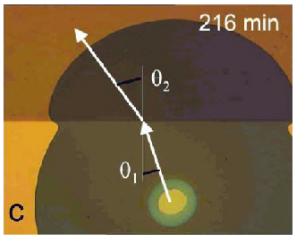
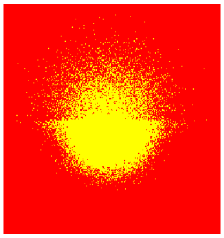
Diffusion with *D(x)*



A. Remhof et al PRL 90(2003)145502



Random walkers

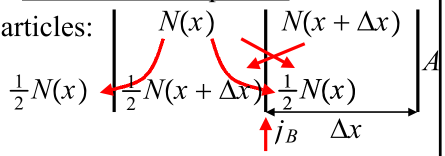
R. J. Wijngaarden
Vrije Universiteit
Amsterdam

Outline

- Standard derivation of the diffusion eqn.
- What if *D(x)* ?
- $j = -D\nabla c$ or $j = -\nabla(Dc)$ or ...
- Equilibrium concentration if *D(x)* ?
- Strategies for bacterial feeding

The diffusion equation

For many particles:



$$j_B = \left[-\tfrac{1}{2}N(x+\Delta x) + \tfrac{1}{2}N(x)\right]/A\tau$$

$$j_B = \frac{(\Delta x)^2}{2\tau}\frac{1}{\Delta x}\left[-\frac{N(x+\Delta x)}{A\Delta x} + \frac{N(x)}{A\Delta x}\right]$$

$$j_B = D\frac{1}{\Delta x}[-c(x+\Delta x) + c(x)] = -D\frac{\partial c}{\partial x} = -D\nabla c$$

continuity eqn. $\frac{\partial c}{\partial t} + \nabla j = 0$

$\frac{\partial c}{\partial t} = D\nabla^2 c$ diffusion eqn.

The diffusion equation

$\frac{\partial c}{\partial t} = D\nabla^2 c$ and $j = -D\,\nabla c$

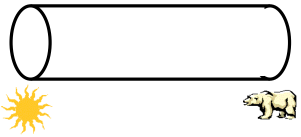
but what if $D = D(x)$?

$j = -D(x)\,\nabla c$ or $j = -\nabla(D(x)c)$?

Next: two routes

- R. Landauer: it depends
- M. Schnitzer: not enough information

$j = -D\,\nabla c$ vs. $j = -\nabla(Dc)$



$pV = nRT$

$\rho = \frac{n}{V} = \left(\frac{p}{R}\right)\frac{1}{T}$

$j = -D\,\nabla c$ with $c =$ const remains constant

hence: $j = -\nabla(Dc)$

$j = -D\,\nabla c$ vs. $j = -\nabla(Dc)$

$pV = nRT$

$\rho = \frac{n}{V} = \left(\frac{p}{R}\right)\frac{1}{T}$

T constant $\Rightarrow c$ const

$j = -D\,\nabla c$ with $c =$ const remains constant

$j = -D\,\nabla c$ or $j = -\nabla(Dc)$

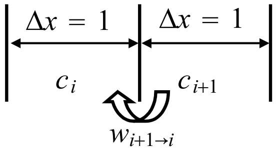
depending on the problem

How do we know what to choose?

Landauer: flux j revisited

c occupation probability

w jump probability



$j = w_{i\to i+1} c_i - w_{i+1\to i} c_{i+1}$

$w_g := \frac{1}{2}(w_{i\to i+1} + w_{i+1\to i})$

$w_u := \frac{1}{2}(w_{i\to i+1} - w_{i+1\to i})$

$j = w_u(c_{i+1} + c_i) - w_g(c_{i+1} - c_i)$

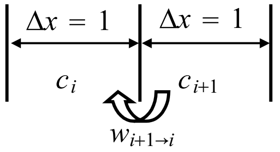
unbalance in jumps between adjacent points

gradient in concentration

Landauer: flux j revisited

c occupation probability

w jump probability



$j = w_u(c_{i+1} + c_i) - w_g(c_{i+1} - c_i)$

$j = v\ c \qquad -D\ \nabla c$

Landauer: flux j revisited

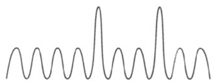
$j = v\ c - D\ \nabla c$

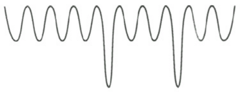
$j = u\ c - \nabla(Dc)$ with $u = v + \nabla D$

