Random Walks and Diffusion

- random motion and diffusion - analytic treatment
- a simplified model: random walks
- Brownian motion: implementation of an algorithm based on the Langevin equation
- Brownian motion: mathematical eqs. & miscellanea

M. Peressi - UniTS - Laurea Magistrale in Physics
Laboratory of Computational Physics - Unit IV

I part:
Random motion and diffusion
-history and analytic treatment-

Random motion

Brownian motion is by now a well-understood problem, and the concepts, techniques and models have proven fruitful in many different fields, from **statistical mechanics** to **econophysics**.   A brief history:

- Robert Brown 1828
- J.C. Maxwell 1867
- Albert Einstein 1905
- Maryan Smoluchowski 1906
- Jean Perrin 1912
- J. Bardeen , C. Herring 1950

Observations of "active molecules" by scientist Robert Brown in 1827

A

BRIEF ACCOUNT

OF

MICROSCOPICAL OBSERVATIONS

Made in the Months of June, July, and August, 1827,

ON THE PARTICLES CONTAINED IN THE POLLEN OF PLANTS;

AND

ON THE GENERAL EXISTENCE OF ACTIVE MOLECULES

IN ORGANIC AND INORGANIC BODIES.

BY

ROBERT BROWN,

F.R.S., Hon. M.R.S.E. and R.I. Acad., V.P.L.S.,

MEMBER OF THE ROYAL ACADEMY OF SCIENCES OF SWEDEN, OF THE ROYAL SOCIETY OF DENMARK, AND OF THE IMPERIAL ACADEMY NATURÆ CURIOSORUM; CORRESPONDING MEMBER OF THE ROYAL INSTITUTES OF FRANCE AND OF THE NETHERLANDS, OF THE IMPERIAL ACADEMY OF SCIENCES AT ST. PETERSBURG, AND OF THE ROYAL ACADEMIES OF PRUSSIA AND BAVARIA, ETC.

Random motion

- random motion of tiny particles had been reported early in scientific literature
- before 1827, random motion was attributed to living particles.
- random motion = "brownian motion", after 1827, when the British botanist **Robert Brown** claimed that even dead particles could exhibit a random motion

~~Random~~ motion "Brownian"

- random motion of tiny particles had been reported early in scientific literature
- <u>before 1827</u>, random motion was attributed to <u>living particles</u>.
- random motion = "brownian motion", <u>after 1827</u>, when the British botanist **Robert Brown** claimed that <u>even dead particles could exhibit a random motion</u>
- What is the origin of the brownian motion? In 1870, Loschmidt suggested that <u>it is caused by thermal agitation</u>

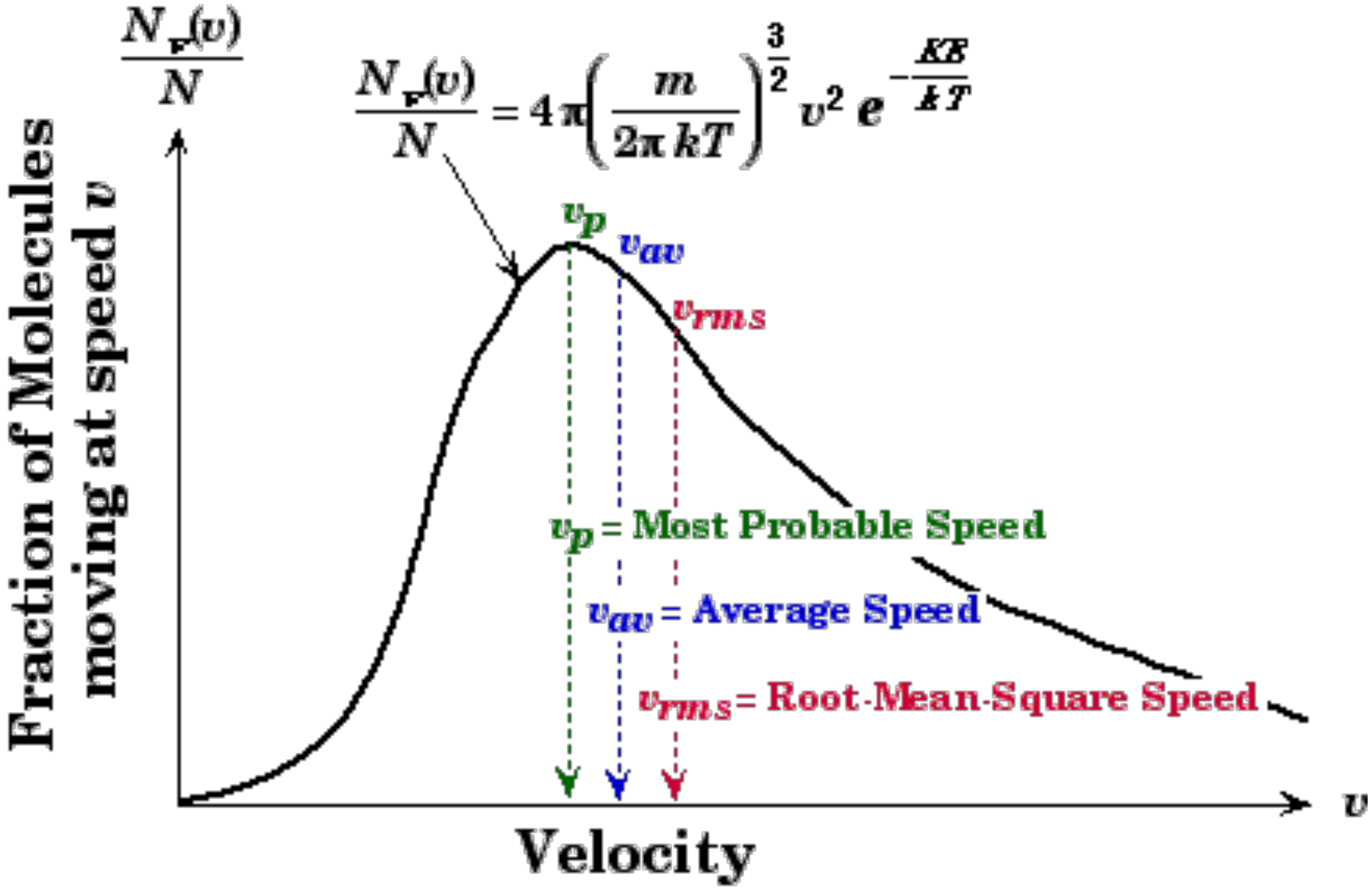
Brownian motion -open questions-

Observations of "active molecules" made by Brown in 1827 led the physics community to **search for the proof that molecules indeed exist.**

At the turn of 20th century, the **atomic nature of matter** was fairly widely accepted among scientists, but not universally (there was **NO direct evidence!**)

Another argument under discussion: **the kinetic theory of gases**

Maxwell-Boltzmann distribution of velocity



$v_p = \sqrt{2\frac{kT}{m}}$ $\quad v_{av} = \sqrt{\frac{8}{\pi}\frac{kT}{m}}$ $\quad v_{rms} = \sqrt{3\frac{kT}{m}}$

Kinetic theory of gases

- Under discussion in ~1900: $\frac{1}{2}m\overline{v^2} = \frac{3}{2}k_B T$???
- Can we prove its validity from the observation of the Brownian motion?
- Could m be obtained from that relationship? In principle yes, provided one can measure v. But v cannot be measured from the erratic trajectory of particles observed at the microscope!
- so... **What can we really measure?**

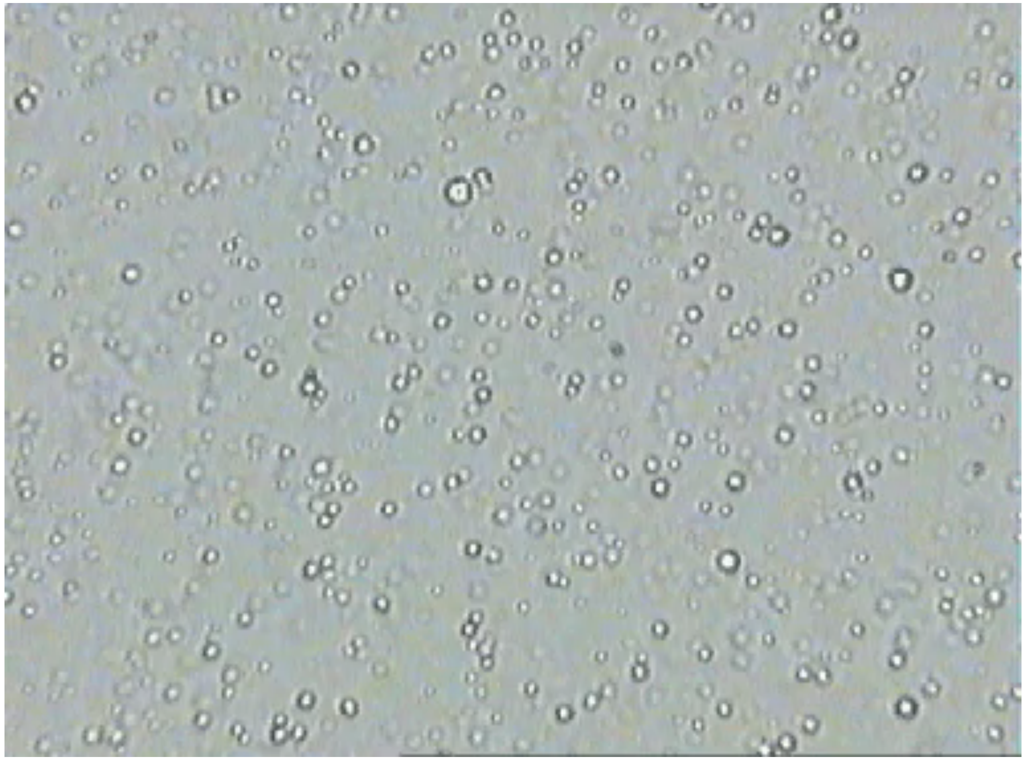
Brownian motion
-Einstein's 1905 paper-

In essence, the Einstein's paper provides:
- evidence for existence of atoms/molecules
- estimation of the size of atoms/molecules
- estimation of the Avogadro's number

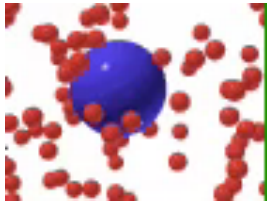
Einstein predicted that **microscopic particles** dispersed in water **undergo random motion as a result of collisions** (stochastic forces) **with water molecules much smaller and light** (not visible on the chosen observation scale).

diameter of Brownian particles: ~ 1 μ, water: ~ 10^{-4} μ

Brownian motion



fat droplets (0.5-3 μm) in milk
http://www.microscopy-uk.org.uk/dww/home/hombrown.htm
credit to David Walker, Micscape



larger particles (blue = fat droplets) jiggle more slowly than smaller (red = water) particles;
only the larger particles are visible

A. Einstein:
"On the Movement of Small Particles Suspended in Stationary Liquids Required by the Molecular-Kinetic Theory of Heat"
Annalen der Physik 19, p. 549 (1905)

...
In this paper it will be shown that, according to the molecular-kinetic theory of heat, **bodies of a microscopically visible size** suspended in liquids must, as a result of thermal molecular motions, **perform motions** of such magnitude that they can be **easily observed with a microscope**. It is possible that the motions to be discussed here are identical with so-called Brownian molecular motion; however, the data available to me on the latter are so imprecise that I could not form a judgment on the question.

If the motion to be discussed here can actually be observed, together with the laws it is expected to obey, then [...] **an exact determination of actual atomic sizes becomes possible.** On the other hand, if the prediction of the motion were to be proved wrong, this fact would provide a far-reaching argument against the molecular-kinetic conception of heat....

