993SM - Laboratory of Computational Physics week IV March 20, 2023

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Using random numbers to simulate random processes:

1) radioactive decay
2) diffusion and random walks

1) Radioactive decay

$N(t)$ Atoms present at time t

λ Probability for each atom to decay in Δt

$\Delta N(t)$ Atoms which decay between t and $t + \Delta t$

$$\Delta N(t) = -\lambda N(t) \Delta t$$

we use the probability λ of decay of each atom
to simulate the behavior of the number of atoms left;
we should be able to obtain (on average):

$$N(t) = N(t = 0) e^{-\lambda t}$$

Radioactive decay: numerical simulation

A scheme for the simulation

1. Assign a value to the decay constant $\lambda \leq 1$ (the probability for each nucleus to decay in a given interval of time Δt)
   λ establishes the time scale; one iteration in the "do loop" corresponds to one time step Δt

2. Start with **Nleft = Nstart**= total number of nuclei at time $t = 0$

3. Basic algorithm: **for each nucleus** left (not yet decayed):
   - Generates a random number $0 \leq x \leq 1$
   - if $x \leq \lambda$, the nucleus decays and **Nleft = Nleft - 1**, otherwise it remains and **Nleft** is unchanged.

4. Repeat for each nucleus

5. Repeat the cycle for the next time step

Note: unbounded loop

```
DO                                    ! loop on time
  DO  i = 1, nleft                    ! loop on all the nuclei left
    call random_number(r)
    IF (r <= lambda) THEN             ! BASIC  ALGORITHM
      nleft = nleft - 1               !  update the nuclei left (*)
    ENDIF
  END DO
WRITE (unit=7,fmt=*) t , nleft
  if (nleft == 0) exit
  t = t + 1
END DO
```

Note: "exit" ≠ "cycle"

(*) Notice that the upper bound of the inner loop (nleft) is changed within the execution of the loop; but with most compilers, in the execution the **loop** goes on up to the **initial value of the upper bound** (nleft); this ensures that the implementation of the algorithm is correct. The program checkloop.f90 is a test for the behavior of the loop. Look also at decay_checkloop.f90. If nleft would be changed (decreased) during the execution, the effect would be an overestimate of the decay rate. CHECK with your compiler!

Programs:

decay.f90
decay_checkloop.f90

checkloop.f90

Details on Fortran: unbounded loops

```
[name:] DO
          exit [name]
```

or

```
[name:] DO
          END DO [name]
```

(name is useful in case of nested loops for explicitly indicating which loop we exit from)

Alternative form: "do while" loop

Always set a condition to exit from a loop! E.g.:

```
DO
 if (condition)exit
END DO
```

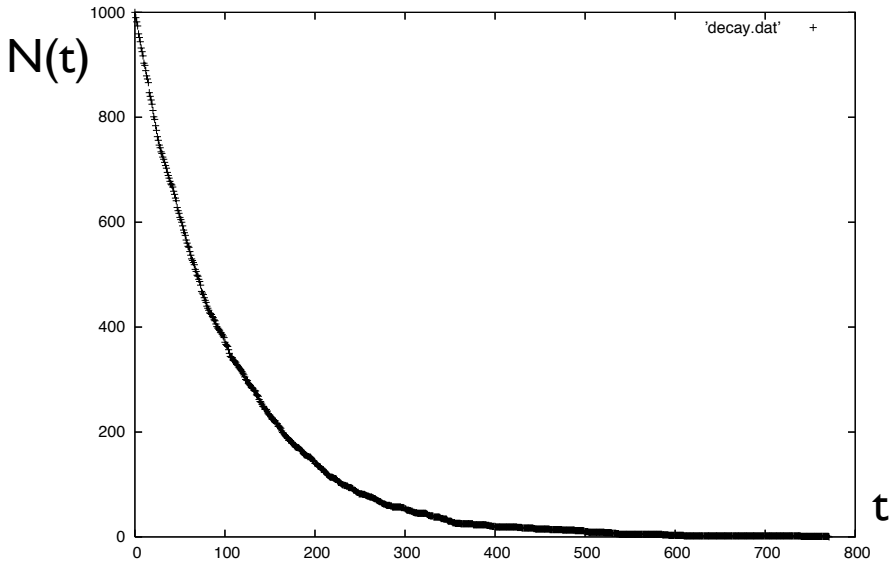
or:

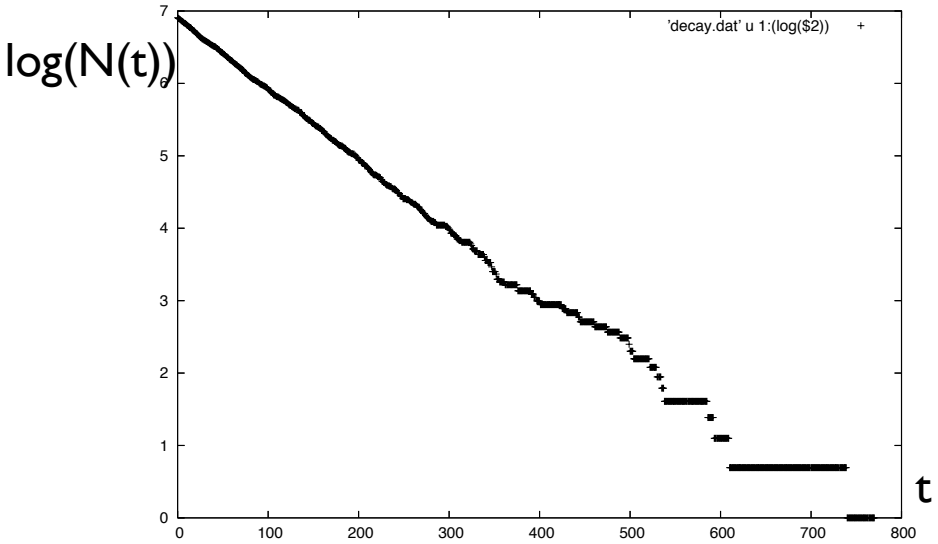
```
DO WHILE (.not. condition)
 ...
END DO
```

NOTE: first is better ("if () ..exit" can be placed everywhere in the loop,
whereas DO WHILE must execute the loop up to the end)

- Additional note:
Difference between EXIT and CYCLE

Radioactive decay:
results of numerical simulation





results of decay simulation (N vs t) with N=1000

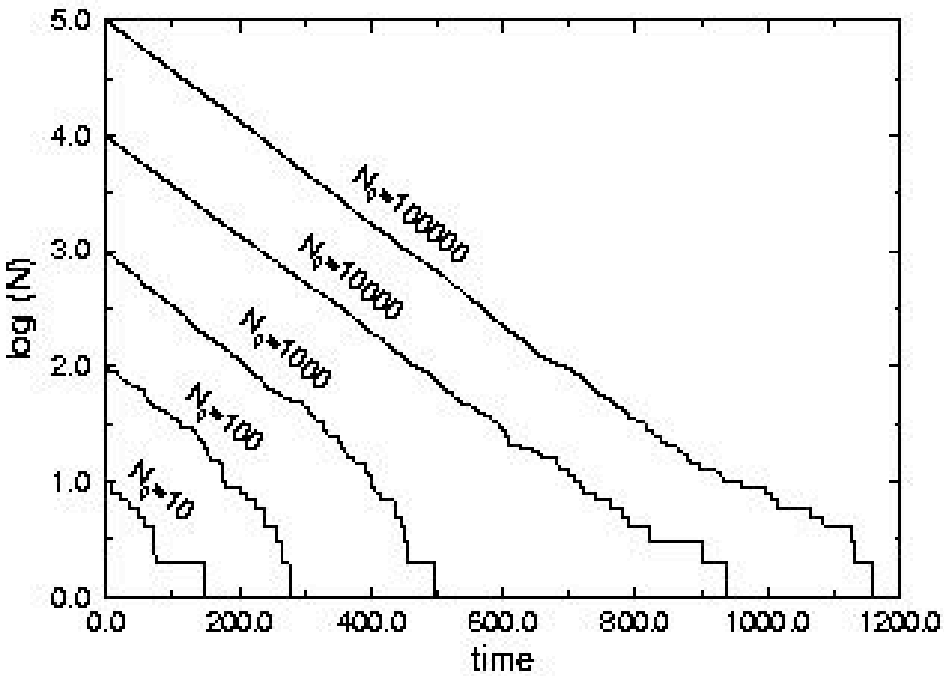
$N(t) \sim N_0 \exp(- a\ t)$

semilog plot (log(N) vs t)

=> $\log(N(t)) = \log N_0 - a\ t$

=> slope is -a

Radioactive decay:
results of numerical simulation



Semilog plots of the results of simulations for the same decay rate and different initial number of atoms:
almost a straight line, but with important deviations (stochastic) for small N

Stochastic simulations give reliable results when obtained:

- on average and for large numbers
- fine discretisation of time evolution

(in the exercise #1: change λ; compare the value obtained from the simulation with the one inserted; does the "quality" of the results change with λ?)

