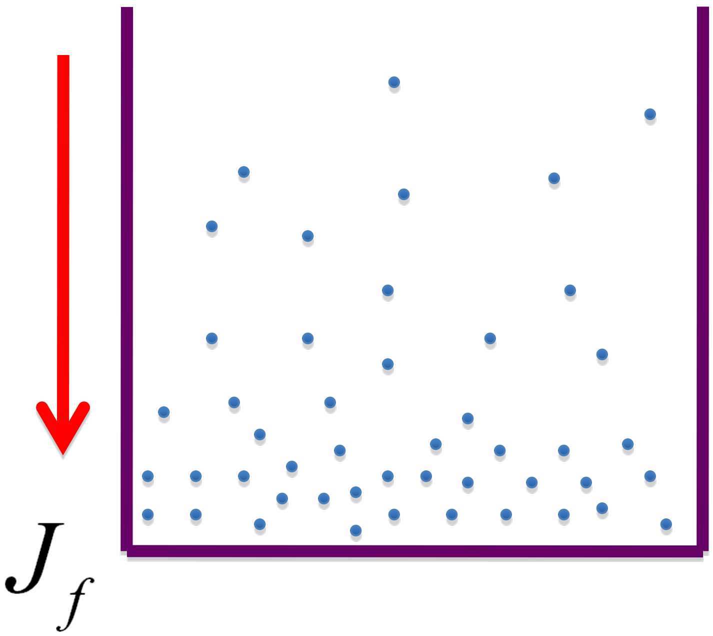
$$C(x) \propto \exp\left(-\frac{gx}{k_B T}\right)$$