*Later Einstein wrote: "**My major aim in this was to find facts which would guarantee as much as possible the existence of atoms of definite finite size**."*

Brownian motion
-Einstein's 1905 paper-

Einstein suggests that **mean square displacements $<\Delta r^2>$** of suspended particles undergoing brownian motion rather then their velocities are suitable **observable and measurable quantities, and directly related to their diffusion coefficient D**:

$$<\Delta r^2> = 2dDt \quad \text{with} \quad D = \mu k_B T = k_B T/(6\pi\eta P)$$

(t time, d dimensionality of the system, μ mobility,
P radius of brownian particles; η solvent viscosity; $k_B = R/N$)

$<\Delta r^2>$ (and therefore D), η, T measurable => obtain P !

Brownian motion
-Einstein's 1905 paper-

Einstein suggests that **mean square displacements $\langle \Delta r^2 \rangle$** of suspended particles undergoing brownian motion rather then their velocities are suitable **observable and measurable quantities, and directly related to their diffusion coefficient D**:

$$\langle \Delta r^2 \rangle \overset{(**)}{=} 2dDt \quad \text{with} \quad D \overset{(*)}{=} \mu k_B T = k_B T/(6\pi\eta P)$$

(t time, d dimensionality of the system, μ mobility,
P radius of brownian particles (???); η solvent viscosity; k_B =R/N)

$\langle \Delta r^2 \rangle$ measurable => from (**) we get D;
η, T measurable => from (*) we obtain P

Diffusion

Part I – Sedimentation Equilibrium

Compare Two Independent Analyses of Final State

First Fick's law (particle diffusion eq.) states that the flux (μWc) goes from regions of high concentration to regions of low concentration, with a magnitude that is proportional to the concentration gradient .

From Mass Transfer Theory:

$$\text{flux} = \underbrace{\mu W c}_{\text{migration in gravity}} \underbrace{- D\frac{dc}{dx}}_{\text{diffusion}} = 0$$

W = net weight of one particle

c = concentration of particles

$$\mu = \text{mobility} = \frac{\text{velocity}}{\text{force}} = \frac{1}{6\pi\eta P}$$

η = viscosity of fluid

P = particle radius

$$c(x) = c_0 \exp\left(-\frac{\mu}{D} W x\right)$$

From Thermodynamics:

$$\underbrace{\frac{d\phi}{dx}}_{\text{gravitational potential}} + \underbrace{RT\frac{d\ln c}{dx}}_{\text{chemical potential}} = 0$$

$\phi = WNx$ = PE per mole

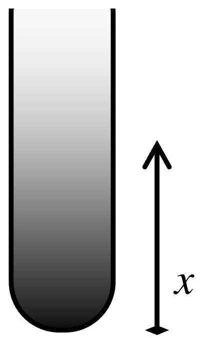
N = Avogadro's number

R = universal gas constant

T = absolute temperature

RT[=]energy/mole

$$c(x) = c_0 \exp\left(-\frac{N}{RT} W x\right)$$



If there is a variation in the potential energy of a system, an energy flow will occur.

Compare: exponentials must be equal! ⇨ $$N = RT\frac{\mu}{D}$$ (*)

N, R, T known; if D is measurable (according to Einstein)

=> Obtain μ; from μ (and η, known) we get particle size P

Brownian motion and diffusion

Fick's law of diffusion (1855): a continuum model

Part II – Statistical Analysis of B.M.

one dimension: d=1
Here: p=c (concentration)

Fick's 2nd law: $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$

Initial Condition: $p(x,0) = \delta(x)$

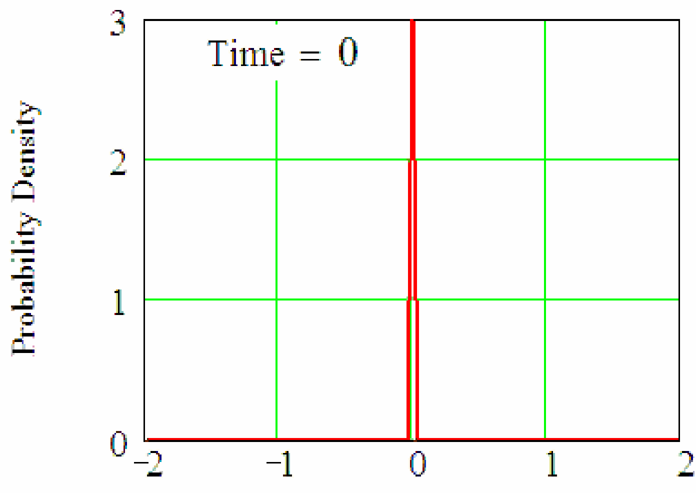
B.C.'s: $p(\pm\infty, t) = 0$

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

remember the gaussian:

$$p(x) = \frac{1}{\sigma}\frac{1}{\sqrt{2\pi}} e^{-x^2/(2\sigma^2)}$$

with $\sigma^2 = 2Dt$



$$1 = \int_{-\infty}^{\infty} p(x,t)\,dx \quad \text{for all } t$$

$$\bar{x}(t) = \int_{-\infty}^{\infty} x p(x,t)\,dx = 0$$

$$\overline{x^2}(t) = \int_{-\infty}^{\infty} x^2 p(x,t)\,dx = 2Dt \qquad (**)$$

The **mean square displacements <Δr²>** of suspended particles are suitable observable quantities and give **D**

ok

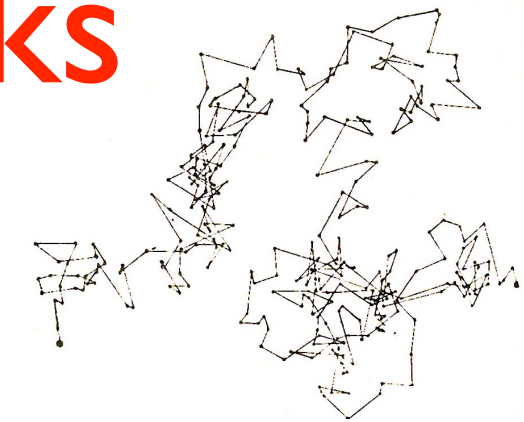
Random motion in nature

- in gases or diluted matter: random motion (after how many collisions on average a particle covers a distance Δr? or which is the distance from the starting point covered on average by a particle after N collisions?)
- in solids: diffusion of impurities (molten metals) or vacancies..., electronic transport in metals...

II part:
Random walks

A very simplified **model**
for many phenomena,
including brownian motion

Random Walks



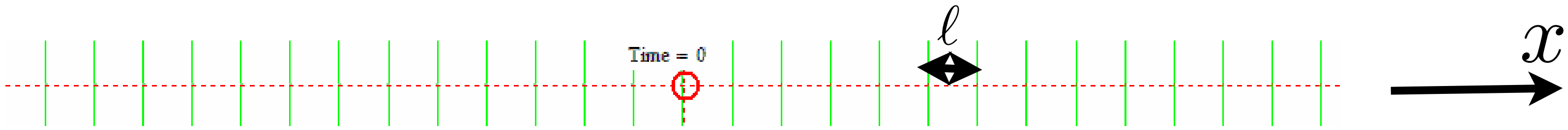
- **traditional** RW ➡ brownian motion
- **modified** (interacting) RW ➡ the motion of the walker depends on his previous trajectory

Scaling properties of RW

Dependence of $\langle R^2(t) \rangle$ on t :

- **normal** behavior: $\langle R^2(t) \rangle \sim t$
  for the brownian motion
- **superdiffusive** behavior: $\langle R^2(t) \rangle \sim t^{2\nu}$ with $\nu > 1/2$
  in models where autointersections are unfavoured
- **subdiffusive** behavior $\langle R^2(t) \rangle \sim t^{2\nu}$ with $\nu < 1/2$
  in models where autointersections are favoured

One-dimensional RW



A walker at each step can go either left or right:

N : number of steps

ℓ : length of the random displacement (random direction)

($s_i = \pm\ell$ relative displacement of the i step)

x_N: displacement from the starting point after N steps

($x_N = \sum_{i=1}^{N} s_i, \quad x_N \in [-N\ell, +N\ell]$)

$p_{\rightarrow}$ $p_{\leftarrow}$: probability of left or right displacement

What can we calculate? **Averaging over walkers**:

$\langle x_N \rangle$: average net displacement after N steps

$\langle x_N^2 \rangle$: average square displacement after N steps

$P_N(x)$: probability for x to be the final net displacement from the starting point after N steps

RW 1D

Exact analytic expressions can be easily derived for $p_{\leftarrow} = p_{\rightarrow}$

$$\langle x_N \rangle = \langle \sum_{i=1}^{N} s_i \rangle = \ldots (\text{if } p_{\leftarrow} = p_{\rightarrow}) \ldots = 0$$

$$\langle x_N^2 \rangle = \langle \left(\sum_{i=1}^{N} s_i \right)^2 \rangle = \langle \sum_{i=1}^{N} s_i^2 \rangle + \langle \sum_{i \neq j} s_i s_j \rangle = \ldots (\text{if } p_{\leftarrow} = p_{\rightarrow}) \ldots = N\ell^2$$

More general:

$$x_N = n_{\leftarrow}(-\ell) + n_{\rightarrow}(+\ell) \ (\text{with } N = n_{\leftarrow} + n_{\rightarrow})$$

$$\langle x_N \rangle = N(p_{\rightarrow} - p_{\leftarrow})\ell \qquad \langle x_N^2 \rangle = [N(p_{\rightarrow} - p_{\leftarrow})\ell]^2 + 4p_{\rightarrow}p_{\leftarrow}N\ell^2$$

therefore:

$$\langle \Delta x^2 \rangle = N\ell^2$$

average over walkers

RW 1D

In general, average quantities can be calculated from $P_N(x)$:

$$\langle x_N \rangle = \sum_{x=-N\ell}^{x=+N\ell} x P_N(x)$$

Let's make an example
of analytical calculation of $P_N(x)$
(N=3 is enough!)
...
(how many
different walks of length N?)

RW 1D

In general, average quantities can be calculated from $P_N(x)$:

$$\langle x_N \rangle = \sum_{x=-N\ell}^{x=+N\ell} x P_N(x)$$

Let's make an example
of analytical calculation of $P_N(x)$
(N=3 is enough!)
...

(There are 2^N different possible walks
of N steps...)

RW 1D

Generalizing the expression for $P_N(x)$:

From:

$$P_1(1) = p_{\rightarrow}; \quad P_1(-1) = p_{\leftarrow}$$
$$P_{N+1}(x) = P_N(x-1)p_{\rightarrow} + P_N(x+1)p_{\leftarrow}$$

we have:

$$P_N(x) = \frac{N!}{\left(\frac{N}{2}+\frac{x}{2}\right)!\left(\frac{N}{2}-\frac{x}{2}\right)!} p_{\rightarrow}^{\frac{N}{2}+\frac{x}{2}} p_{\leftarrow}^{\frac{N}{2}-\frac{x}{2}}$$

number of steps

$n \setminus x$	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$	0	$\frac{1}{2}$				
2				$\frac{1}{4}$	0	$\frac{2}{4}$	0	$\frac{1}{4}$			
3			$\frac{1}{8}$	0	$\frac{3}{8}$	0	$\frac{3}{8}$	0	$\frac{1}{8}$		
4		$\frac{1}{16}$	0	$\frac{4}{16}$	0	$\frac{6}{16}$	0	$\frac{4}{16}$	0	$\frac{1}{16}$	
5	$\frac{1}{32}$	0	$\frac{5}{32}$	0	$\frac{10}{32}$	0	$\frac{10}{32}$	0	$\frac{5}{32}$	0	$\frac{1}{32}$

$P_N(x)$ for $p_{\leftarrow} = p_{\rightarrow}$

(Pascal triangle)

RW 1D

$$P_N(x) = \frac{N!}{\left(\frac{N}{2}+\frac{x}{2}\right)!\left(\frac{N}{2}-\frac{x}{2}\right)!} p_{\rightarrow}^{\frac{N}{2}+\frac{x}{2}} p_{\leftarrow}^{\frac{N}{2}-\frac{x}{2}}$$

Can be generalized to large N (put $N = t/\Delta t$, then $\Delta t \to 0$, continuum limit):

$$P(x, N\Delta t) = \sqrt{\frac{2}{\pi N}} e^{-x^2/(2N)} \qquad (*)$$

which looks like a Gaussian.