2) Diffusion and Random Walks

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

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

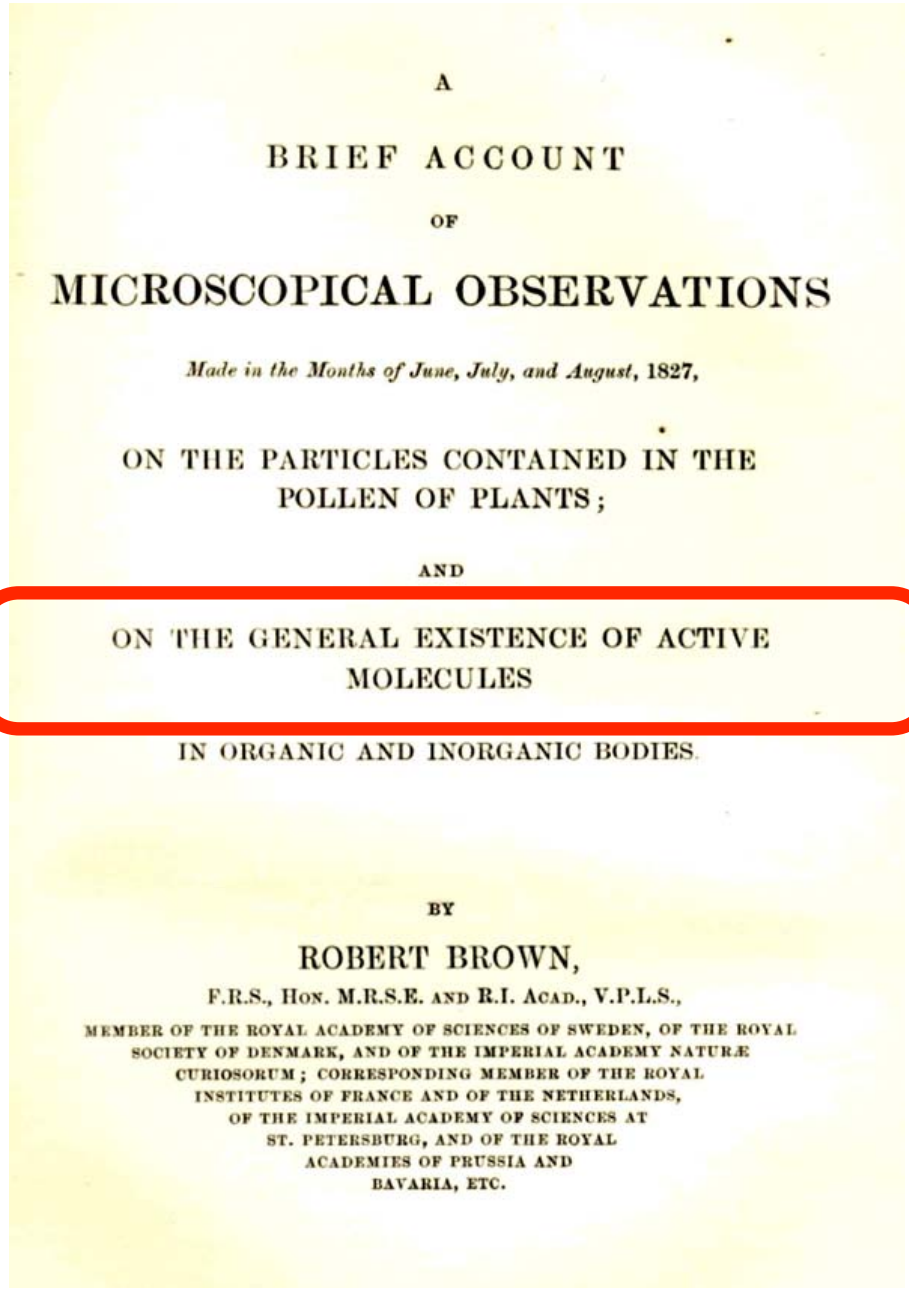
Random motion

- 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
- 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
- What is the origin of the brownian motion?
  In 1870, Loschmidt suggested that it is caused by thermal agitation

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.

Brownian motion
-open questions-

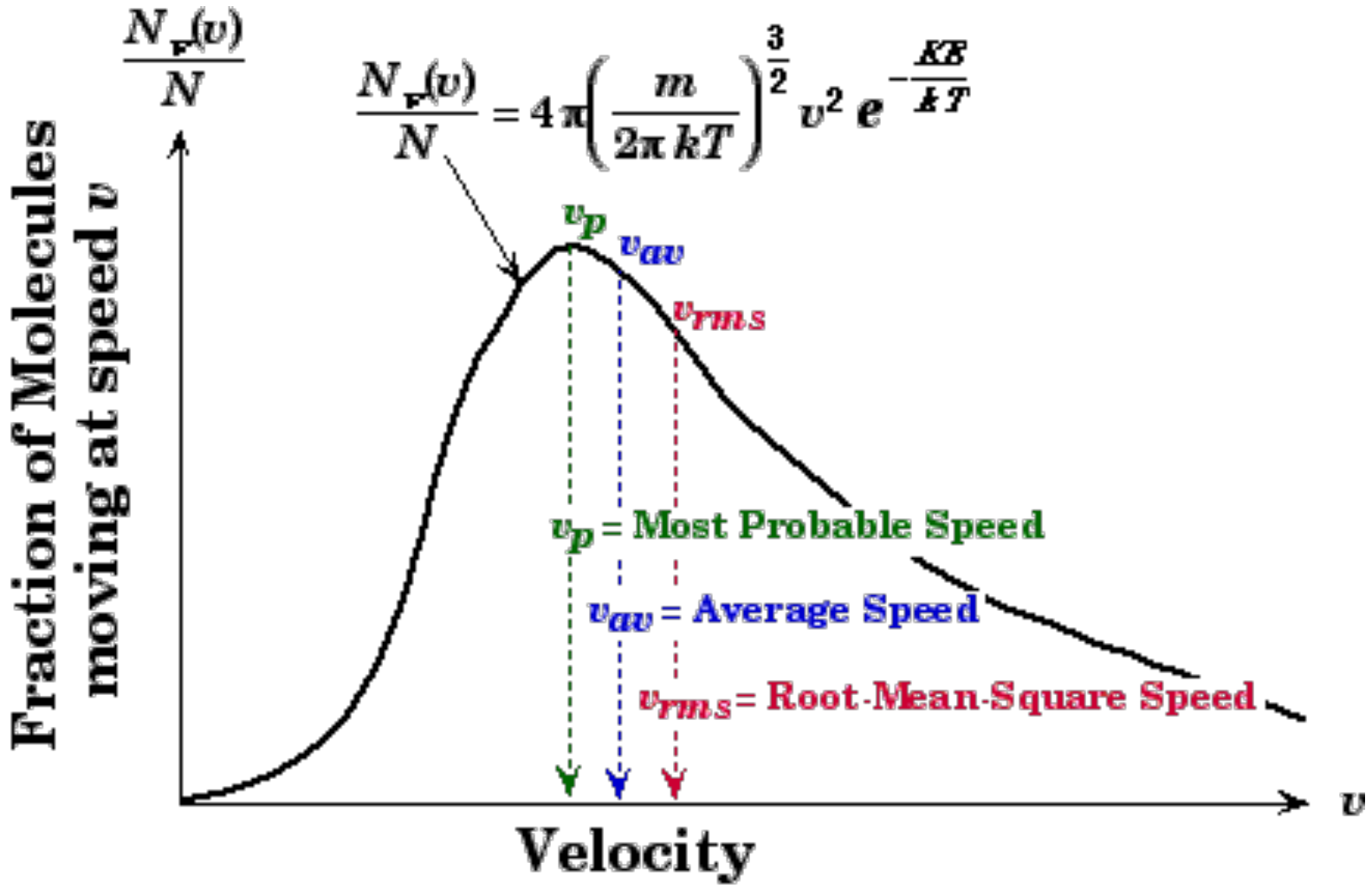
Observations of "active molecules" made by Brown in 1827 led the physics community to **search for the proof that molecules indeed exist.**

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**

(1860) (1872)

Maxwell-Boltzmann distribution of velocity



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

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?**

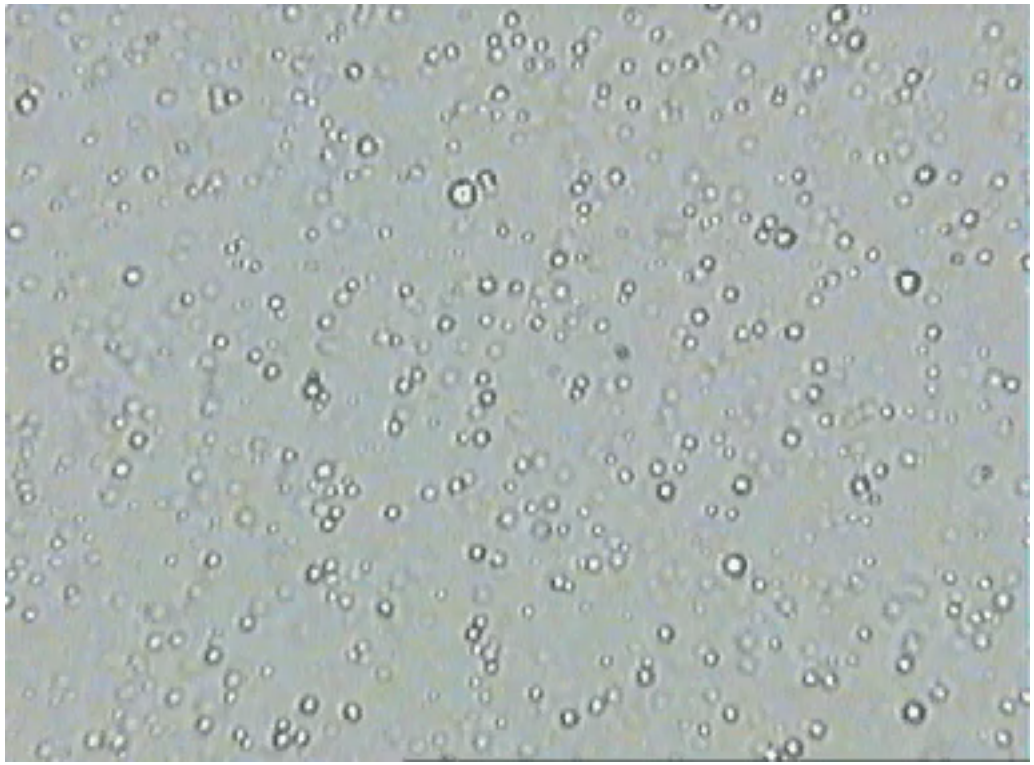
Brownian motion
-Einstein's 1905 paper-

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

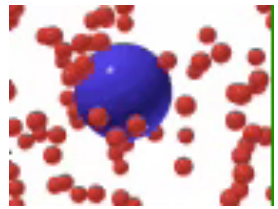
Einstein predicted that **microscopic particles** dispersed in water **undergo random motion as a result of collisions** (stochastic forces) **with water molecules much smaller and light** (not visible on the chosen observation scale).

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

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

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

$\langle \Delta r^2 \rangle$ (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;
Once D is known, since η, T are measurable => from (**) we obtain P

Diffusion

Derivation of the diffusion coefficient: $D = \mu k_B T$

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

μ = mobility $= \dfrac{\text{velocity}}{\text{force}} = \dfrac{1}{6\pi\eta P}$

η = viscosity of fluid

P = particle radius

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

From Thermodynamics:

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

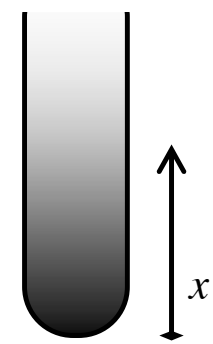
$\phi = WNx$ = PE per mole

N_A = Avogadro's number

R = universal gas constant } $k_B = \frac{R}{N_A}$

T = absolute temperature

RT[=]energy/mole



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

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

Compare: exponentials must be equal! ⇨ $D = \mu k_B T$ (*)

Brownian motion and diffusion

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

Part II – Statistical Analysis of B.M.