v : drift unbalance between adjacent points exchange

u : drift unbalance in 2 directions from a single point outflow

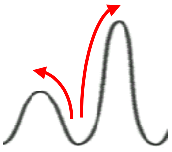
Random barriers Random traps



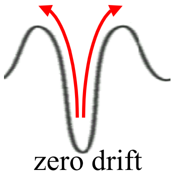


asymmetric outflow
$u \neq 0$

symmetric outflow
$u = 0$

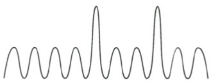


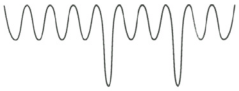
net drift



zero drift

Random barriers Random traps



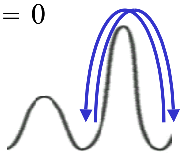


asymmetric outflow
$u \neq 0$

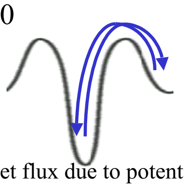
symmetric exchange
$v = 0$

symmetric outflow
$u = 0$

asymmetric exchange
$v \neq 0$

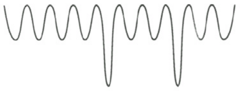


zero flux due to potential



net flux due to potential

Random barriers Random traps



asymmetric outflow
$u \neq 0$
drift

symmetric exchange
$v = 0$
flux due to potential

symmetric outflow
$u = 0$

asymmetric exchange
$v \neq 0$

$j = v\ c - D\ \nabla c$

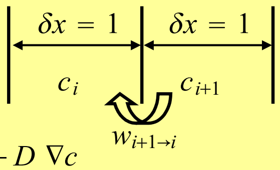
$j = u\ c - \nabla(Dc)$

$j = -D\ \nabla c$ | $j = -\nabla(Dc)$

Big names; probability flux

c occupation probability

w jump probability

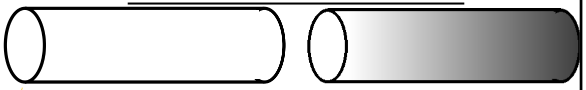


$\frac{\partial c}{\partial t} = -\nabla j$ with $j = v\,c - D\,\nabla c$

Fokker-Planck equation (probability flux)

The Smoluchowski equation

What do we have to choose?



$j = -\nabla(Dc)$ $\quad$ $j = -D\,\nabla c$

We choose using the known result

But how can one know *a proiri* what to choose?

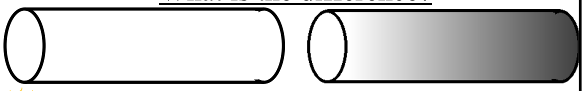
Landauer 

Mark Schnitzer, PRE 48 (1993) 2553

Chemotaxis of *Escherichia coli*

Enthousiasm leads to hunger

What is the difference?



$j = -\nabla(Dc)$ $\quad$ $j = -D\,\nabla c$

free path length δ $\quad$ determined by iron wool

free time interval τ

δ constant	$\delta = \delta(x)$
$\tau = \tau(x)$	τ constant

$$D = \frac{\delta^2}{2\tau}$$

$D(x)$ in both boxes can be the same !

one must know $\delta(x)$ and $\tau(x)$ separately

A diffusion equation for the case *D(x)*

Define new variables:

particle speed $v(x) := \frac{\delta(x)}{\tau(x)}$

collision rate $\alpha(x) := \frac{1}{\tau(x)}$

Ignore distributions of v and α

General case: $v \to \bar{v}$ and $\alpha \to \bar{\alpha}$

A diffusion equation for the case *D(x)*

At a collision: 50% chance to change direction

R density of right-moving particles →

L density of left-moving particles ←

$$\frac{\partial R}{\partial t} = -\frac{\partial(vR)}{\partial x} - \frac{\alpha R}{2} + \frac{\alpha L}{2}$$

heaping up due to non-uniform velocity $\quad$ loss by flipping $\quad$ gain by flipping

$$\frac{\partial L}{\partial t} = +\frac{\partial(vL)}{\partial x} + \frac{\alpha R}{2} - \frac{\alpha L}{2}$$

A diffusion equation for the case *D(x)*

$$\frac{\partial R}{\partial t} = -\frac{\partial(vR)}{\partial x} - \frac{\alpha R}{2} + \frac{\alpha L}{2}$$

$$\frac{\partial L}{\partial t} = +\frac{\partial(vL)}{\partial x} + \frac{\alpha R}{2} - \frac{\alpha L}{2}$$

local density $c := R + L$

flux $j = v\sigma$ with $\sigma := R - L$

adding : $\frac{\partial c}{\partial t} = -\frac{\partial(v\sigma)}{\partial x} = -\frac{\partial j}{\partial x}$

subtracting : $\frac{\partial \sigma}{\partial t} = -\frac{\partial(vc)}{\partial x} - \alpha\sigma$