Why?

Let's describe the RW problem with a space/time differential equation...

RW 1D: Diffusion - continuum limit

(case $p_{\leftarrow} = p_{\rightarrow}$)

$$P(i,N) = \frac{1}{2}P(i+1,N-1) + \frac{1}{2}P(i-1,N-1)$$

Defining: $t = N\tau,\, x = i\ell$ we have:

$$P(x,t) = \frac{1}{2}P(x+l,t-\tau) + \frac{1}{2}P(x-l,t-\tau)$$

We rewrite this by subtracting $P(x,t-\tau)$ and dividing by τ

$$\frac{P(x,t) - P(x,t-\tau)}{\tau} = \frac{P(x+l,t-\tau) + P(x-l,t-\tau) - 2P(x,t-\tau)}{2\tau}$$

we get

$$\frac{\partial P(x,t)}{\partial t} \approx \frac{l^2}{2\tau}\frac{\partial^2 P(x,t)}{\partial x^2}$$

In the limit $\tau \to 0, l \to 0$ but where the ratio l^2/τ is finite, this becomes an exact relation.

RW 1D: Diffusion - continuum limit

The fundamental solution of the continuum diffusion equation of the previous slide, defining $D = \frac{\ell^2}{2\tau}$ is:

$$P(x,t) = \sqrt{\frac{1}{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right).$$

The discretized solution of the RW problem:

$$P_N(x) = \sqrt{\frac{2}{\pi N}} \exp\left(-\frac{x^2}{2N}\right)$$

considering $t = N\tau$ and the definition of D, can be rewritten as:

$$P(x,t) = \sqrt{\frac{1}{\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

a part from the normalization which is a factor of 2 larger in this form because of the spatial discretization that excludes alternatively odd or even values of x.
The solution is therefore a Gaussian distribution with $\sigma^2 = 2Dt$ which describes a pulse gradually decreasing in height and broadening in width in such a manner that its area is conserved.

RW 1D: Diffusion - continuum limit

physical meaning!
(hint: try to simulate a number of particles
initially concentrated at 0 and
evolving according to the RW model:
... the ‘cloud’ is progressively expanding)

RW 1D: simulation

The basic algorithm:

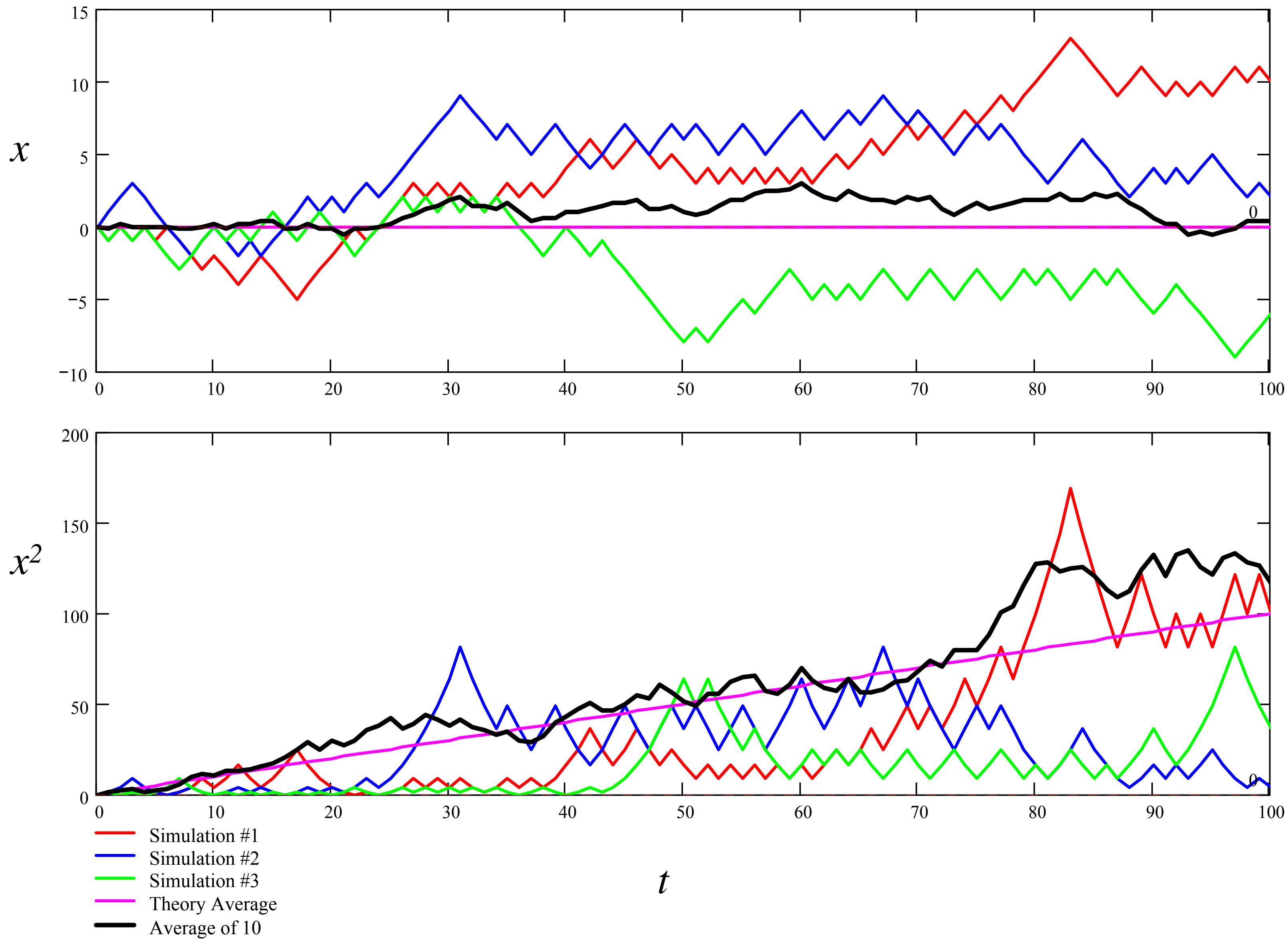
ix = position of the walker
x_N, x2_N = cumulative quantities
rnd(N) = sequence of N random numbers

(1 run= 1 particle= 1 walker)

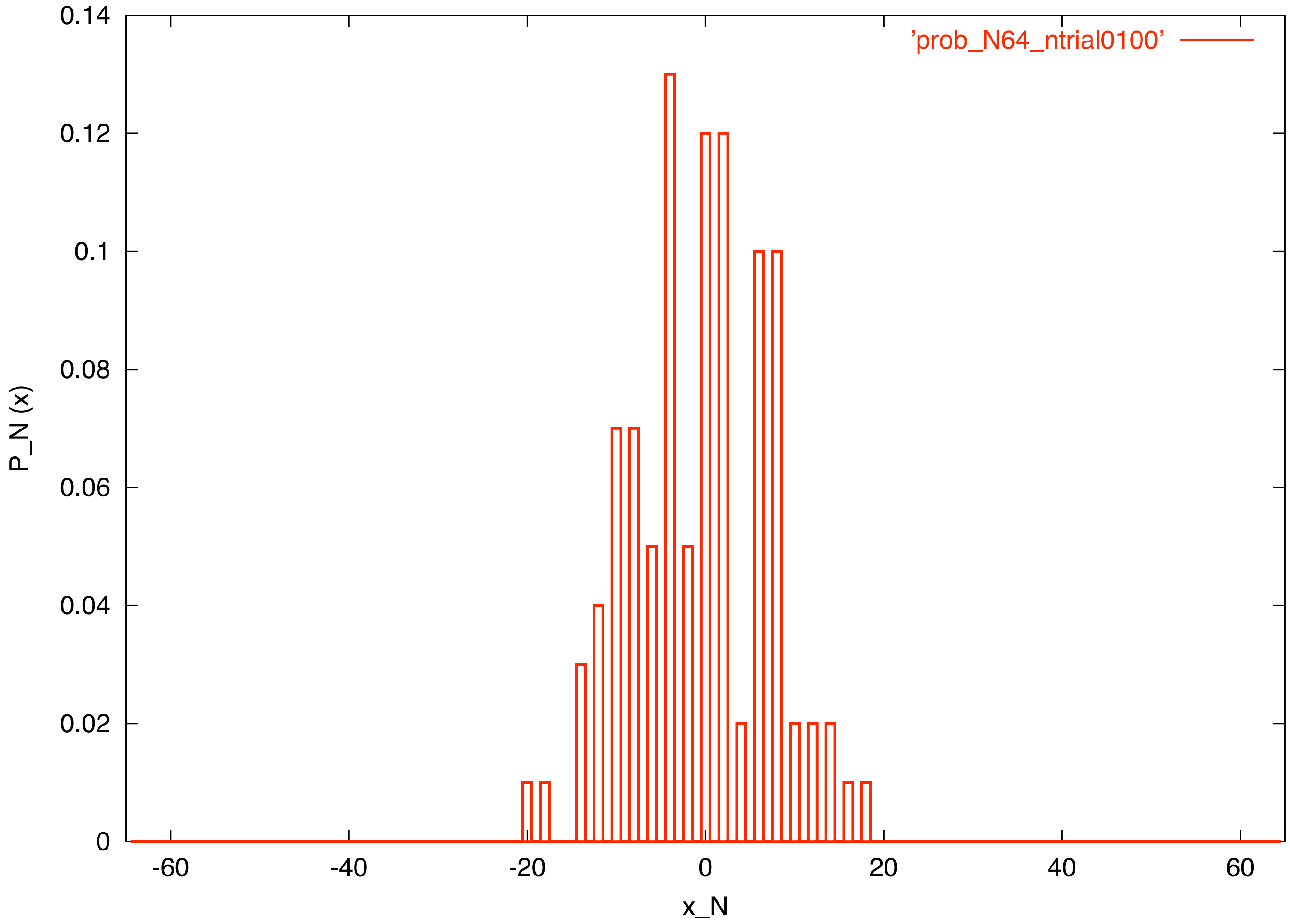
```
do irun = 1, nruns
   ix = 0 ! initial position of each run
   call random_number(rnd) ! get a sequence of random numbers
   do istep = 1, N
      if (rnd(istep) < 0.5) then ! random move
         ix = ix - 1 ! left
      else
         ix = ix + 1 ! right
      end if
      x_N (istep) = x_N (istep) + ix
      x2_N(istep) = x2_N(istep) + ix**2
   end do
   P_N(ix) = P_N(ix) + 1 ! accumulate (only for istep = N)
end do
```

Note:
x_N and x2_N are NOT reset to zero, but summed over the runs (walkers)