Here: 1D (d=1)

p=concentration

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

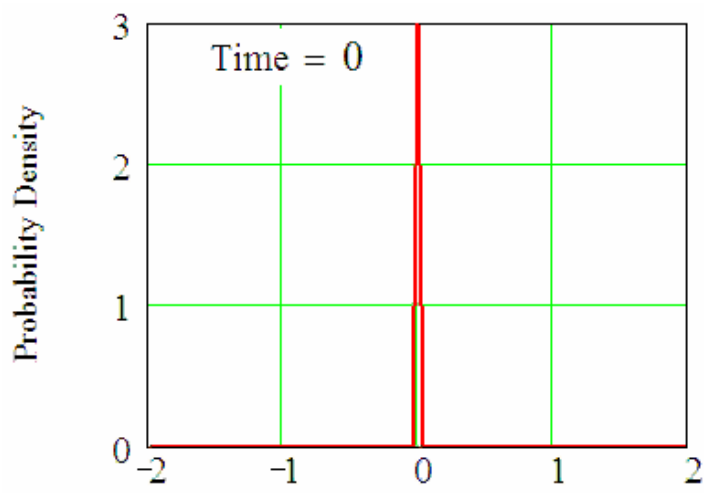
Initial Condition: $p(x,0) = \delta(x)$

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

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

gaussian with $\sigma^2 = 2Dt$

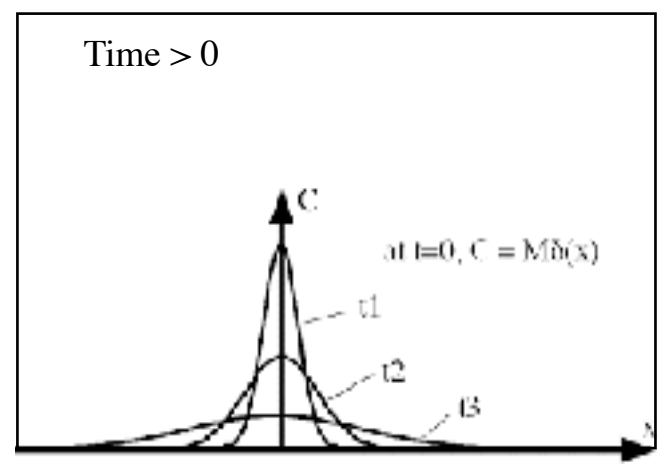
$$p(x) = \frac{1}{\sigma}\frac{1}{\sqrt{2\pi}}\, e^{-x^2/(2\sigma^2)}$$



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

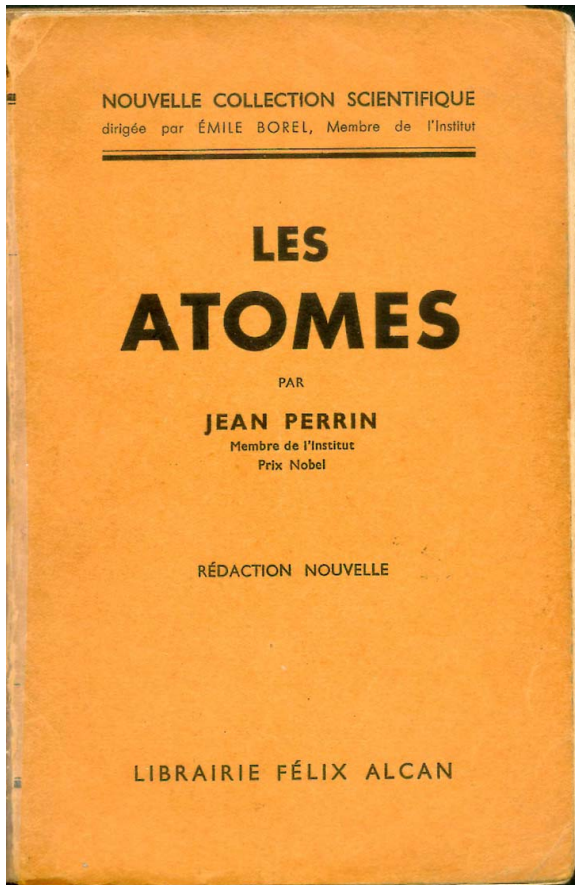
$$\bar{x}(t) = \int_{-\infty}^{\infty} x p(x,t)\,dx = 0$$

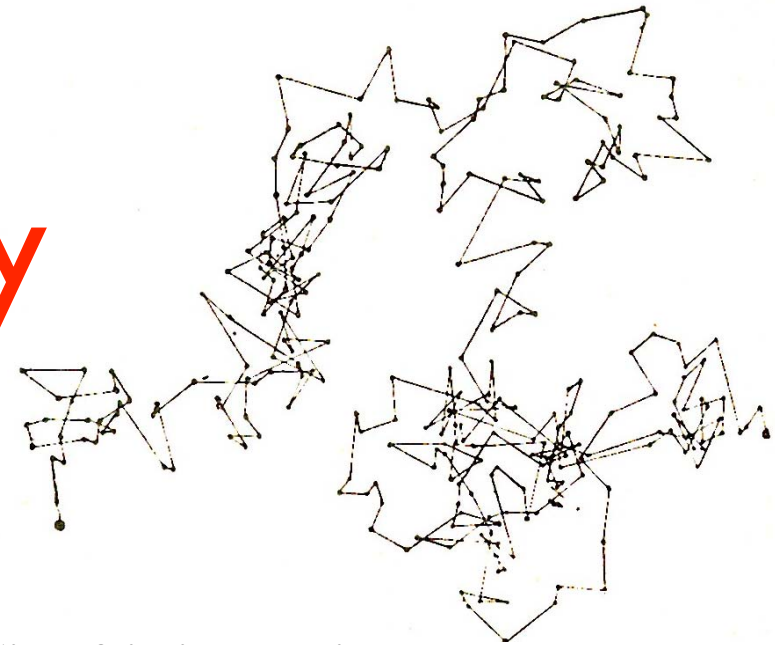
$$\overline{x^2}(t) = \int_{-\infty}^{\infty} x^2 p(x,t)\,dx = 2Dt \qquad (**)$$



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

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)

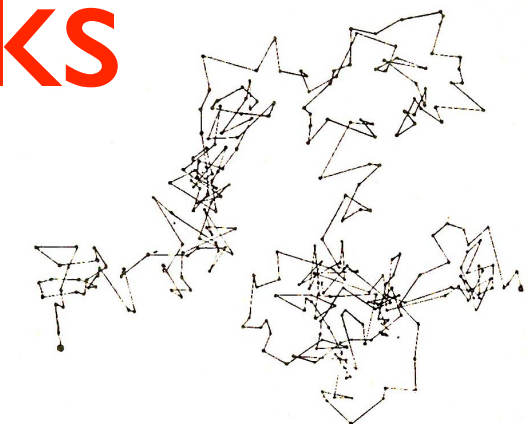
Random motion in nature

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

Random walks

A very simplified **model**
for the brownian motion
and many phenomena

Random Walks



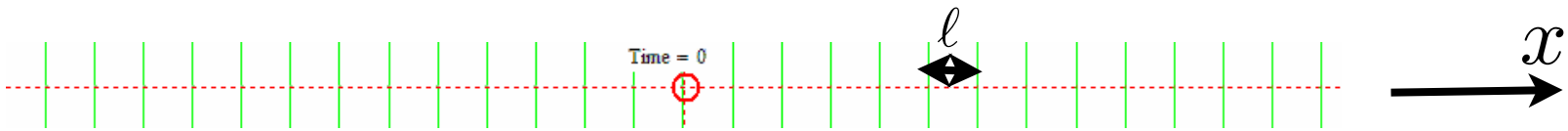
- **traditional** RW ➡ brownian motion
- **modified** (interacting) RW ➡ the motion of the walker depends on his previous trajectory

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, if $p_{\leftarrow} \neq p_{\rightarrow}$:

$$\langle x_N \rangle = n_{\leftarrow}(-\ell) + n_{\rightarrow}(+\ell) \quad \text{with} \quad n_{\leftarrow} = Np_{\leftarrow} \text{ and } n_{\rightarrow} = Np_{\rightarrow}$$

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

therefore:

$$\langle \Delta x_N^2 \rangle = \langle x_N^2 \rangle - \langle x_N \rangle^2 = 4p_{\rightarrow}p_{\leftarrow}N\ell^2$$

We expect this behavior for averages over many walkers

RW 1D

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

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

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

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 $P_N(x)$:

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

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

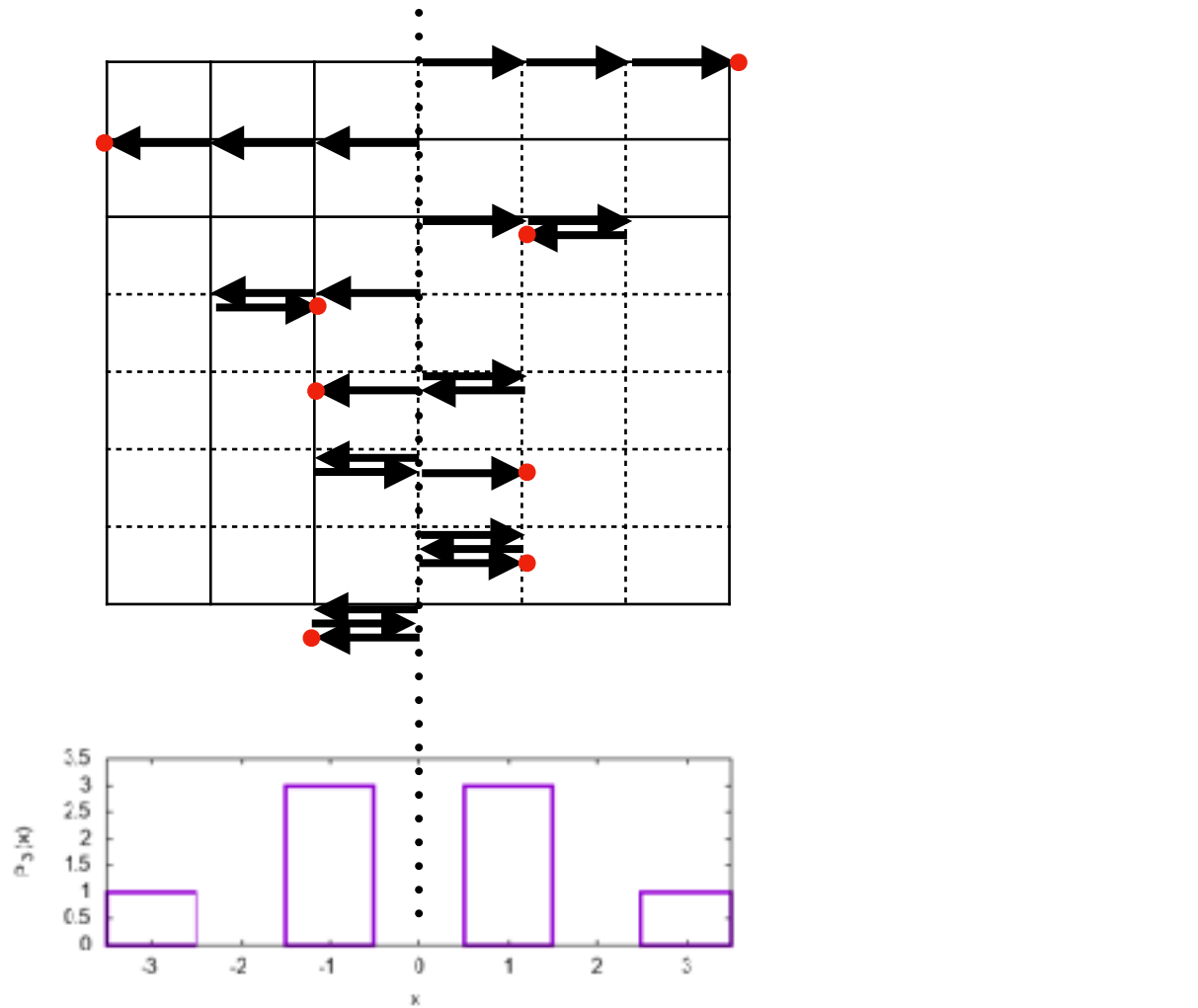
Let's make an example
of analytical calculation of $P_N(x)$
(N=3 is enough!)

...

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

RW 1D

N = 3 => 8 possible different walks



$$\Rightarrow P_3(0) = P_3(\pm 2) = 0; \quad P_3(\pm 1) = 3,\ P_3(\pm 3) = 1$$

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 (a part from the normalization).
Why?
Let's describe the RW problem with a space/time differential equation...

