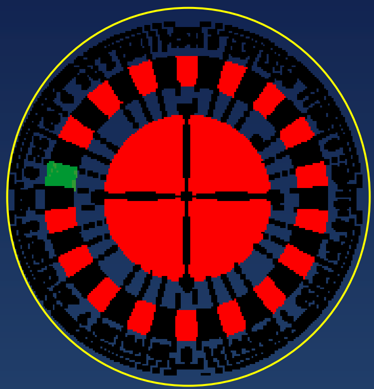
"Monte Carlo" <u>Simulations</u>

(the real things)



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Computational Physics for Undergraduates
BS Degree Program: Oregon State University

"Engaging People in Cyber Infrastructure"
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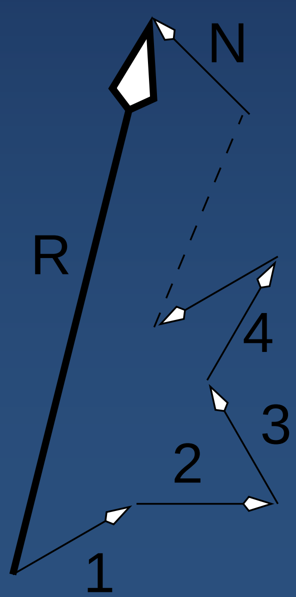
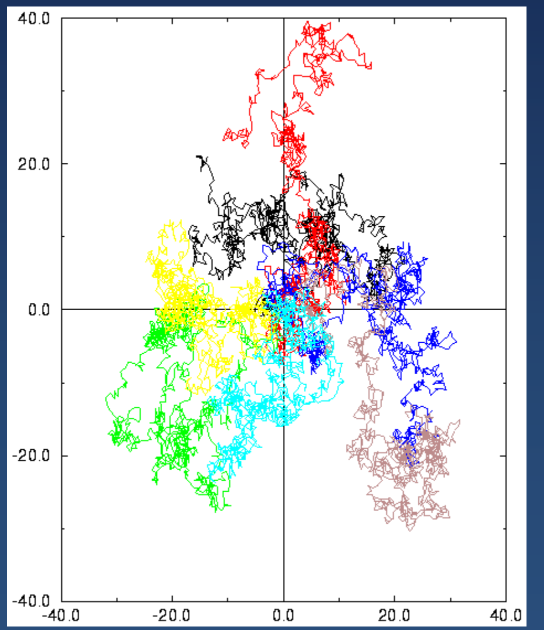
Prob 1: Random Walk Simulation

Diffusion Limited Aggregation
Applet

- Random walks in nature
  - Brownian motion (perfume)
  - electron transport
- Problem: N collisions

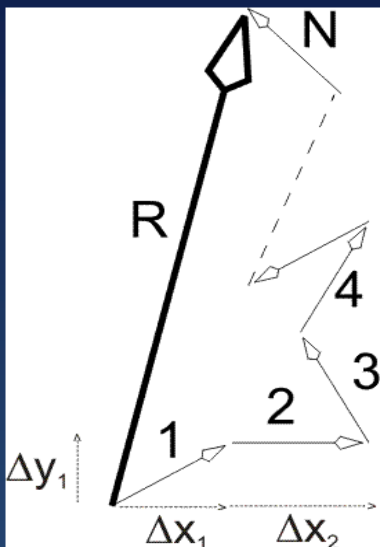
  to travel R?
- Model: walk N steps of r
  - random directions





Random Walk Theory

How far from origin after *N* steps?



$$R^2 = (\Delta x_1 + \cdots + \Delta x_N)^2 + (x \rightarrow y) \quad (1)$$

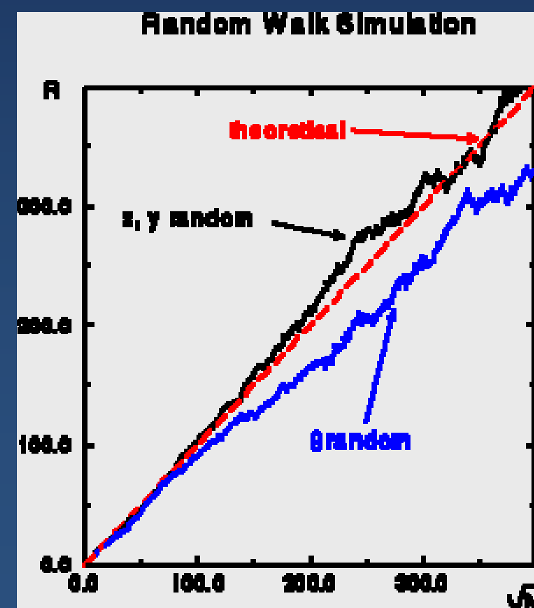
$$= \Delta x_1^2 + \cdots + \Delta x_N^2 + 2\Delta x_1 \Delta x_2 + \cdots + (x \rightarrow y) \quad (2)$$