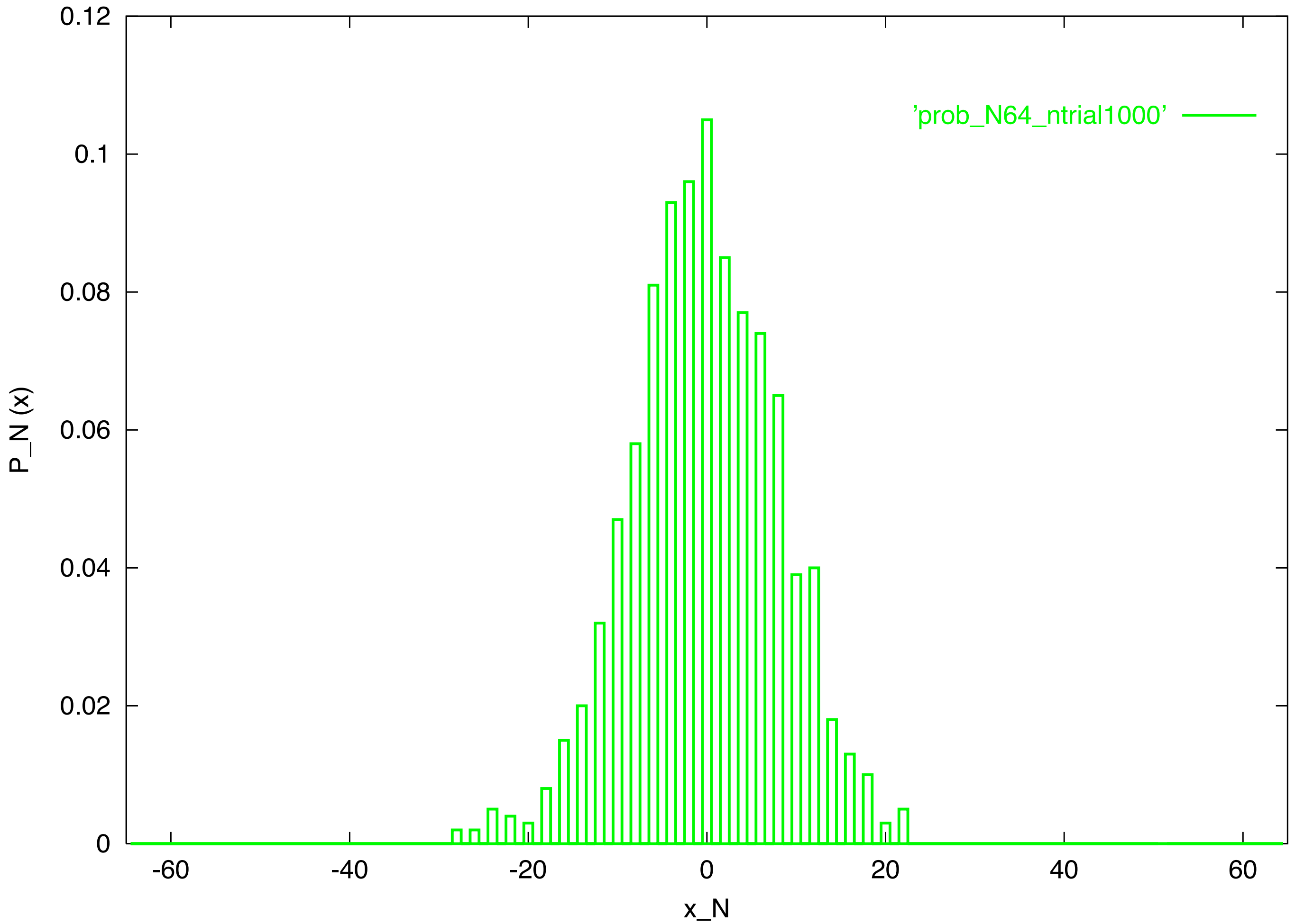
RW 1D: simulation



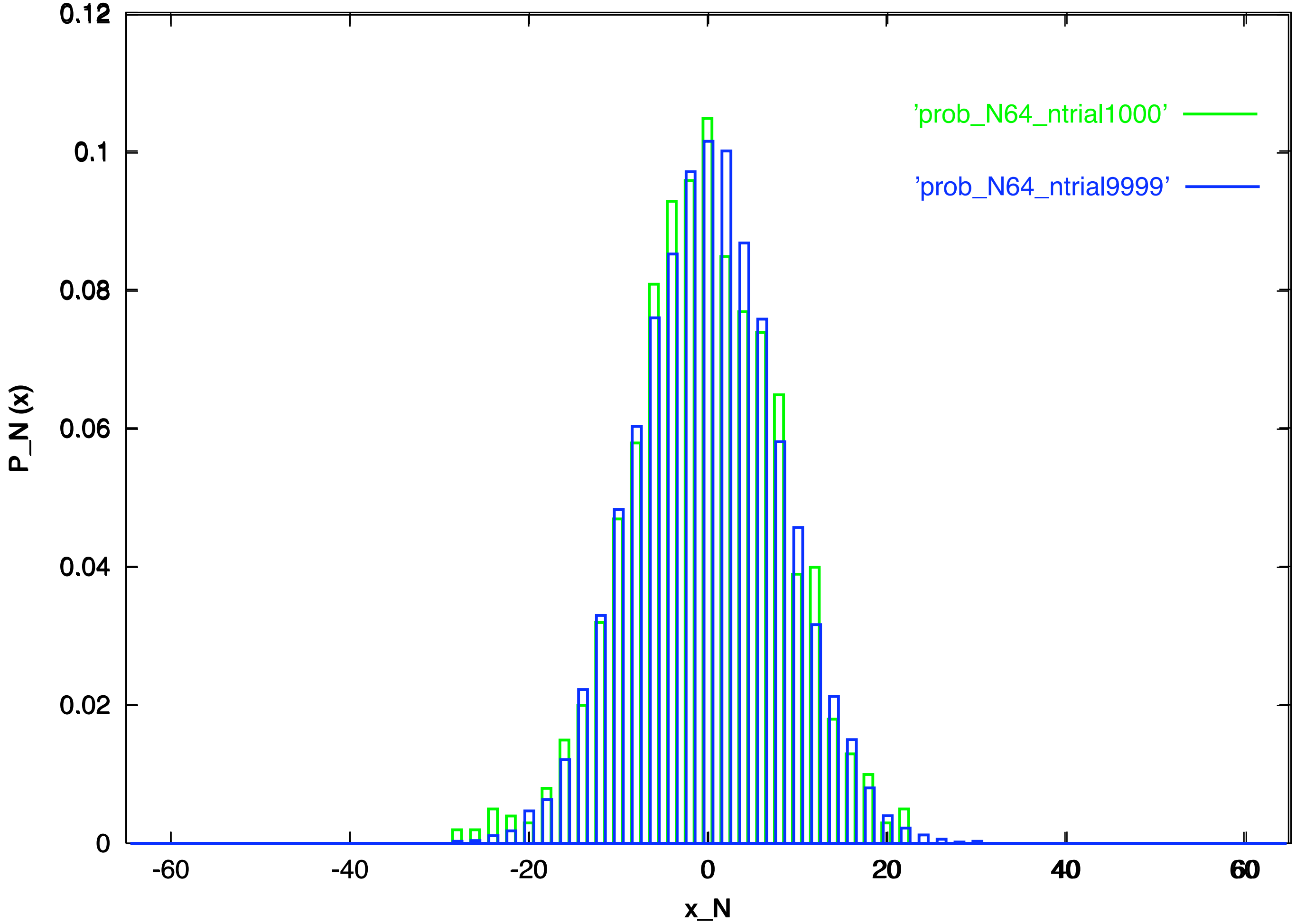
RW 1D: simulation



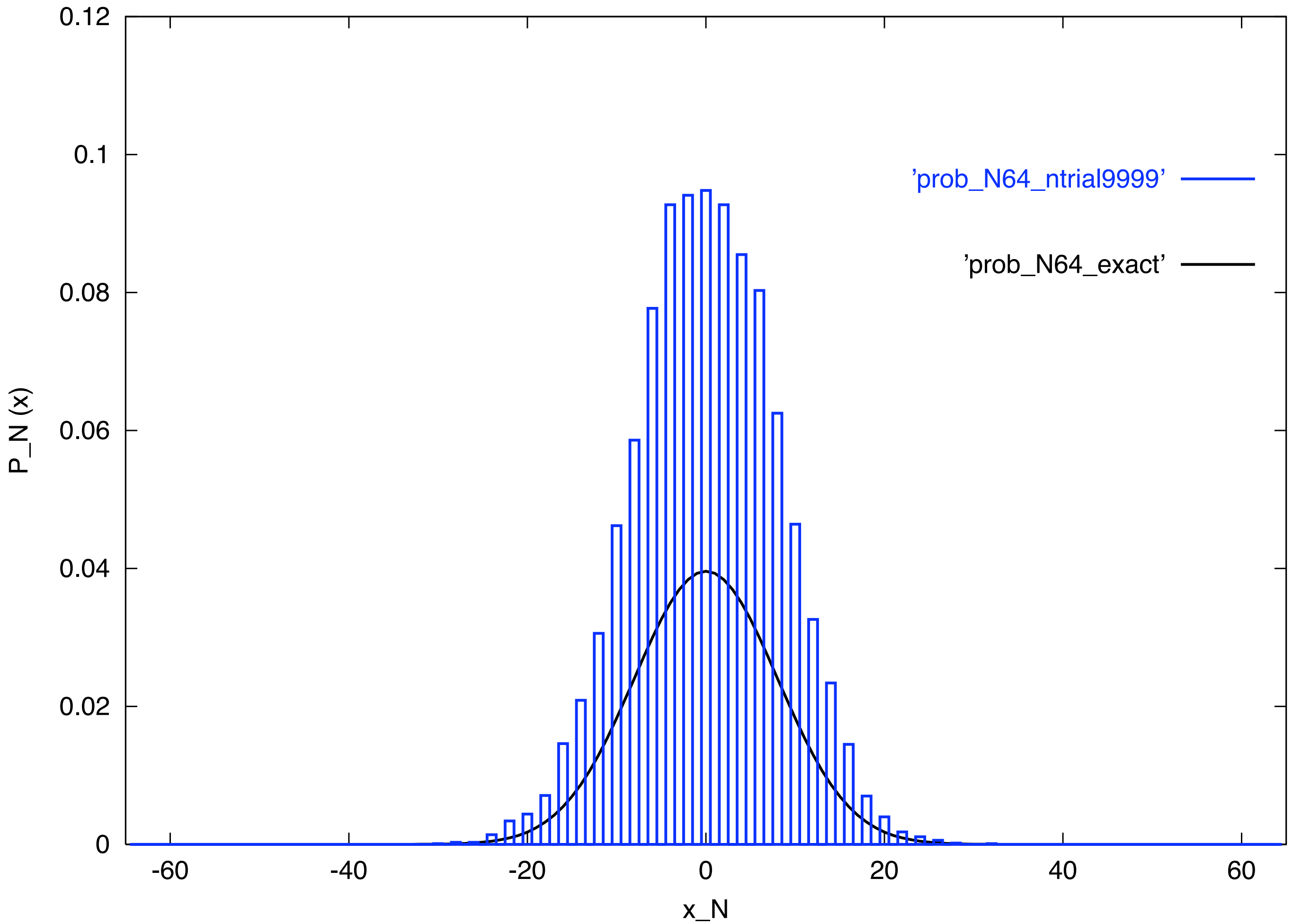
RW 1D: simulation



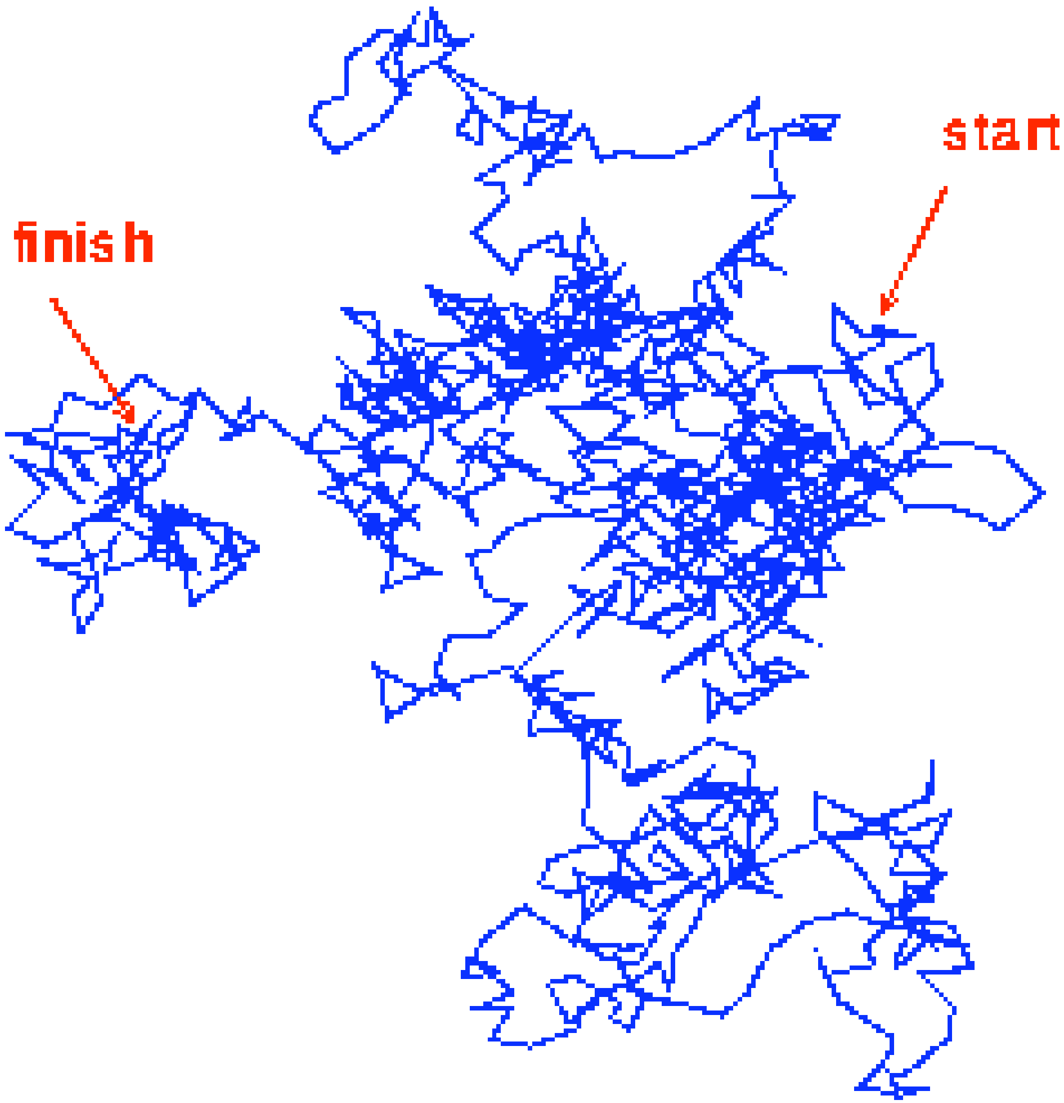
RW 1D: simulation



RW 1D: simulation

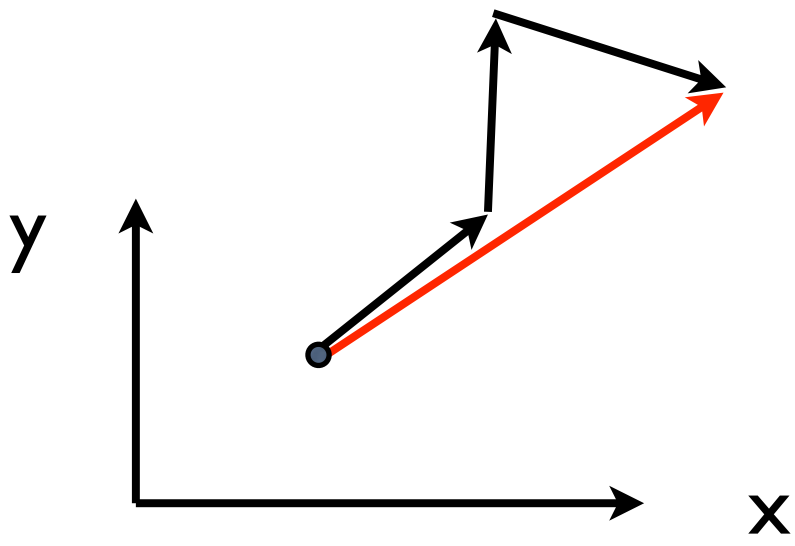


Random Walks



In the continuum space, or discretised on a lattice…

Random Walks 2D

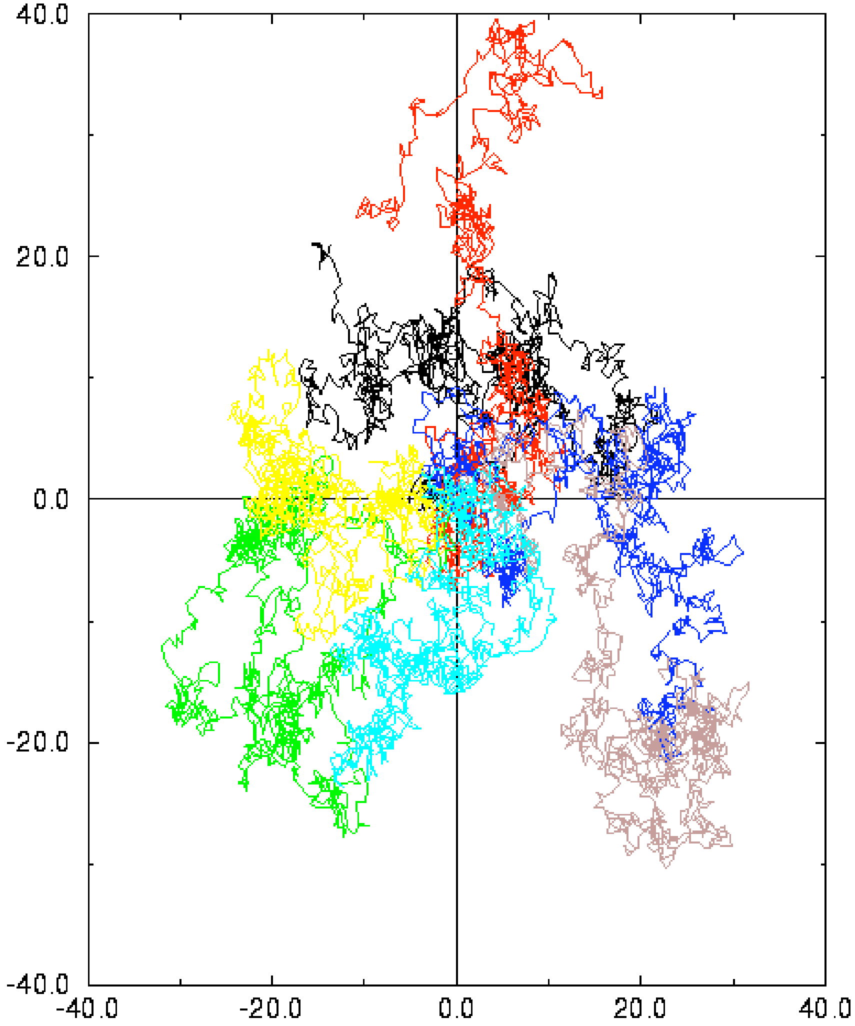


$$\langle R_N^2 \rangle = \langle (\Delta x_1 + ... + \Delta x_N)^2 + (\Delta y_1 + ... + \Delta y_N)^2 \rangle = ... = N \langle \Delta x_i^2 + \Delta y_i^2 \rangle = N \ell^2$$

$$\langle R^2 \rangle \propto N$$

also in 2D! (and in general in each dimension)

Random Walks 2D



Theory predicts that $\langle R^2 \rangle \propto N$, but this holds only for averages on many walkers!

Random Walks 2D

Generating 2-D random unit steps

1. Choose θ a random number in the range $[0, 2\pi]$ and then set $x = \cos\theta, y = \sin\theta$.

2. Choose a random value for Δx in the range $[-1, 1]$ and $\Delta y = \pm\sqrt{1 - \Delta x^2}$ (choose the sign randomly too).