RW 1D: Diffusion - continuum limit

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

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

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

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

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

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

$\frac{\ell^2}{2\tau} \to D$

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: 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)

```
ix = 0 ! initial position of each walker
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  ! now ix is the updated position of the individual walker
end do
```

Now ix is the final position of the walker

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 walker
  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  ! now ix is the updated position of the individual walker
   end do

    x_N = x_N + ix
    x2_N = x2_N + ix**2

end do
```

Let's sum over many walkers
(note that x_N and x2_N must not be not reset to zero!)
This accounts for the final positions only after N steps

RW 1D: simulation

The basic algorithm:

ix = position of the walker

x_N, x2_N = cumulative quantities

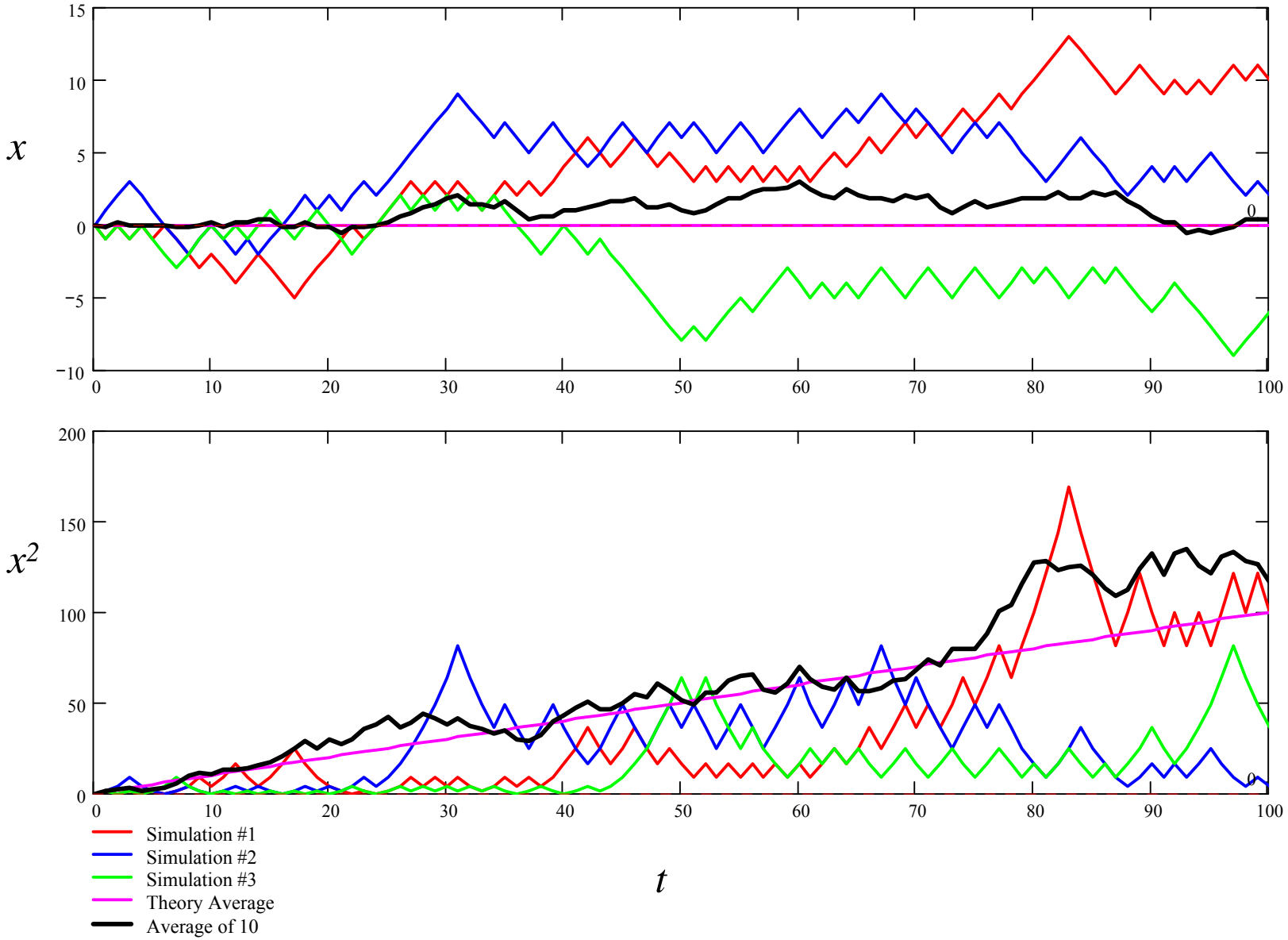
rnd(N) = sequence of N random numbers

(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
```

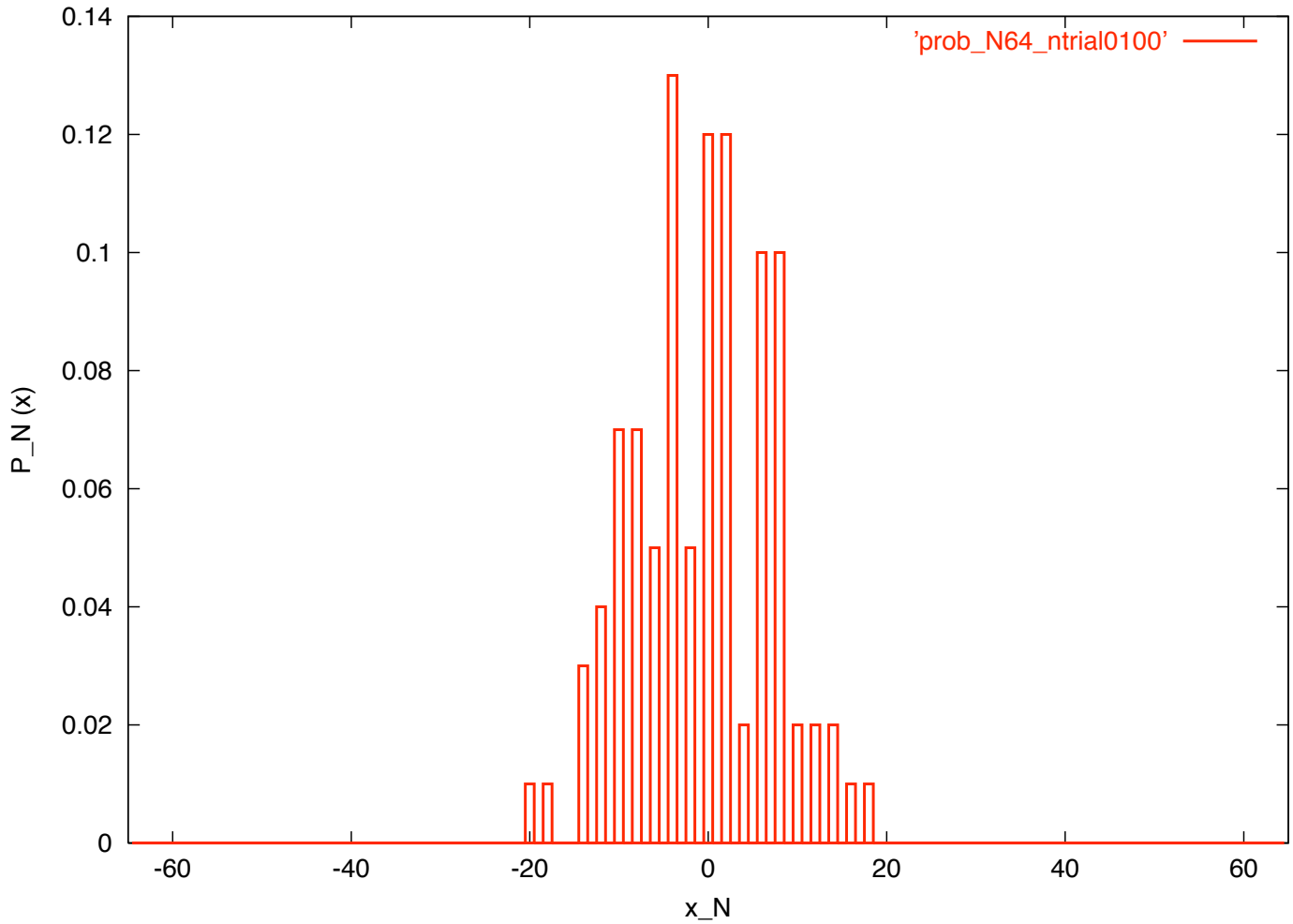
But we can monitor what happens for each intermediate step by using arrays x_N() and x2_N() and including the calculation inside the loop on the steps