A diffusion equation for the case *D(x)*

$$\frac{\partial c}{\partial t} = -\frac{\partial(v\sigma)}{\partial x} = -\frac{\partial j}{\partial x}$$

$$\frac{\partial \sigma}{\partial t} = -\frac{\partial(vc)}{\partial x} - \alpha\sigma$$

differentiating and combining

$$\frac{\partial^2 c}{\partial t^2} = -\frac{\partial\left(v\frac{\partial\sigma}{\partial t}\right)}{\partial x} = \frac{\partial}{\partial x}\left(v\frac{\partial(vc)}{\partial x}\right) + \frac{\partial(\alpha j)}{\partial x}$$

$$\frac{\partial^2 c}{\partial t^2} = \frac{\partial}{\partial x}\left(v\frac{\partial(vc)}{\partial x}\right) + \frac{\partial(\alpha j)}{\partial x} \text{ Telegraph equation}$$

The telegraph equation

$$\frac{\partial^2 c}{\partial t^2} = \frac{\partial}{\partial x}\left(v\frac{\partial(vc)}{\partial x}\right) + \cancel{\frac{\partial(\alpha j)}{\partial x}} \qquad \alpha = \frac{1}{\tau}$$

$t << \tau$ wavelike eqn: ballistic regime

The telegraph equation

$$\cancel{\frac{\partial^2 c}{\partial t^2}} = \frac{\partial}{\partial x}\left(v\frac{\partial(vc)}{\partial x}\right) + \frac{\partial(\alpha j)}{\partial x} \qquad \alpha = \frac{1}{\tau}$$

$t << \tau$ wavelike eqn: ballistic regime

$\tau << t << \frac{L^2}{\tau v^2} = \frac{t^2_{ballistic}}{\tau}$ non-equilibrium

$t >> \frac{L^2}{\tau v^2}$ equilibrium: $R = L, j = 0$

Next: $t >> \tau$ ignore $\frac{\partial^2 c}{\partial t^2}$ or ballistic particles

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The telegraph equation

$$0 = \frac{\partial}{\partial x}\left(v\frac{\partial(vc)}{\partial x}\right) + \frac{\partial(\alpha j)}{\partial x}$$

Integrate:

$$\boxed{j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\frac{\partial v}{\partial x}}$$

flux due to diffusion

flux due to drift

$$v_{drift} = -\frac{v}{\alpha}\frac{\partial v}{\partial x}$$

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} + v_{drift}c$$

$j = v\ c - D\ \nabla c$

Landauer

The case $v \neq v(x)$ and $\alpha \neq \alpha(x)$

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\cancel{\frac{\partial v}{\partial x}}$$

const

$$j = -D\frac{\partial c}{\partial x}$$

in equilibrium: $j = 0$

$$\frac{\partial c}{\partial x} = 0$$

$$c = c_0 \neq c_0(x)$$

The case $v \neq v(x)$ and $\alpha = \alpha(x)$

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\cancel{\frac{\partial v}{\partial x}}$$

$$j = -\frac{v^2}{\alpha(x)}\frac{\partial c}{\partial x} = -D(x)\frac{\partial c}{\partial x}$$

in equilibrium: $j = 0$

$$\frac{\partial c}{\partial x} = 0$$

$$c = c_0 \neq c_0(x)$$

The case $v = v(x)$ and $\alpha = \alpha(x)$ but $\frac{v(x)}{\alpha(x)} = \text{const}$

mean free path

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\frac{\partial v}{\partial x}$$

$$j = -\frac{\partial(Dc)}{\partial x} \text{ with } D = \frac{v^2(x)}{\alpha(x)}$$

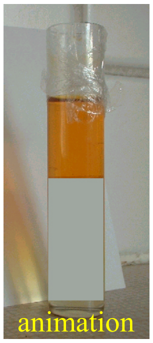
$$\left[\text{check: } j = -\frac{\partial\left(\frac{v}{\alpha}v\ c\right)}{\partial x} = -\frac{v}{\alpha}\frac{\partial\left(v\ c\right)}{\partial x}\right]$$

in equilibrium: $j = 0$

$$Dc = \text{const}$$

$$c(x) \sim \frac{1}{D(x)} \sim \frac{\alpha(x)}{v(x)}\frac{1}{v(x)} \sim \frac{1}{v(x)}$$