3. Choose separate random values for $\Delta x, \Delta y$ in the range $[-1, 1]$ (but not $\Delta x = 0, \Delta y = 0$). Normalize $\Delta x, \Delta y$ so that the step size is 1.

4. Choose a direction (N, E, S, W) randomly as the step direction (no trigonometric functions are then needed). Note, choosing one of four directions is equivalent to choosing a random *integer* on [0,3].

5. Choose separate random values $\Delta x, \Delta y$ in the range $[-\sqrt{2}, \sqrt{2}]$

   (NOTE: The average step size is...)

TEST DIFFERENT ALGORITHMS!

WHAT IS THE BEST? THE ONE WHICH GIVES THE BEST BEHAVIOR?

WHAT IS THE MOST EFFICIENT?

Generating 2D random unit steps
Comment on the algorithm n. 5 (p. 39 of the slides)

Indicating with x and y the individual displacements,

$p(x) = \dfrac{1}{2\sqrt{2}}$ for $|x| < \sqrt{2}$ and 0 otherwise; the same for $p(y)$;

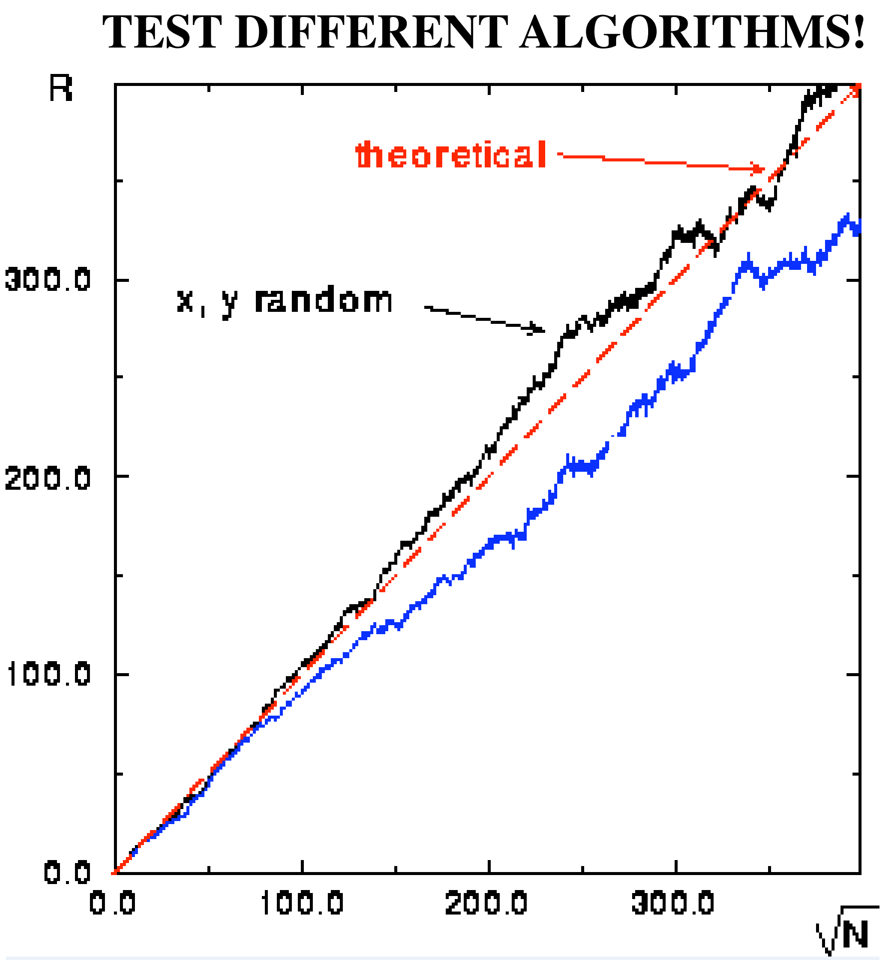
the average step size is:

$$\sqrt{\langle x^2 + y^2 \rangle} = \int_{-\sqrt{2}}^{\sqrt{2}} \int_{-\sqrt{2}}^{\sqrt{2}} (x^2 + y^2)\, p(x)\, p(y)\, dx\, dy = ... = \frac{2}{\sqrt{3}}$$

Therefore, with x and y generated in this way, the behaviour of the simulated $\langle \Delta R_N^2 \rangle$ should be $\frac{4}{3} N$ (since $\langle \Delta R_N^2 \rangle = N\ell^2$).