RW 1D: simulation

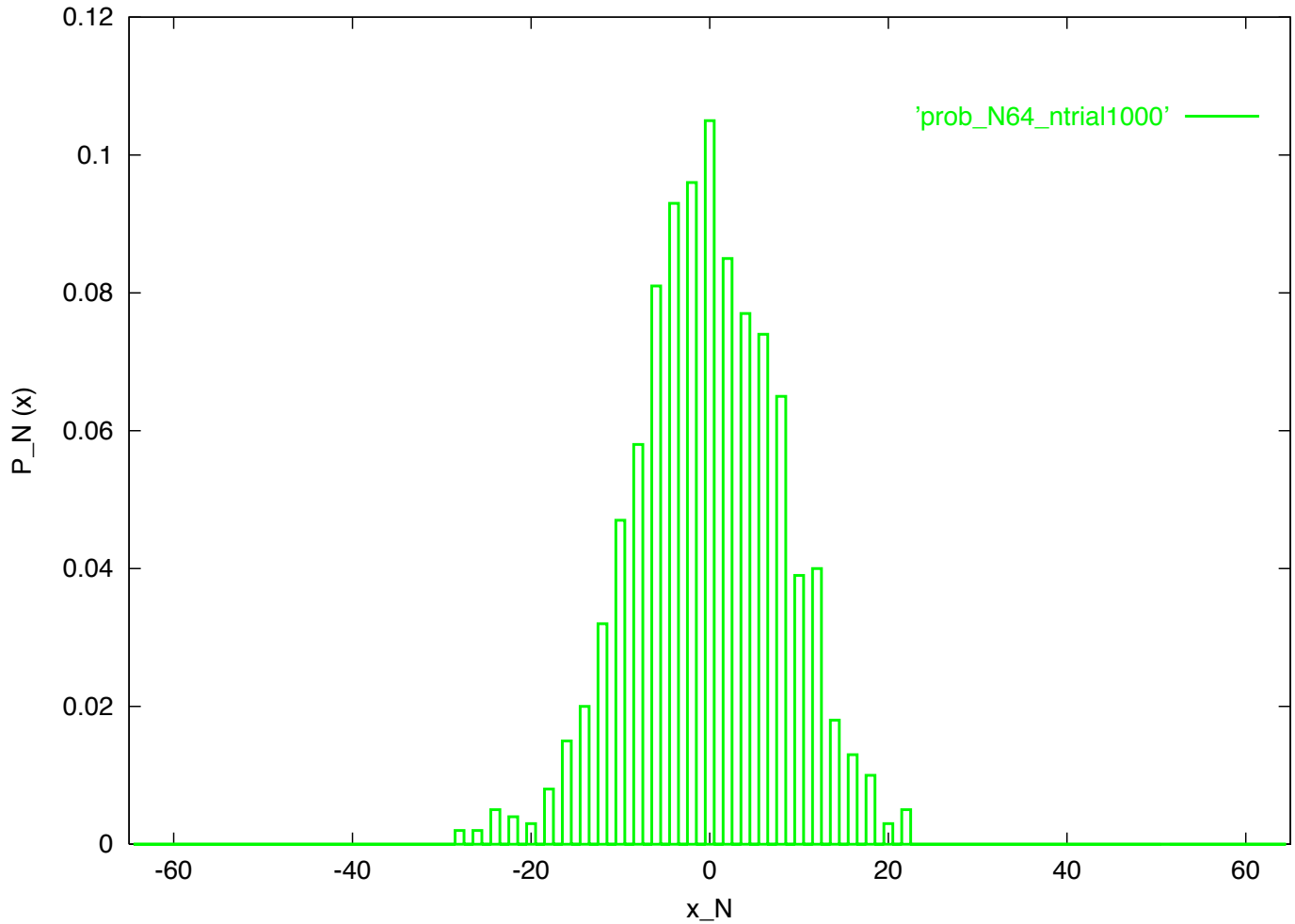


10

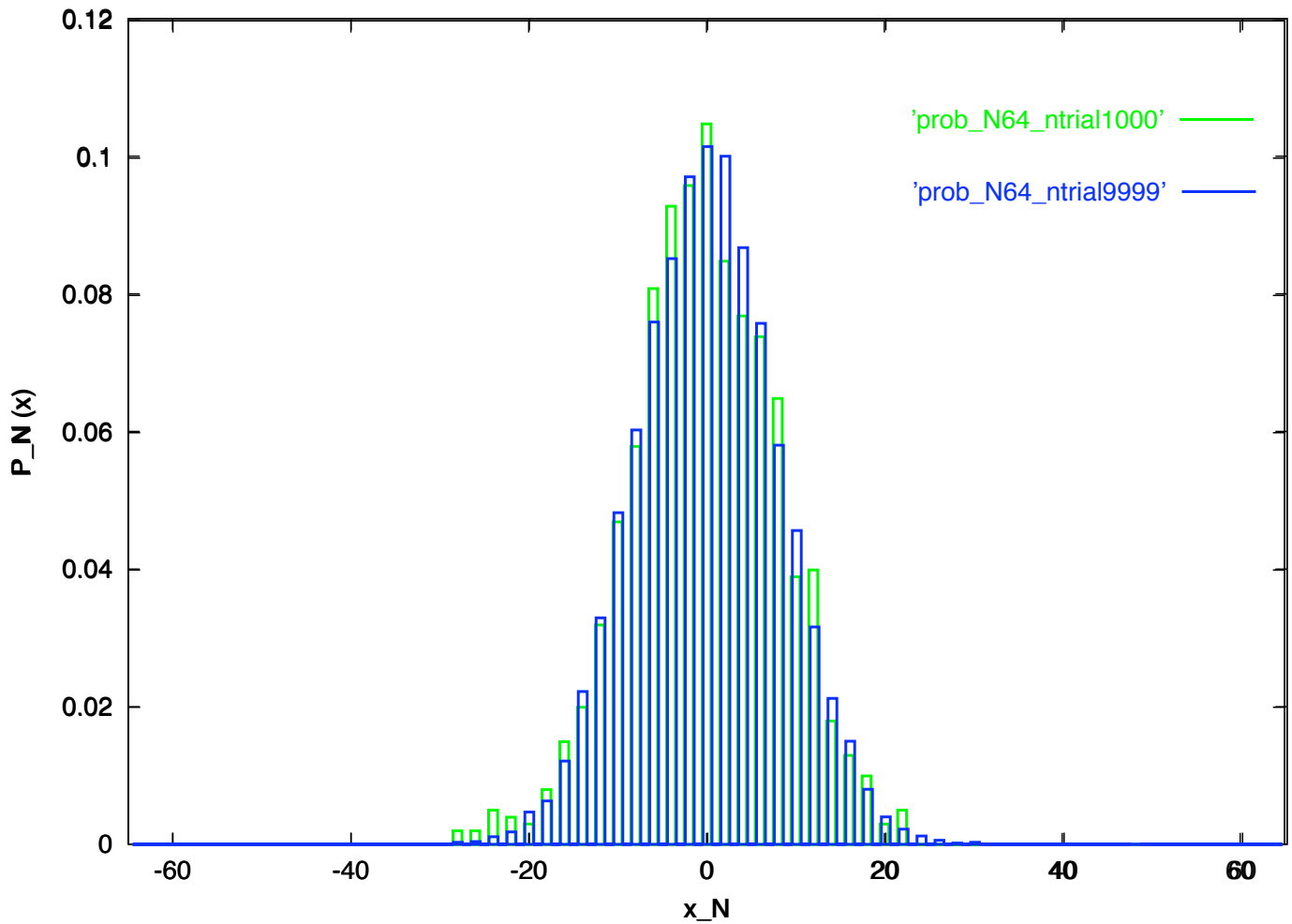
RW 1D: simulation



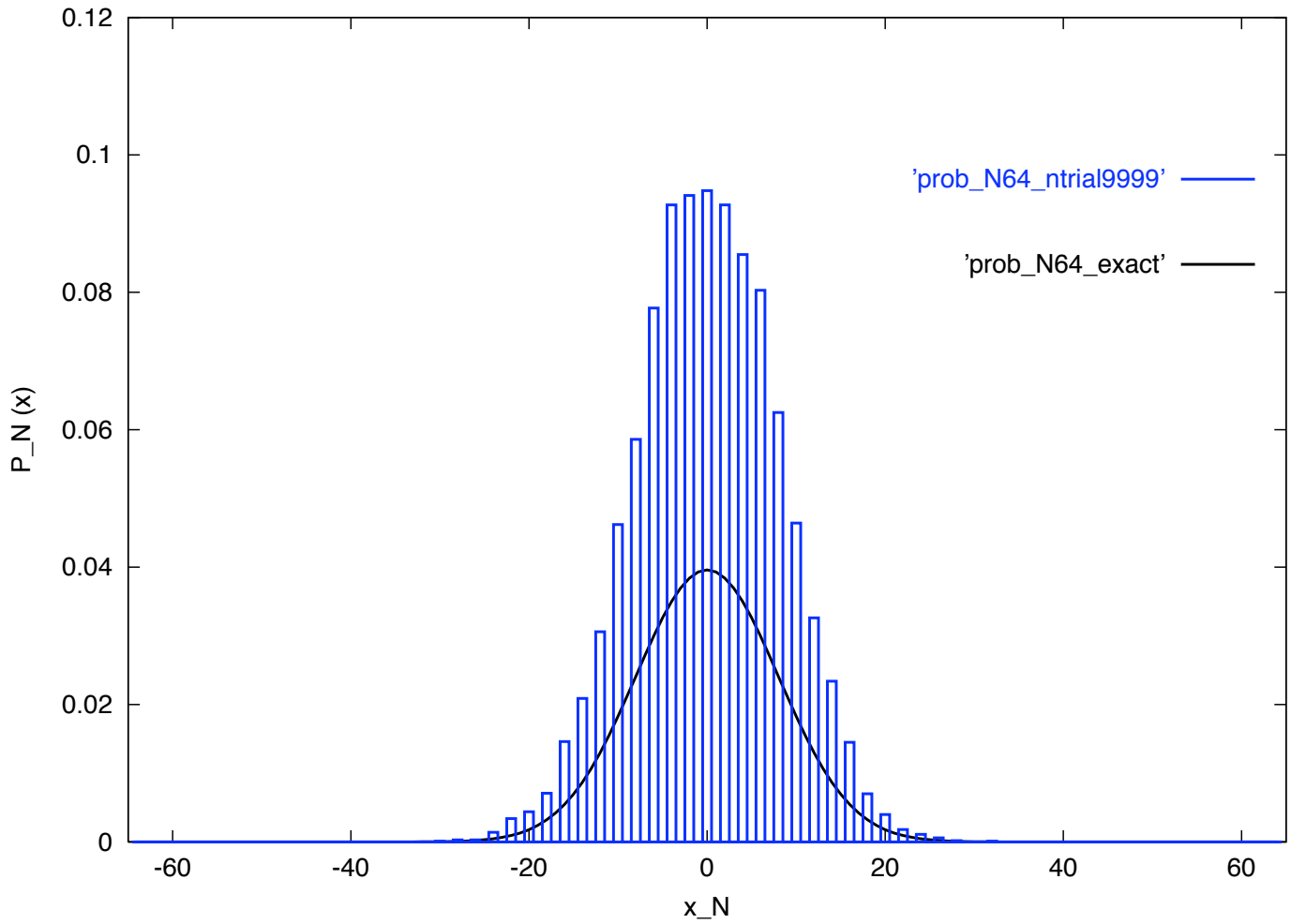
RW 1D: simulation



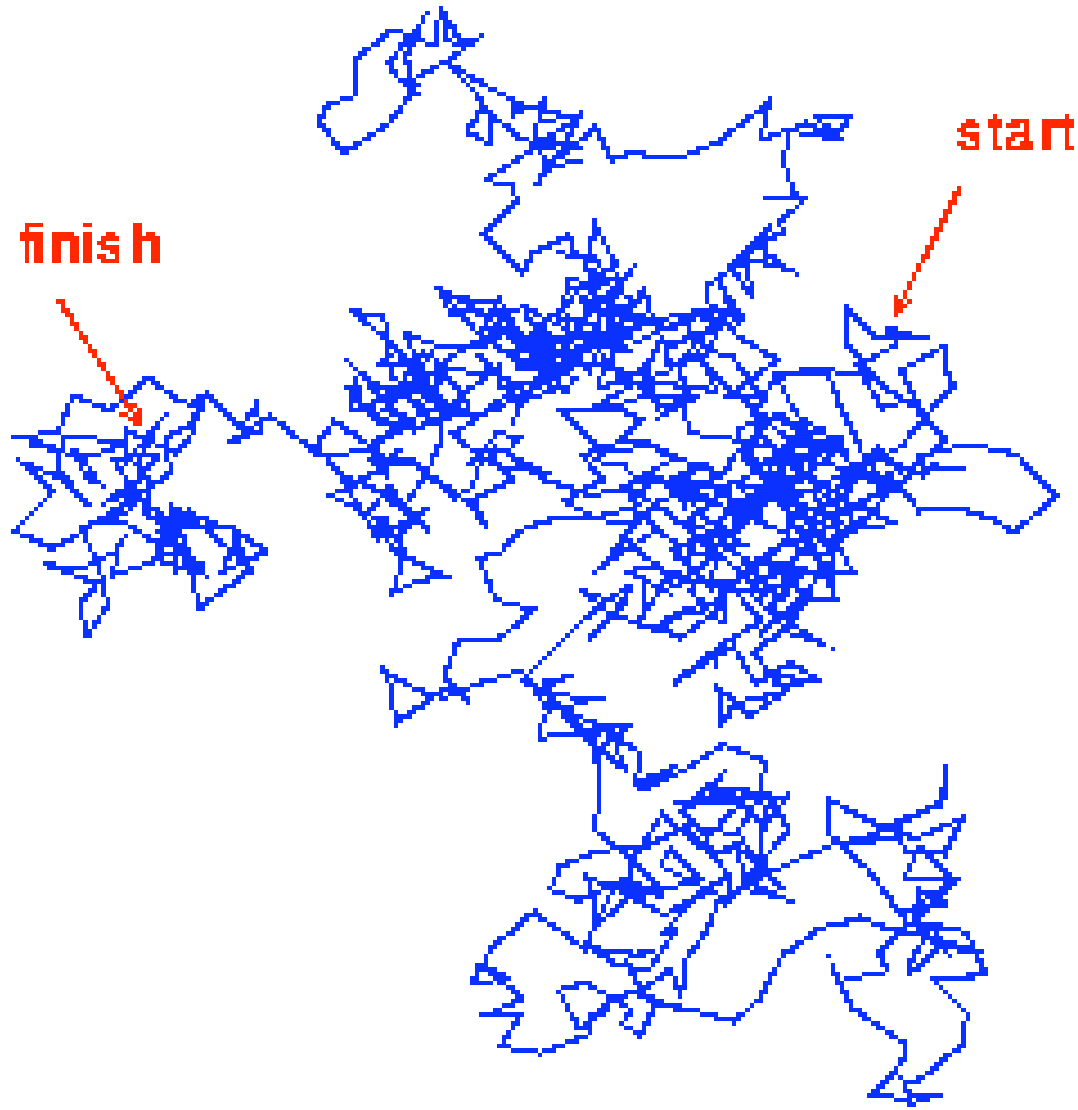
RW 1D: simulation



RW 1D: simulation

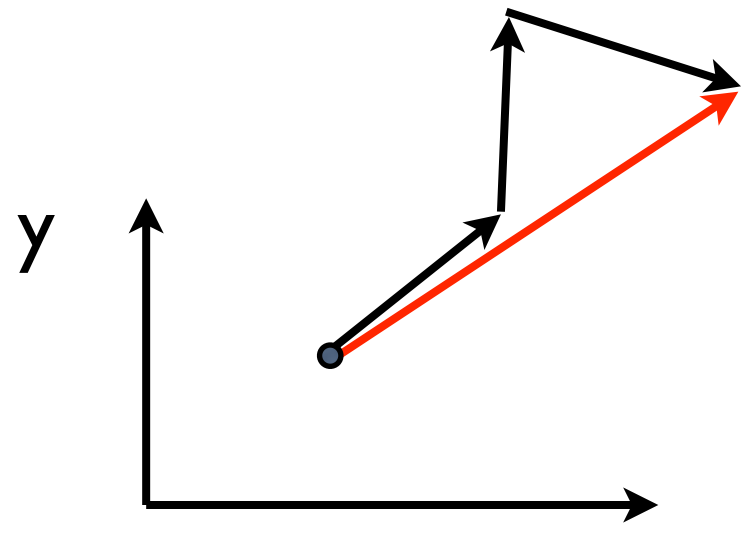


Random Walks 2D



In the continuum space, or discretised on a lattice…

Random Walks 2D

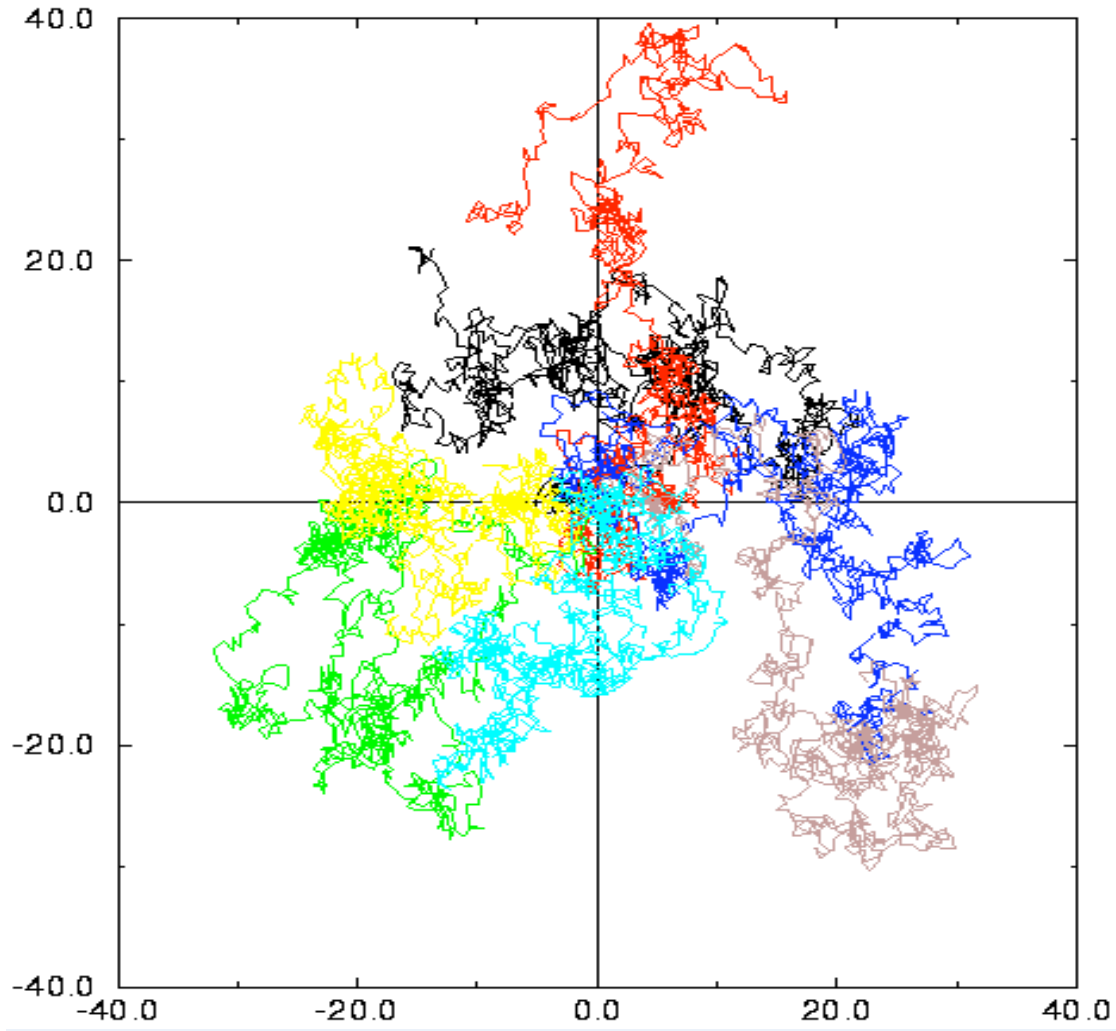


$$\langle \Delta R_N^2 \rangle = \langle (\Delta x_1 + ... + \Delta x_N)^2 + (\Delta y_1 + ... + \Delta y_N)^2 \rangle = ... = N \langle \Delta x_i^2 + \Delta y_i^2 \rangle = N \ell^2$$

$$\langle \Delta R_N^2 \rangle \propto N$$

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

Random Walks 2D