Current due to the force

$$\vec{J}_f = C\vec{v}$$

$$\vec{v} = \frac{\vec{f}}{6\pi\eta a}$$

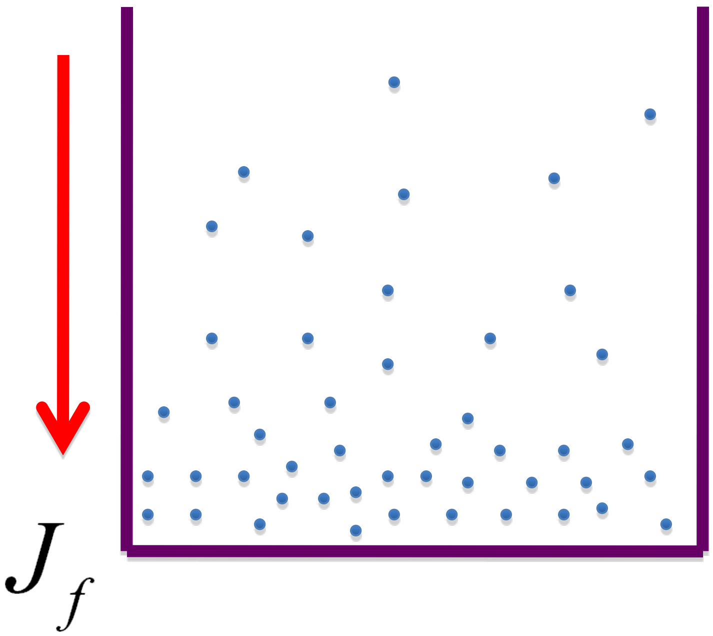


Current due to the force

$$\vec{J}_f = C\vec{v}$$

$$\vec{v} = \frac{-g\hat{x}}{6\pi\eta a}$$

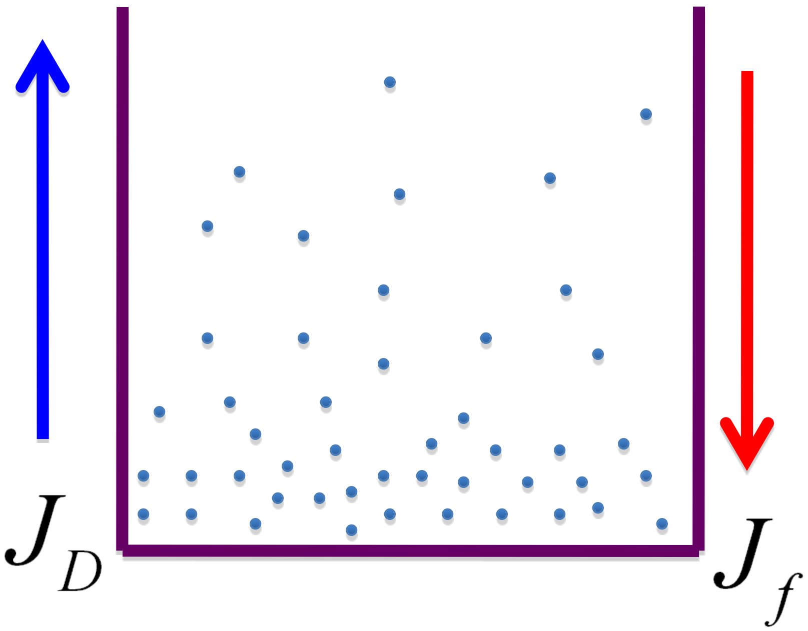
$$\vec{J}_f = -C\frac{g\hat{x}}{6\pi\eta a}$$



Diffusion

$$\vec{J}_D = -D\vec{\nabla}C$$

$$\vec{J}_D = -D\frac{\partial C}{\partial x}\hat{x}$$



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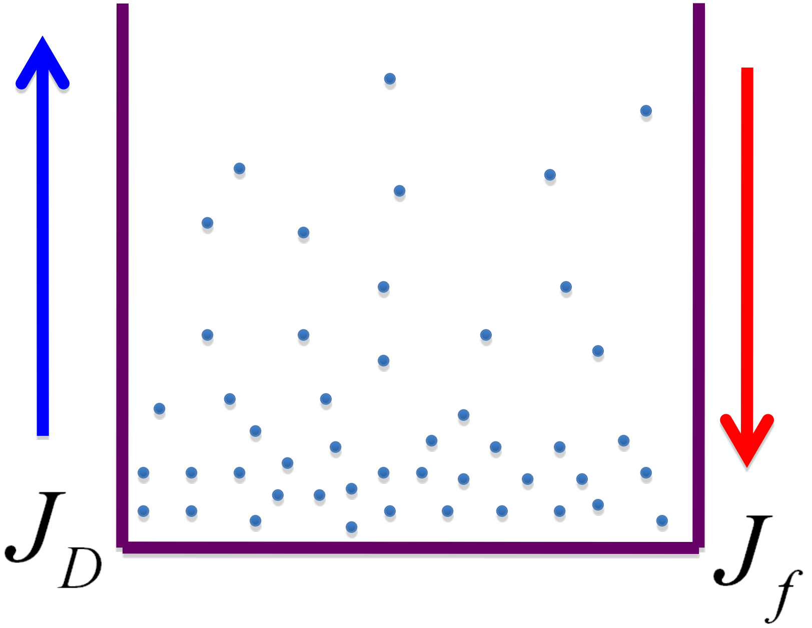
Diffusion

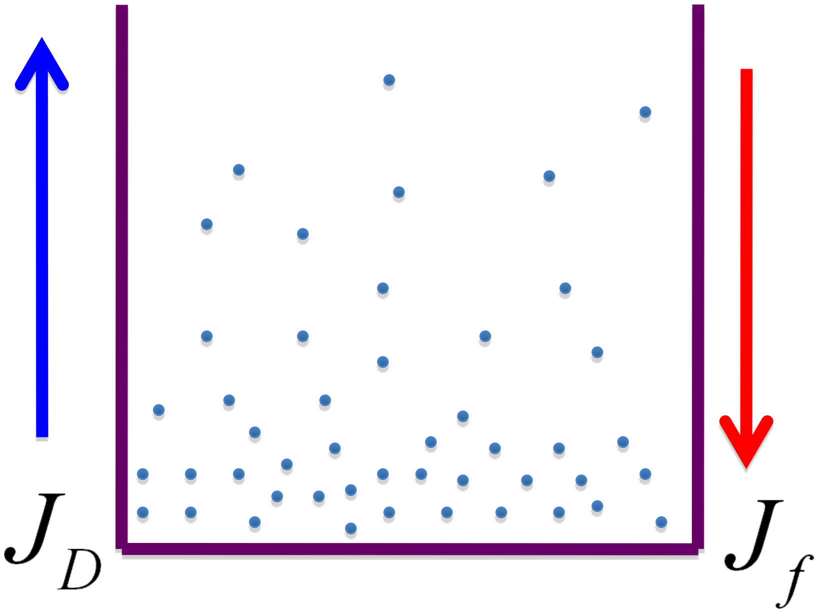
$$\vec{J}_D = -D\frac{\partial C}{\partial x}\hat{x}$$