In which extension you should generate x and y in order to have on average a unitary step size?

Random Walks 2D



Theory predicts that $\langle R^2 \rangle \propto N$, but this holds only for averages on many walkers! Consider this before extracting your conclusions…

Random Walks 2D

0	0.0000000	0.0000000
10	0.2242774	3.7794106
20	-1.7333623	1.3218992
30	-1.4481916	-3.1119978
40	-2.2553353	-3.5246484
50	-3.8911035	-6.6665235
60	-3.6508965	-8.0110636

.....

↑

```
if (mod(i,10)==0) then
   WRITE (...) i,x,y
end if
```

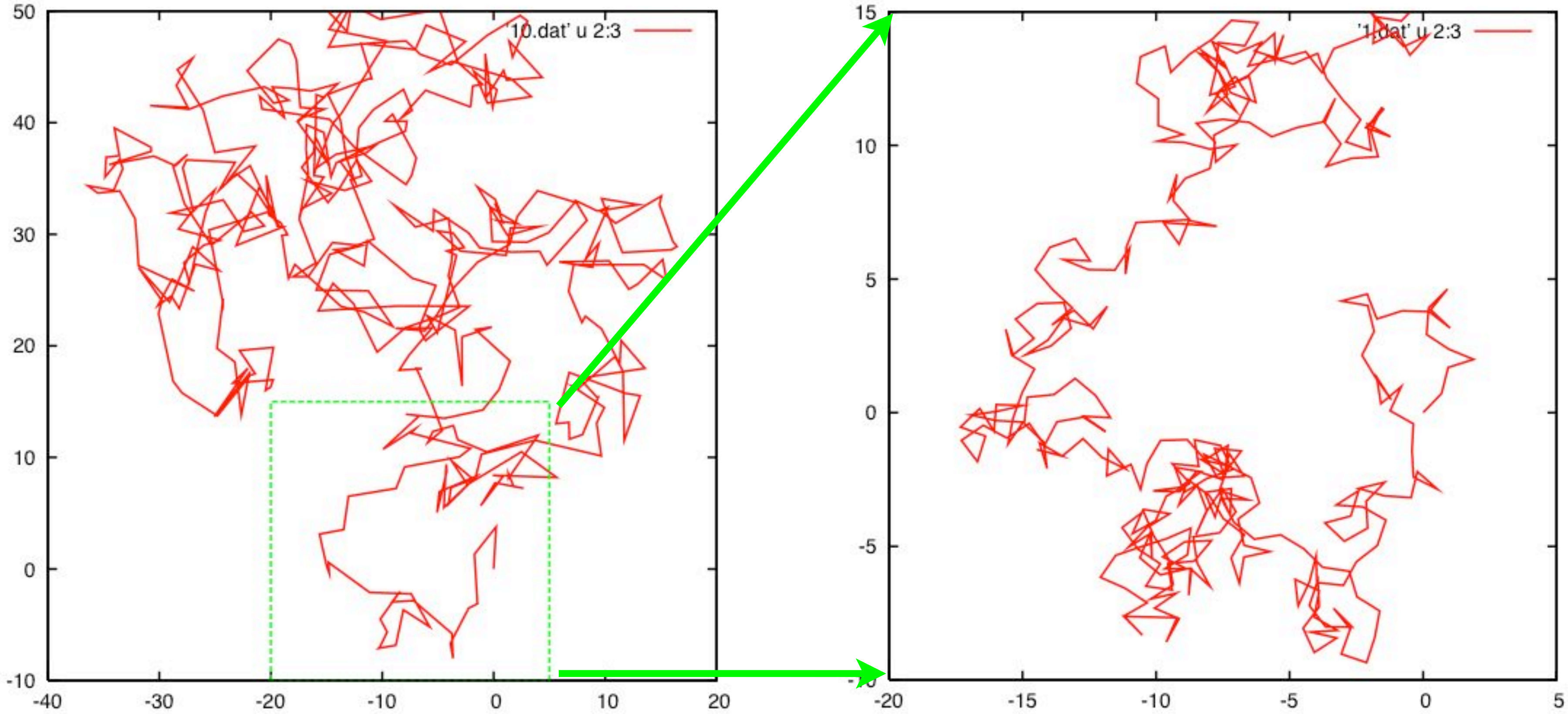
```
WRITE (...) i,x,y
```
→

0	0.0000000	0.0000000
1	0.6946244	0.7193726
2	0.9359566	1.6898152
3	1.8891419	1.9922019
4	0.9642899	2.3725290
5	0.1308700	2.9251692
6	0.2071800	3.9222534
7	0.9160752	4.6275673
8	0.2856980	3.8512783
9	1.0143363	3.1663797
10	0.2242774	3.7794106
11	-0.7752404	3.8104627
12	-1.7280728	3.5069659
13	-2.0930278	4.4379911
14	-3.0587580	4.1784425
15	-2.0729706	4.0104446
16	-1.8304152	3.0403070
17	-2.2890768	2.1516960
18	-1.7717266	1.2959222
19	-1.1920205	0.4810965
20	-1.7333623	1.3218992
21	-1.5798329	0.3337551

.....

Random Walks 2D

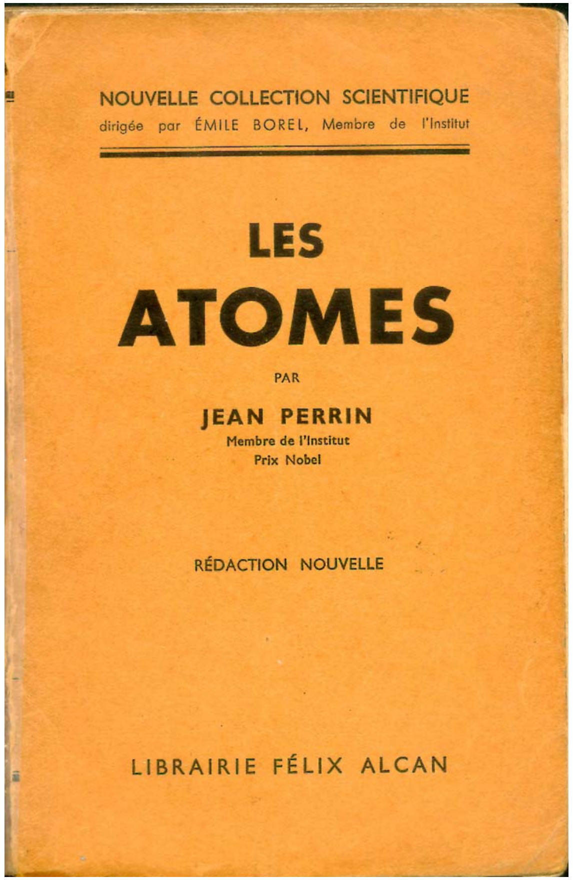
self-similarity!

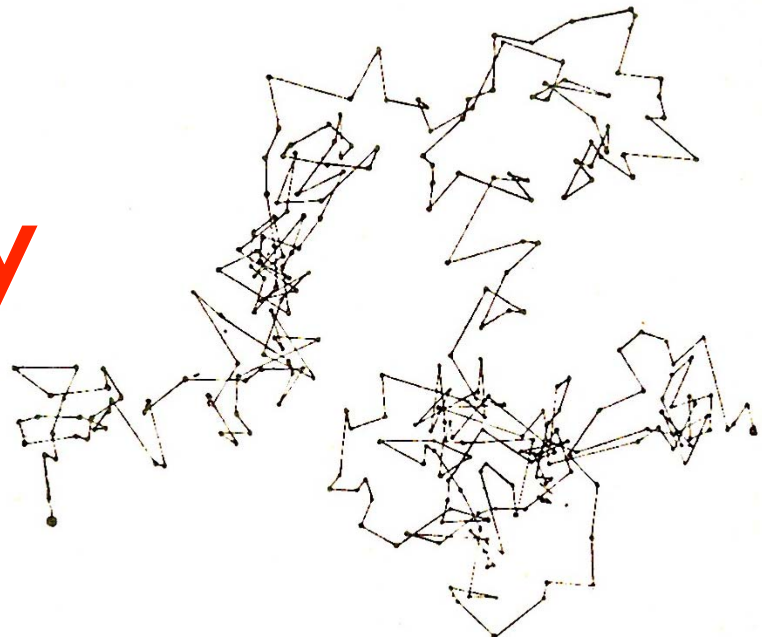


plot every 10 steps

plot every step

Brownian motion and fractal trajectory





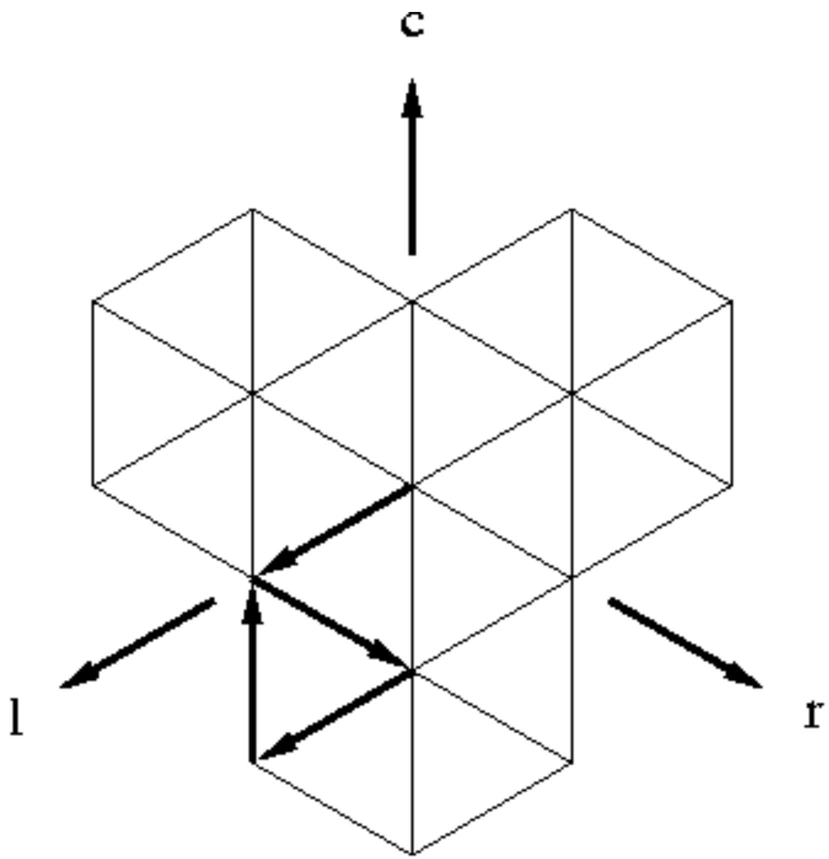
Si on faisait des pointés à des intervalles de temps 100 fois plus rapprochés, chaque segment serait remplacé par un contour polygonal relativement aussi compliqué que le dessin entier, et ainsi de suite. *On voit comment s'évanouit … la notion de trajectoire.*