Theory predicts that $\langle \Delta R_N^2 \rangle \propto N$, 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 Δx, Δy in the range $[-1, 1]$(but not $\Delta x = 0, \Delta y = 0$). Normalize Δx, Δy 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 Δx, Δy in the range $\left[-\sqrt{3/2}, \sqrt{3/2}\right]$

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

Indicating with x and y the individual displacements,

$$p(x) = \frac{1}{2\sqrt{3/2}} \quad \text{for} \quad |x| < \sqrt{3/2} \text{ or } 0 \text{ otherwise; the same for } p(y)$$

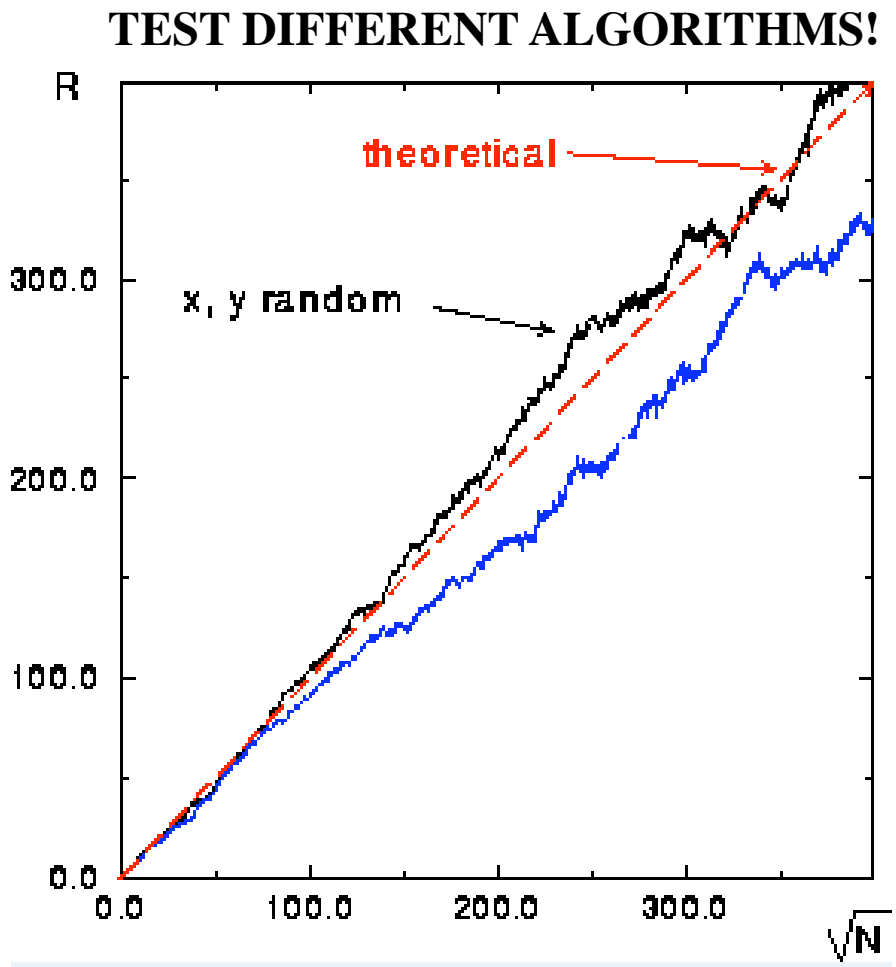
the average step size is:

$$\langle x^2 + y^2 \rangle = \int_{-\sqrt{3/2}}^{\sqrt{3/2}} \int_{-\sqrt{3/2}}^{\sqrt{3/2}} (x^2 + y^2)\ p(x)p(y)\ dx\ dy = \ldots = 1$$

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

(the code rw2d-with-averages-3methods.f90 checks this)