$$C \propto \exp\left(-\frac{gx}{k_B T}\right)$$

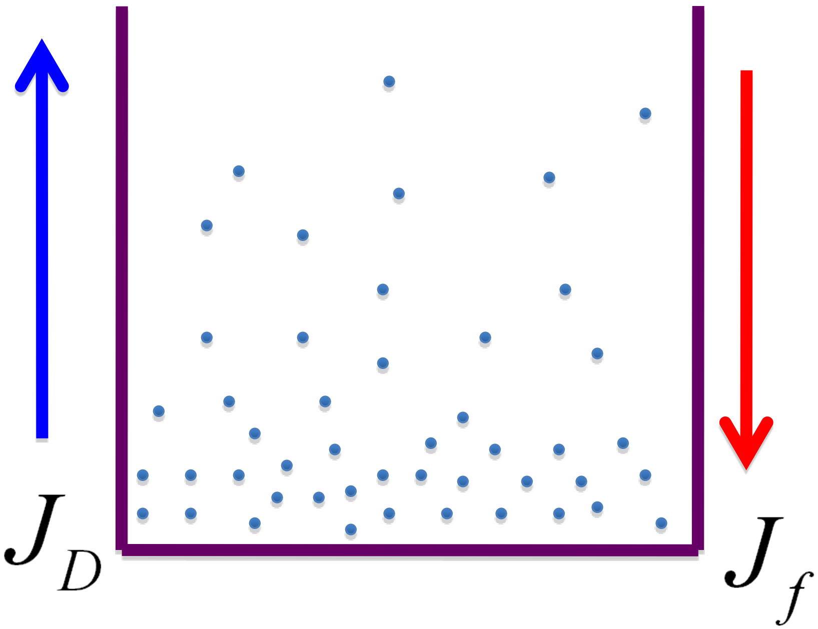
$$\vec{J}_D = DC\frac{g}{k_B T}\hat{x}$$



When both the currents balance, we reach equilibrium.



Equilibrium=net current zero



$$\vec{J}_D + \vec{J}_E = 0$$

$$\vec{J}_D = -\vec{J}_E$$

Einstein's relation

$$\vec{J}_D = DC\frac{g}{k_B T}\hat{x}$$

$$\vec{J}_f = -C\frac{g\hat{x}}{6\pi\eta a}$$

$$\vec{J}_D = -\vec{J}_f$$

$$DC\frac{g}{k_B T} = C\frac{g}{6\pi\eta a}$$

$$\Rightarrow D = \frac{k_B T}{6\pi\eta a}$$

Summary

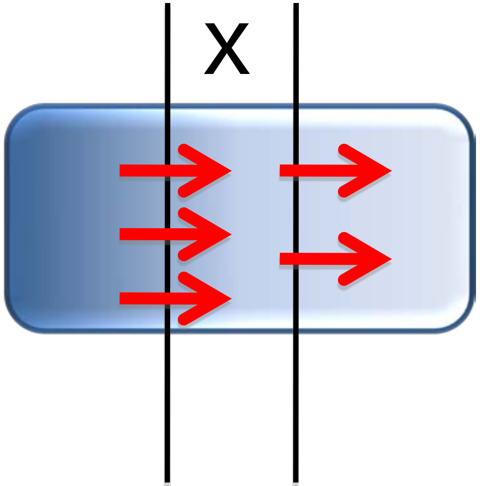
Two important relations

$$\langle x^2 \rangle = 2Dt$$

$$D = \frac{k_B T}{6\pi\eta a}$$

Diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = -\vec{\nabla} \bullet \vec{J}$$



$$\vec{J} = -D\frac{\partial C}{\partial x}\hat{x}$$

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, c(x)\, dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2\, c(x)\, dx$$

Summary

- Divergence
- Continuity equation
- Diffusion equation
- Mean-square position