Jean Perrin

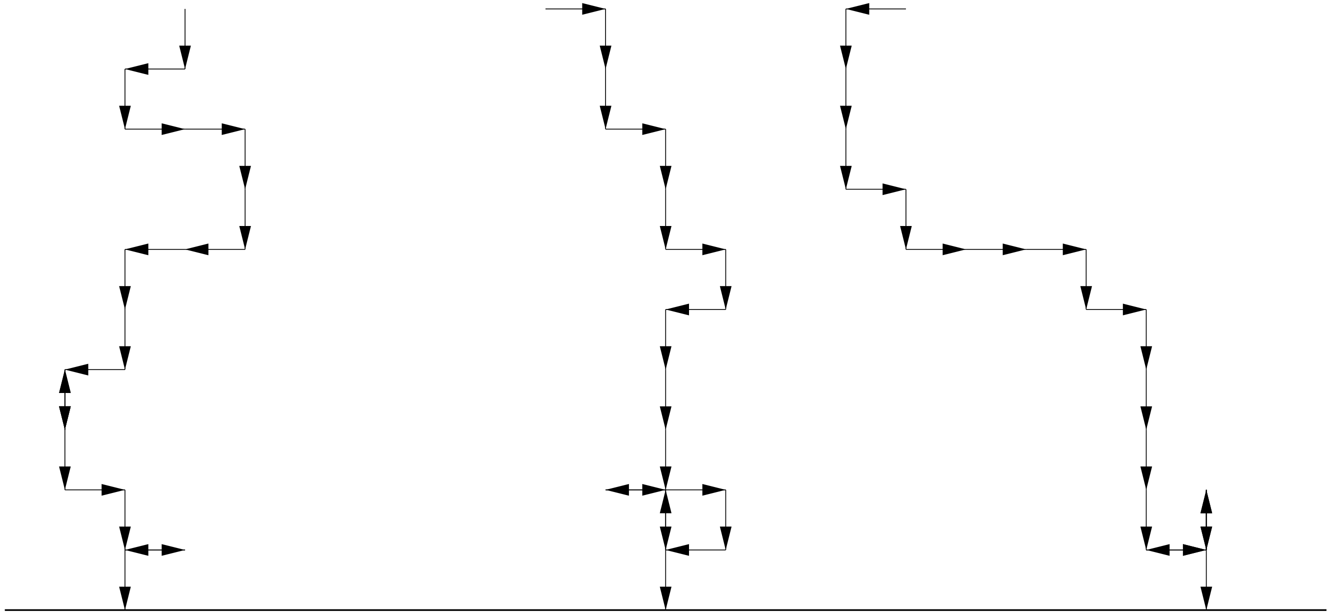
(1912)

Random Walks 2D

on a triangular lattice



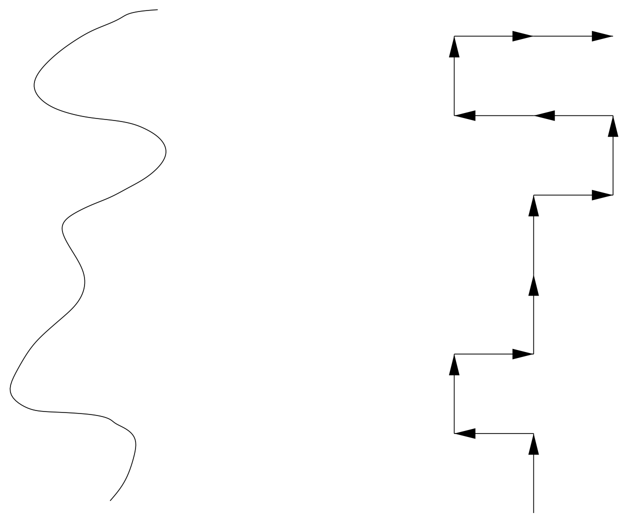
Other Random Walks



Examples of the random path of a raindrop to the ground

The probability of a step down is larger than the probability of a step up; furthermore, this is a *restricted RW*, i.e. limited by boundaries

Self-avoiding Random Walks



(a) (b)

a) Schematic illustration of a linear polymer in a good solvent :
head-tail mean square distance is (in 3D):

$$\langle \Delta R_N^2 \rangle \sim N^{2\nu} \qquad \nu = 0.592$$

b) Simulation with a SAW on a square lattice:
2D model gives $\nu = 3/4$
(independent on details such as monomers and solvent structures)

Other Random Walks

- RW with traps
- persistent RW (a *correlated random walk* in which the walker has probability α of continuing in the same direction as the previous step) => superdiffusive behaviour
- ….

Some programs:

on

$/home/peressi/comp-phys/IV-random-walk/f90

[do: $cp /home/peressi/.../f90/* .]

or on https://moodle2.units.it

rw1d.f90

rw2d.f90

rw2zoom.f90

contour, pl => see following slide

‘pl’: macro for gnuplot for plotting trajectories
(suppose column 1 is ‘time’, 2 is x, 3 is y)
and check self-similarity:

```
set term postscript color
set size square
set out '1.ps'
p [-20:5][-10:15] '1.dat' u 2:3 w l
set out '10.ps'
p [-40:20][-10:50] '10.dat' u 2:3 w l, 'contour' u 1:2 w l
```

Use:
gnuplot$ load ‘pl’

III part:
algorithm for the
Brownian motion
(Langevin treatment)

Other program:

on

$/home/peressi/comp-phys/IV-random-walk/f90

[do: $cp /home/peressi/.../f90/* .]

brown.f90

The numerical approach:
the ingredients

Here: NOT Einstein's, but Langevin's (1906) approach arriving at a Newtonian equation of motion including a *random* force due to the solvent

See: De Grooth BG, Am. J. Phy. 67, 1248 (1999)

Ingredients:

* large Brownian particles - solvent interactions described by: **elastic collisions** between large particle (mass *M*, velocity *V*) and small (solvent) particles (*m, v*);

* **momentum and energy conservation** at each collision

$$MV+mv = MV'+mv'$$

$$MV^2/2+mv^2/2 = MV'^2/2+mv'^2/2$$

The numerical approach:
the equation of motion

After **reasonable assumptions** *(many collisions (i) in a time interval Δt, where V_i are the same..., m<<M..., ...)* =>

arrive at a simple expression for $M\Delta V/\Delta t = M(V'-V)/\Delta t$:

$$Ma = F_s - \gamma V(t)$$

F_s : stochastic force, i.e. the cumulative effect, in the time interval, of many collisions with smaller particles

$-\gamma V(t)$: drag force, opposite to $V(t)$ $(\gamma > 0)$; γ can be expressed (using Stokes' formula for a sphere of radius P) as:

$$\gamma = 6\pi\eta P$$

(both forces have the same origin, in the collisions with the smaller particles)

The numerical approach:
discretization of the equation of motion

$$Ma = F_s - \gamma V(t)$$

Rewritten as: $M\Delta V/\Delta t = \Delta V_s /\Delta t - \gamma\, V(t)$

=> $V_{q+1} = V_q + \Delta V_s - \gamma(\Delta t/M)V_q$

with:

$\Delta V_s = 2mv/M = (\ldots) = 1/M\ v/|v|\ \sqrt{(2\gamma k_B T/n)}$;

At each collision v/|v| is -1 or +1 => after N collisions ???

the result is a **gaussian random variable**

w_q centered in 0, s.d.$=\sqrt{(N/2)}$ => (see also next lectures)

The numerical approach:
discretized equations for positions and velocities

$$V_{q+1} = V_q - (\gamma/M)V_q\Delta t + w_q(\sqrt{(2\gamma k_B T\Delta t)})/M$$

$$X_{q+1} = X_q + V_{q+1}\Delta t$$

- the hearth of our numerical approach
- can be easily implemented for iterative execution

NOTE : we are NOT imposing any specific time dependence behavior: it will come out as an "**experimental**" result of the simulation

The numerical approach:
Input parameters - I

$$V_{q+1} = V_q \,[1 - (\gamma/M)\Delta t] + w_q(\surd(2\gamma k_B T\Delta t))/M$$

- physical parameters of the system: **T** and γ
  (through η and P: $\gamma = 6\pi\eta P$)

The numerical approach:
Input parameters - II

$$V_{q+1} = V_q [1 - (\gamma/M)\Delta t] + w_q(\sqrt{(2\gamma k_B T\Delta t)})/M$$

- time step Δt : cannot be fixed a priori!

Some suggestions from physical and rough numerical considerations

[$(\gamma/M)\Delta t < 1$ to reproduce the situation of $T \approx 0$ (damped motion)

Δt too small: too long numerical simulations necessary…

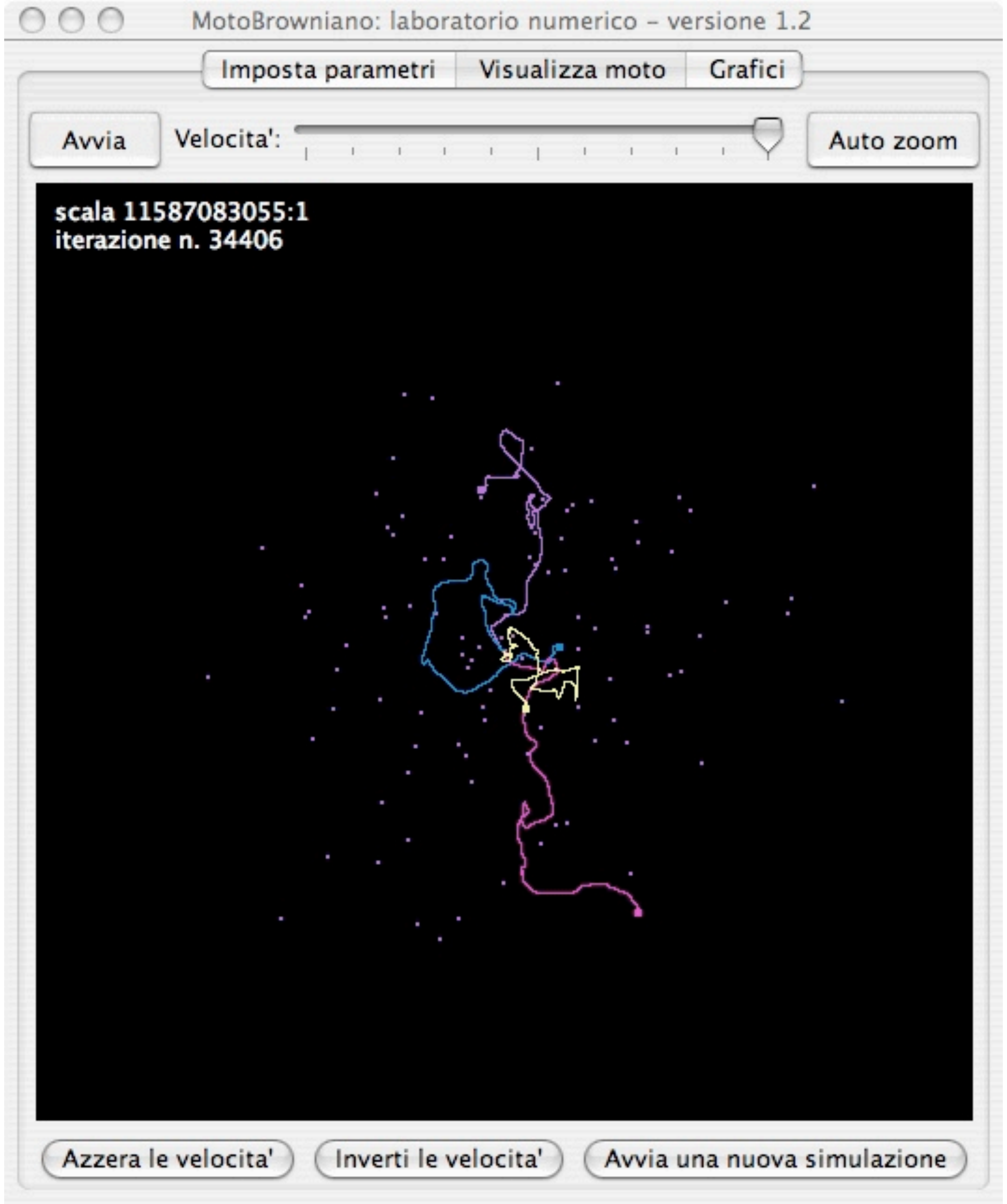
Δt too large: serious numerical uncertainties…]

Our numerical work:

choice of Δt is analogous of an instrument calibration !!!

suggestion: start from small Δt *s.t.* $\gamma\Delta t/M \ll 1$, increase Δt until important changes in the diffusion coefficient are observed.