Random Walks 2D



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

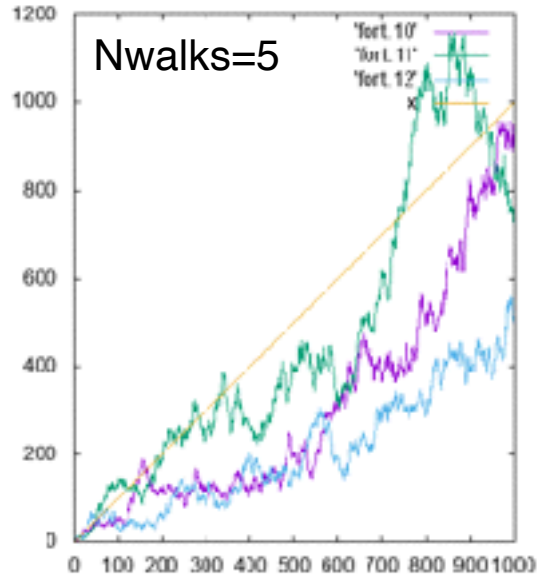
Random Walks 2D

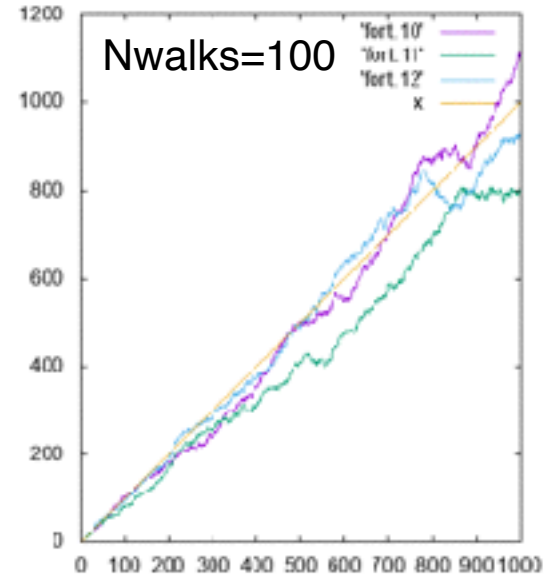
<ΔR^2> vs Nsteps

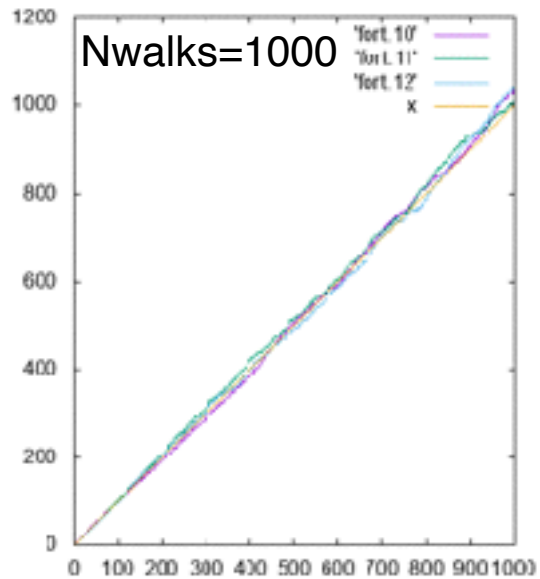
Test algorithm
n. 1 (fort.10)
n. 3 (fort.11)
n. 5 (fort.12)