Experiment



after 0 days

after 1 day

after 7 days

The case $v = v(x)$ and $\alpha \neq \alpha(x)$

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\frac{\partial v}{\partial x}$$

$$j = -D\frac{\partial c}{\partial x} - \frac{c}{2}\frac{\partial D}{\partial x} \text{ with } D = \frac{v^2(x)}{\alpha}$$

$$\left[\text{check: } j = -\frac{v^2(x)}{\alpha}\frac{\partial c}{\partial x} - \frac{c}{2}\frac{\partial\left(\frac{v^2(x)}{\alpha}\right)}{\partial x}\right]$$

in equilibrium: $j = 0$

$$\frac{1}{c}\frac{\partial c}{\partial x} = -\frac{1}{2}\frac{1}{D}\frac{\partial D}{\partial x}$$

$$\ln c = \ln D^{-\frac{1}{2}} + \text{const}$$

$$c(x) \sim \frac{1}{\sqrt{D(x)}} \sim \frac{1}{v(x)}$$

The case $v = v(x)$ and $\alpha = \alpha(x)$ and $\frac{v(x)}{\alpha(x)} \neq \text{const}$

No general Ficks Law

$$j = -\frac{v^2}{\alpha}\frac{\partial c}{\partial x} - \frac{vc}{\alpha}\frac{\partial v}{\partial x}$$

in equilibrium: $j = 0 = -v\frac{\partial c}{\partial x} - c\frac{\partial v}{\partial x}$

$$\frac{1}{c}\frac{\partial c}{\partial x} = -\frac{1}{v}\frac{\partial v}{\partial x}$$

$$c(x) \sim \frac{1}{v(x)} \quad \Leftarrow \quad \ln c = \ln v^{-1} + \text{const}$$

Cells that speed up at high attractant concentration move away from it

Enthousiasm leads to hunger

Connection with random walk simulation

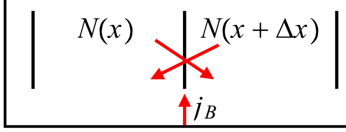
Schnitzer uses v and α

Simulation uses only variable steplength

Lançon, Europhys Lett 2001

$$\Delta x = \pm\sqrt{2D\Delta t}$$

is that at the start or end or ...?



Connection with random walk simulation

$$\Delta x = \pm\sqrt{2D(x+\beta\Delta x)\Delta t}$$

D at start	Ito convention	$\beta = 0$
D at end	isothermal convention	$\beta = 1$
D at middle	Stratonovich convention	$\beta = \frac{1}{2}$

$$D(x+\beta\Delta x) = D(x) + \beta\frac{\partial D}{\partial x}\Delta x$$

$$\Delta x = \pm\sqrt{2\left[D(x) + \beta\frac{\partial D}{\partial x}\Delta x\right]\Delta t}$$

$$\Delta x = \beta\frac{\partial D}{\partial x}\Delta t \pm \sqrt{2D(x)\Delta t}$$

Connection with random walk simulation

$$\langle\Delta x\rangle = \left\langle\beta\frac{\partial D}{\partial x}\Delta t\right\rangle + \cancel{\left\langle\pm\sqrt{2D(x)\Delta t}\right\rangle}$$

Net drift for $\beta \neq 0$

$$v_{drift} = \beta\frac{\partial D}{\partial x}$$

What about the flux?

We discussed Δx from a point x

$$\underset{x}{\bullet}\longrightarrow D(x+\beta\Delta x)$$

e.g. $\beta = 1$: take the endpoint

$$v_{drift} = \beta\frac{\partial D}{\partial x}$$

Flux is through a plane: towards a point x

$$\underset{x}{\bullet}\longleftarrow D(x+(1-\beta)\Delta x)$$

e.g. $\beta = 1$: take the endpoint

$$j = -c(1-\beta)\frac{\partial D}{\partial x}$$

What about the flux?

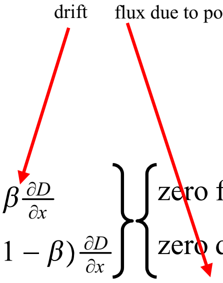
$$j = -c(1-\beta)\frac{\partial D}{\partial x}$$

$$\left.\begin{array}{c}\text{demanding in equilibrium } c = \text{constant}\\ \downarrow\\ j = 0\end{array}\right\}\Rightarrow \beta = 1$$

Constant concentration if stepsize determined by ***end***point

$$\left.\begin{array}{l}v_{drift} = \beta\frac{\partial D}{\partial x}\\ j = -c(1-\beta)\frac{\partial D}{\partial x}\end{array}\right\}\left\{\begin{array}{l}\text{zero flux} \Leftrightarrow \text{non-zero drift}\\ \text{zero drift} \Leftrightarrow \text{non-zero flux}\end{array}\right.$$

What about the flux?