Running the code…



$k_BT=4\cdot10^{-21}J$, $M=1.4\cdot10^{-10}kg$,

$\gamma\approx8\cdot10^{-7}Ns/m$

Snapshot of a numerical simulation of the Brownian motion in 2D of many large particles. The trajectories of four of them are shown

Discovering the results

We can prove by numerical experiments:

(i) the linear behavior of the mean square displacement $<R^2>$ with time:

$$<R^2> = 2dD\ t$$

(i) the validity of the Einstein relation between the slope of this line and the solvent parameters (temperature and drag coefficient):

$$<R^2> = (2d\ k_B T\ /\ \gamma)\ t$$

IV part:

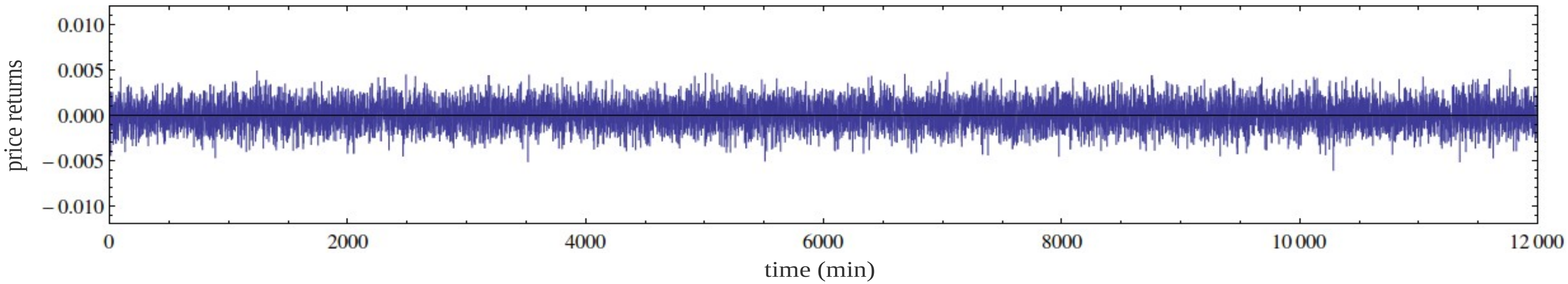
Brownian motion in finance

-

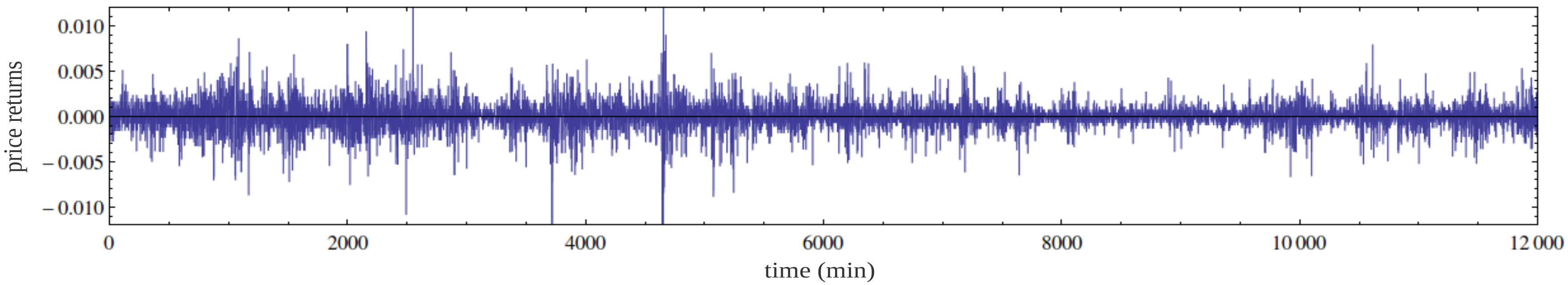
mathematical formulation

Brownian motion in finance

Simulated Returns (Geometric Brownian Motion)



Real Returns (Financial Time-Series)



Cont, *Empirical properties of asset returns, stylized facts and statistical issues*, 2001

Random Walk in Finance

- **Geometric Brownian motion:** μ: drift; σ: volatility; ε: random variable following normal distribution with unit variance

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

- **Let the 2nd term be 0,**

$$S(t) = S_0 \exp(\mu t)$$

- **Let the 1st term be 0, then for $U = \ln S$ ($dU = dS/S$)**

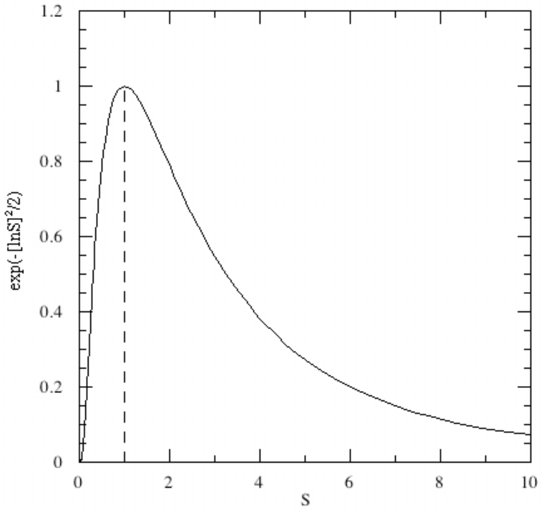
$$dU = \sigma \varepsilon \sqrt{dt}$$

$$U(t) - U(0) = \sigma \sqrt{\Delta t} \sum_{i=1}^{N} \varepsilon_i$$

- **Central-limit theorem states that $\Sigma_i \varepsilon_i$ is normal distribution with variance N; let $t = N\Delta t$**

$$U(t) - U(0) = \sigma \sqrt{t} \varepsilon$$

- **Log-normal distribution**

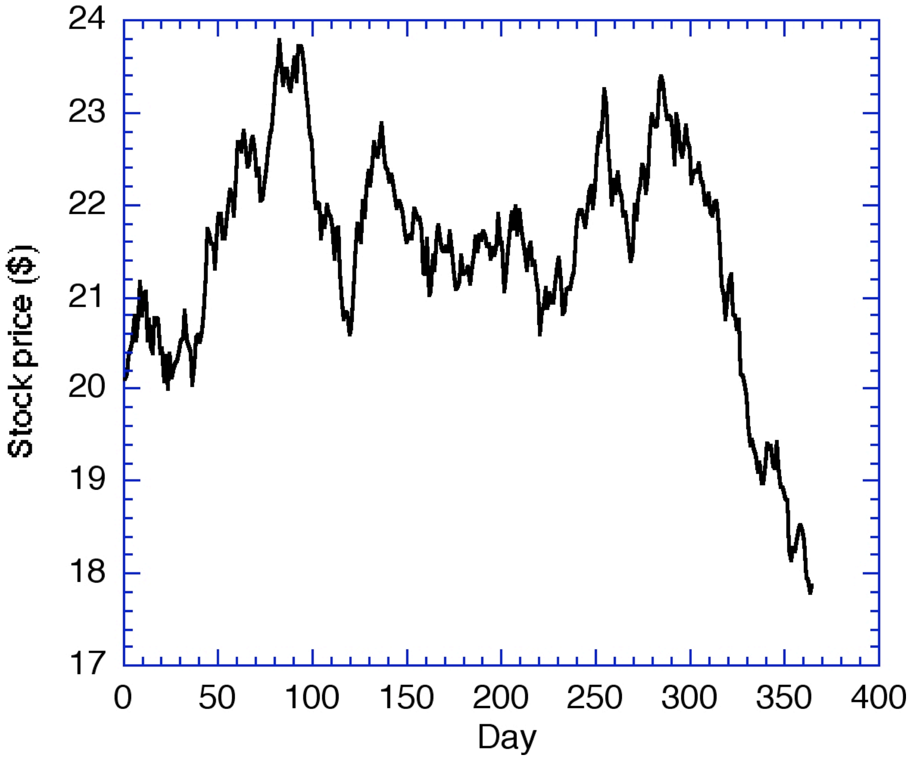


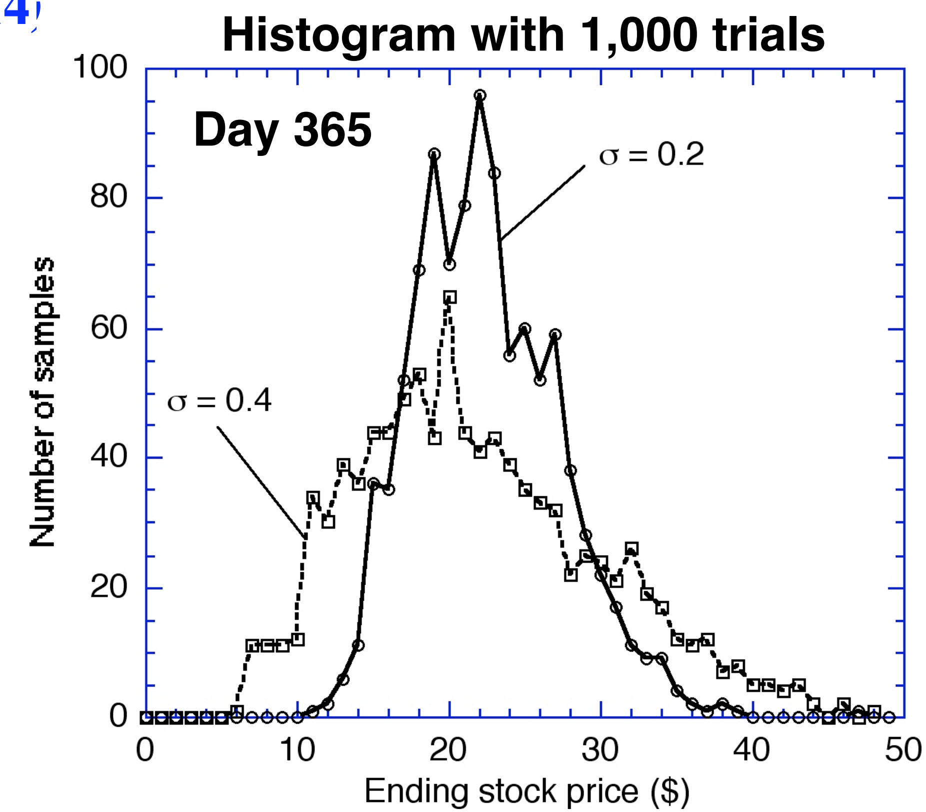
credits: Nakano

MC Simulation of Stock Price

$$\frac{dS}{S} = \mu dt + \sigma\sqrt{dt}\xi$$

$\mu = 0.14$





Stochastic Model of Stock Prices

Basis of Black-Scholes analysis of option prices

$$dS = \mu S dt + \sigma S \varepsilon \sqrt{dt}$$

The Bank of Sweden Prize in Economic Sciences in Memory of Alfred Nobel 1997

"for a new method to determine the value of derivatives"

Robert C. Merton

1/2 of the prize

USA

Myron S. Scholes

1/2 of the prize

USA

Computational stock portfolio trading