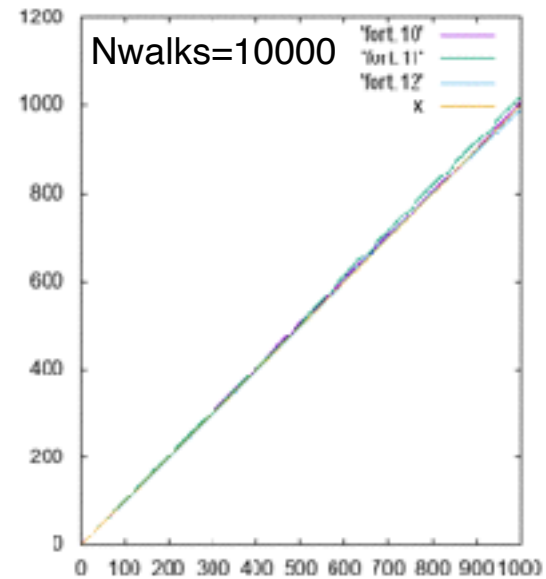
with
Nsteps = 1000

averaged over
A different number of Nwalks









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
```

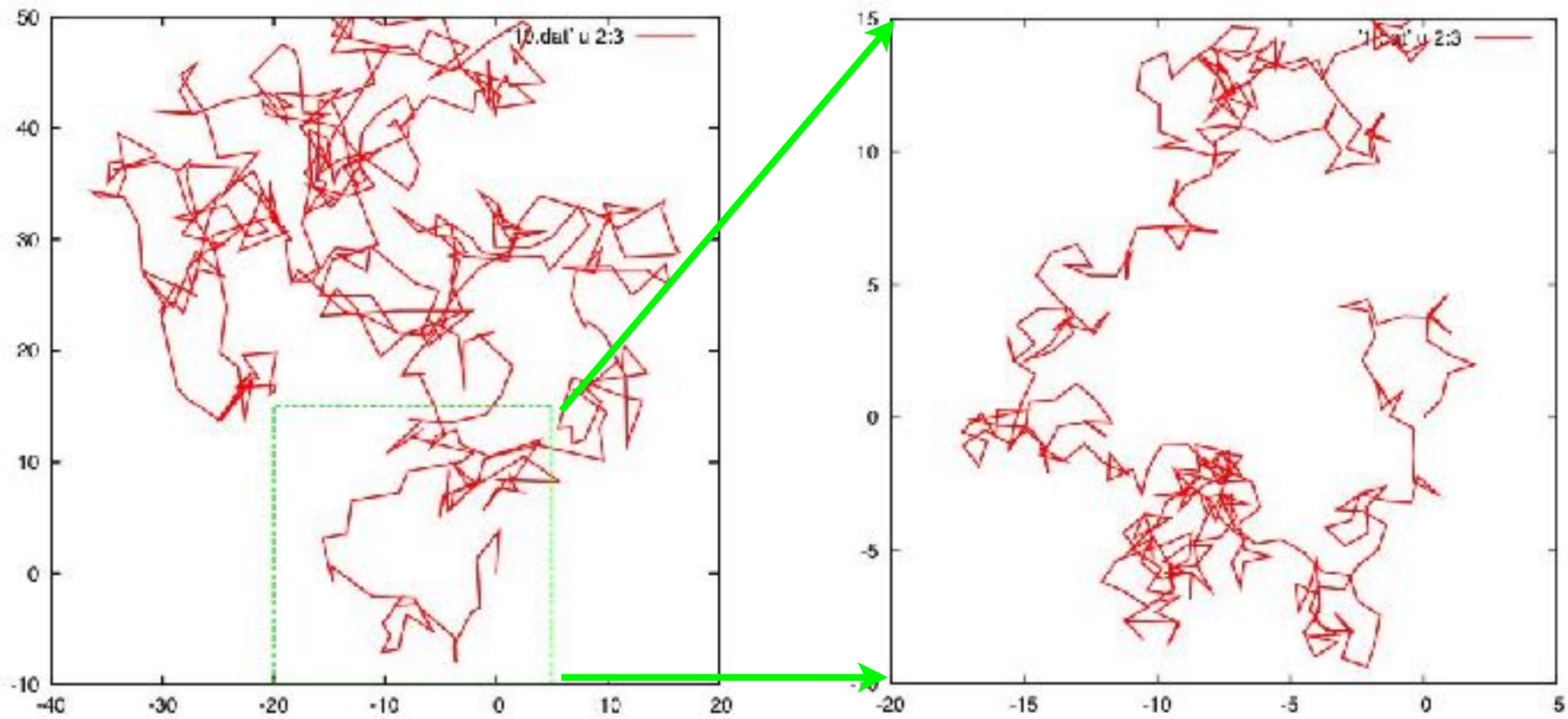
WRITE (...) i,x,y

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!

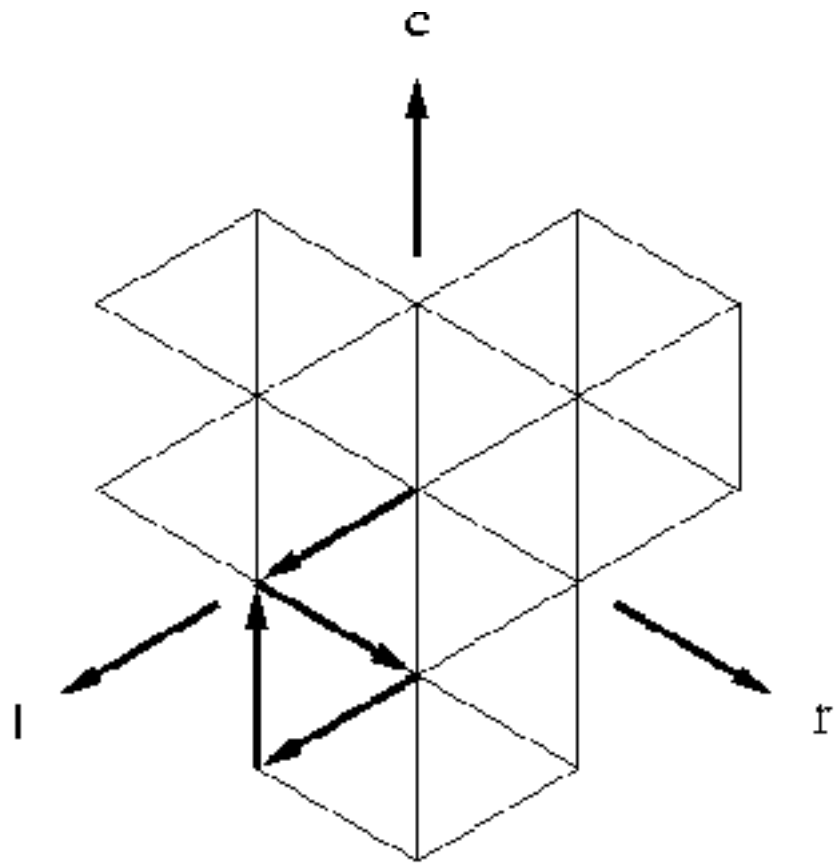


plot every 10 steps

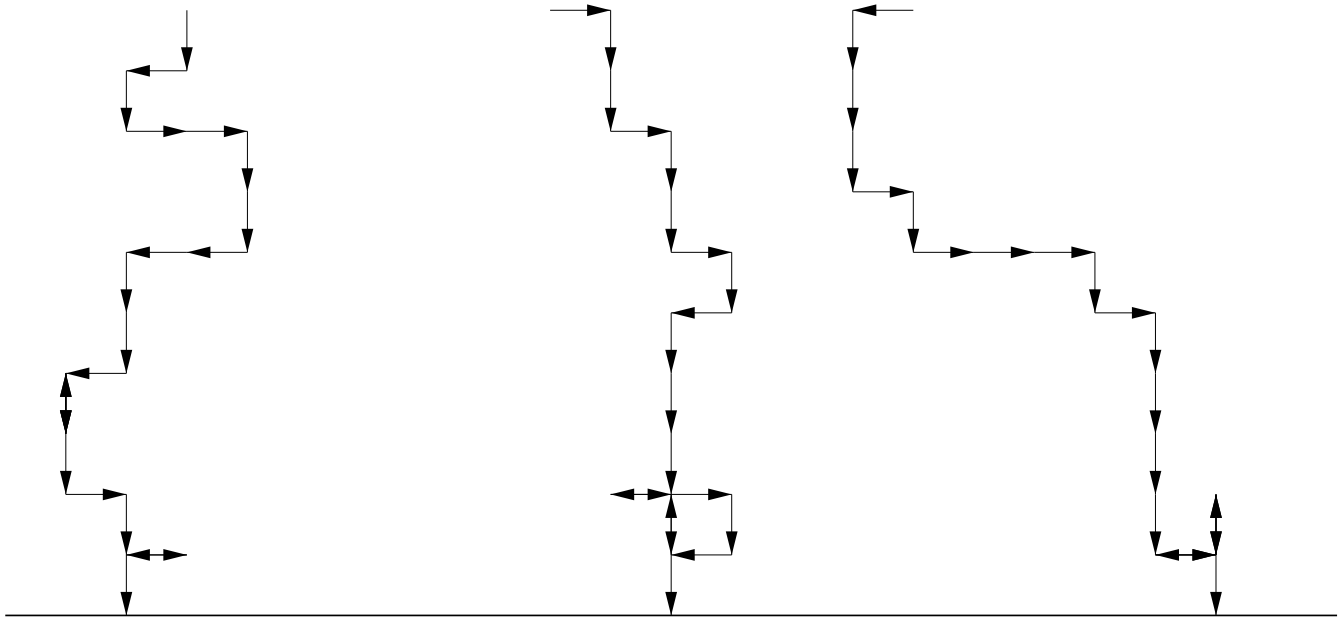
plot every step

Random Walks 2D

on a triangular lattice



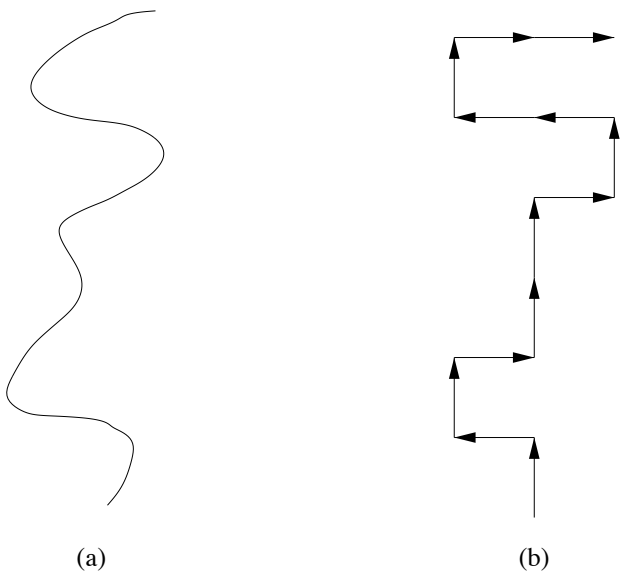
Other Random Walks



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) 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 https://moodle2.units.it

rw1d.f90
rw2d.f90
rw2-with-averages-1method.f90
rw2-with-averages-3methods.f90
rw2zoom.f90

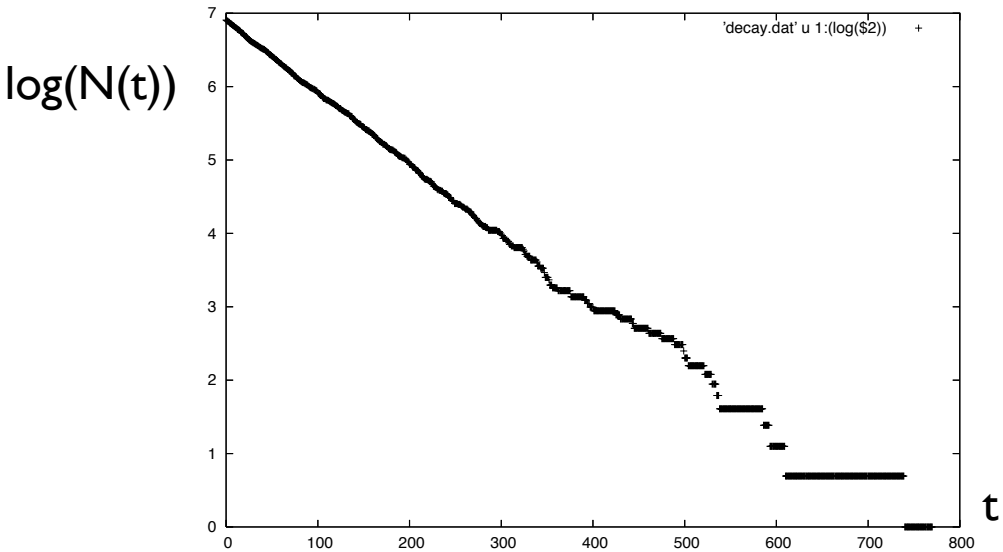
contour, pl => see following slide

‘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’

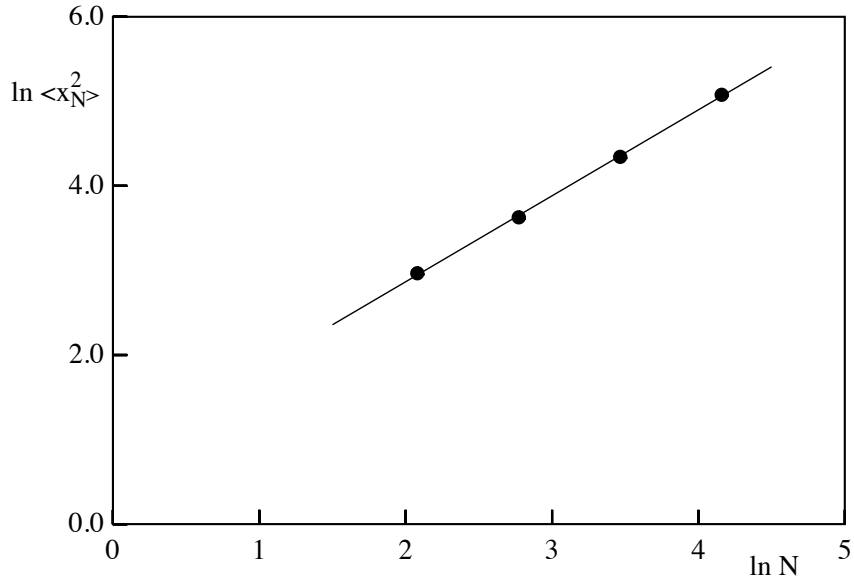
Examples - linear regression



radioactive decay:
$N(t) \sim N_0 \exp(- a\ t)$

fit with exp. ok, but even better:

$\log(N(t)) = \log N_0 - a\ t$
(semilog plot)



Random walk:
$\langle x^2_N \rangle \sim N^a$

$\log \langle x^2_N \rangle = a \log N$
(log-log plot)

LINEAR FIT is more robust!

Other random processes: order and disorder

A box is divided into two parts communicating through a small hole. One particle randomly can pass through the hole per unit time, from the left to the right or viceversa.

$N_{left}(t)$: number of particles present at time t in the left side
Given $N_{left}(0)$, what is $N_{left}(t)$?

(more on that in a future Lecture)

last part *(optional)*: algorithm for the Brownian motion (Langevin treatment)

(see code: 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

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

- 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...

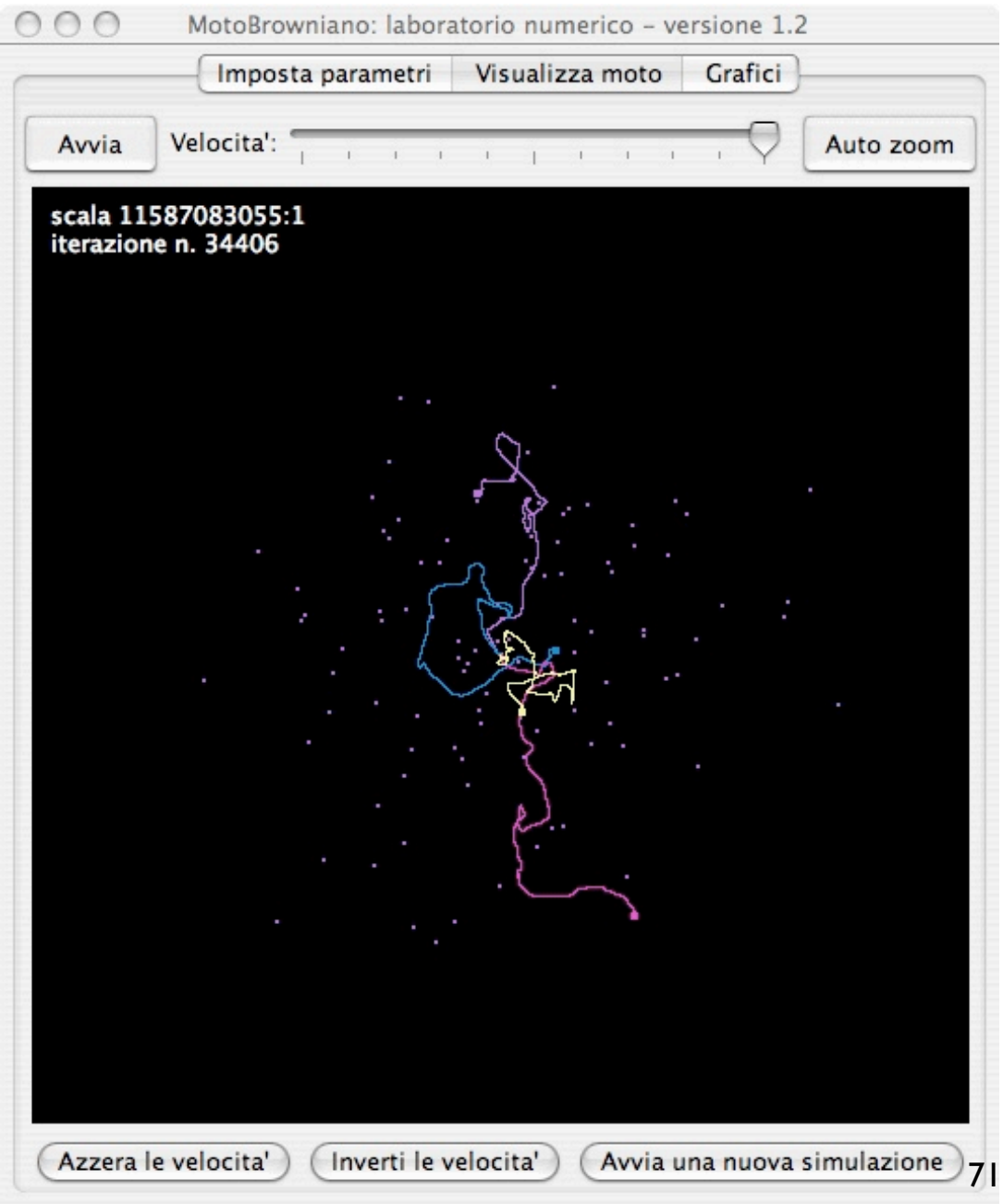
Δt too large: serious numerical uncertainties...]

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…



$k_B T = 4 \cdot 10^{-21}$ J, $M = 1.4 \cdot 10^{-10}$ kg,

$\gamma \approx 8 \cdot 10^{-7}$ 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 $\langle R^2 \rangle$ with time:

$$\langle R^2 \rangle = 2dD\ t$$

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

$$\langle R^2 \rangle = (2d\ k_B T\ /\ \gamma)\ t$$