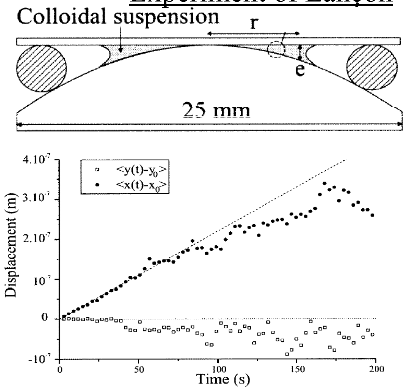


$$\text{Landauer}\quad \underset{\text{drift}}{\underset{\downarrow}{u}} = \underset{\text{flux due to potential}}{\underset{\downarrow}{v}} + \frac{\partial D}{\partial x}$$

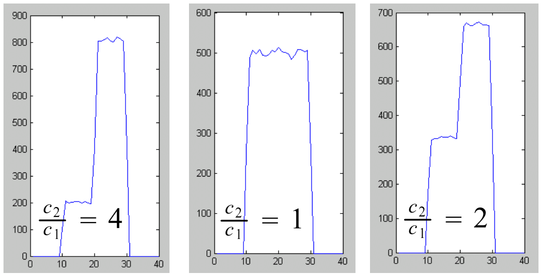
$$\left.\begin{array}{l}v_{drift} = \beta\frac{\partial D}{\partial x}\\ j = -c(1-\beta)\frac{\partial D}{\partial x}\end{array}\right\}\left\{\begin{array}{l}\text{zero flux} \Leftrightarrow \text{non-zero drift}\\ \text{zero drift} \Leftrightarrow \text{non-zero flux}\end{array}\right.$$

$$v_{flux} = -(1-\beta)\frac{\partial D}{\partial x} = \beta\frac{\partial D}{\partial x} - \frac{\partial D}{\partial x}$$

Experiment of Lançon

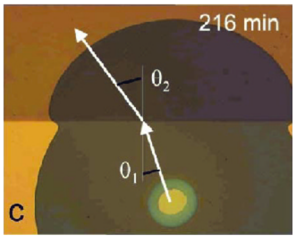


Equilibrium concentrations vs. stepsize $\frac{D_1}{D_2} = 4$

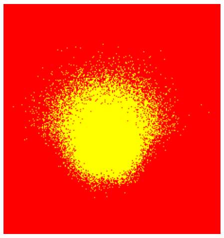


start	end	average
$\beta = 0$	$\beta = 1$	$\beta = \frac{1}{2}$
Ito	isothermal	Stratonovich

Diffusion with *D(x)*



A. Remhof et al PRL



Random walkers

Extensions

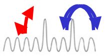
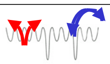
Schnitzer:

- Direction dependent velocity
- Higher dimensional cases
- Distributions in v and α
- Feeding strategy: lower tumbling if $\frac{\partial c}{\partial x} > 0$
- Bacterium has memory: *c(t)*

References

Schnitzer, PRE 48 (1993) 2553
Landauer, Helv.Phys.Acta 56(1983)847
Collins *et al.*, Am.J.Phys 65(1997)230
Krug, Europhys.Lett 60 (2002)788
Lançon *et al.*, Europhys.Lett 54(2001)28
Tan, APL 73 (1998) 2678

Summary

$\alpha = C$ $v = C$	$\alpha = \alpha(x)$ $v = C$	$\alpha = \alpha(x)$ $v(x) \sim \alpha(x)$	$\alpha = C$ $v = v(x)$	$\alpha = \alpha(x)$ $v = v(x)$
$j = -D\frac{\partial c}{\partial x}$	$j = -D(x)\frac{\partial c}{\partial x}$ 	$j = -\frac{\partial(Dc)}{\partial x}$ 	$j = -D\frac{\partial c}{\partial x} - \frac{c}{2}\frac{\partial D}{\partial x}$	No law
$c = C$	$c = C$	$c \sim \frac{1}{D}$	$c \sim \frac{1}{\sqrt{D}}$	$c \sim \frac{1}{v}$
trivial				difficult
	$\beta = 1$ $v_{drift} = \frac{\partial D}{\partial x}$	$\beta = 0$ $v_{drift} = 0$	$\beta = \frac{1}{2}$ $v_{drift} = \frac{1}{2}\frac{\partial D}{\partial x}$	
	Isothermal *D* at end	Ito *D* at start	Stratonovich *D* in middle	