Random: all directions,
average for large numbers

$$R^2 \simeq \Delta x_1^2 + \cdots + \Delta x_N^2 + \Delta y_1^2 + \cdots + \Delta y_N^2 \quad (3)$$

$$= N\langle r^2 \rangle, \quad (4)$$

$$\Rightarrow \boxed{R \simeq \sqrt{N} r_{\text{rms}}} \quad (5)$$



Each step with root-mean-square length *r*

Virtual Lab

- Use computer to “simulate” a random walk
- Computer = “virtual” lab

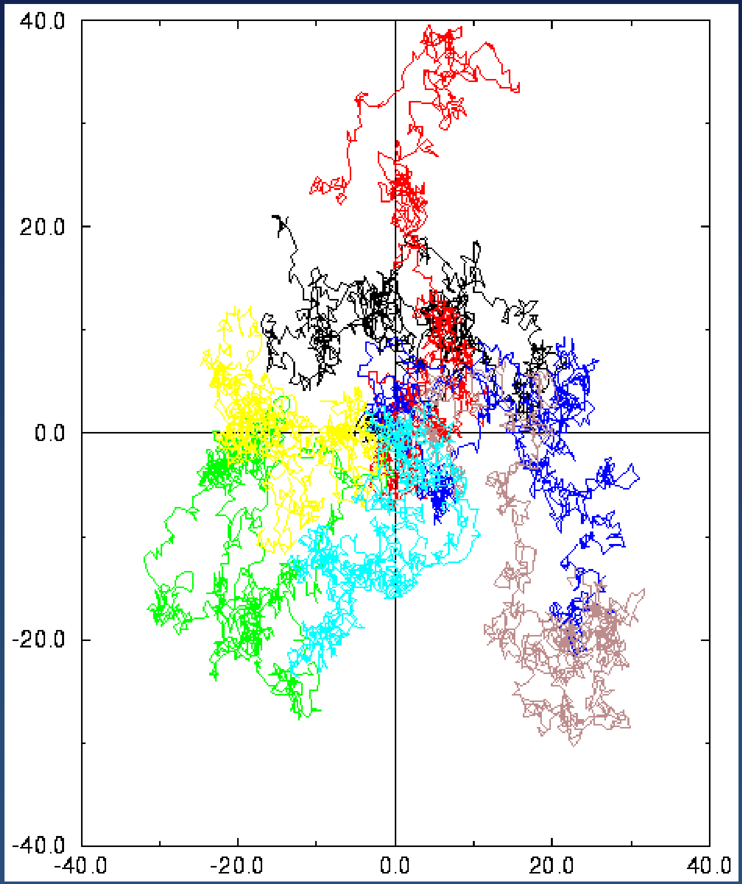
Random Walk Simulation

1. Is $R_{rms} = \sqrt{< R^2 >} \propto \sqrt{N}$?
2. Need ensure much randomness
3. Both random Δx & Δy
4. Range [-1, 1]
5. Normalize each step $r = 1$:

$$\Delta x = \frac{1}{L}\Delta x', \qquad \Delta y = \frac{1}{L}\Delta y', \qquad (1)$$

$$L = \sqrt{\Delta x'^2 + \Delta y'^2} \qquad (2)$$

6. Plot several <u>independent</u> 1000-steps walks
7. Do these look random?



Random Walk Simulation (specifics)

8. Good Statistics: N = # steps single trial,
   different seeds
   $K \approx \sqrt{N}$ = number trials

9. Calculate squared-distance each K trials

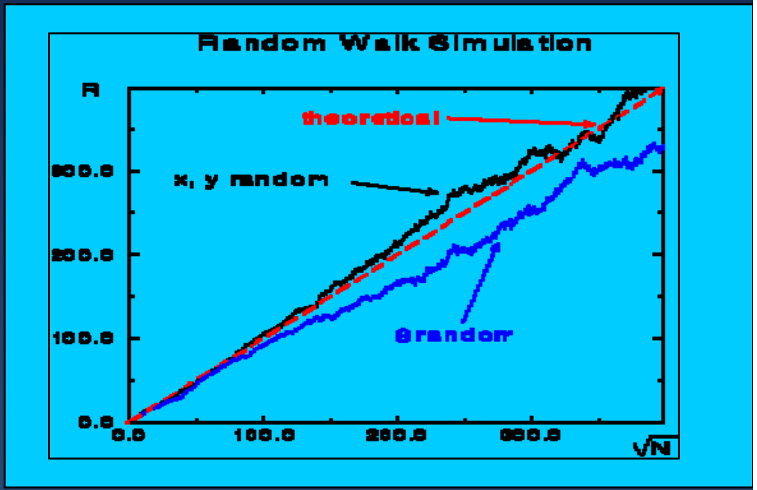
$$R_k^2(N) = \left(\sum_{i=1}^{N} \Delta x_i\right)^2 + \left(\sum_{i=1}^{N} \Delta y_i\right)^2 \qquad (1)$$

Then average trials: mean squared R

$$\langle R^2(N)\rangle = \frac{1}{K}\sum_{k=1}^{K} R_k^2(N) \qquad (2)$$

Then, root mean squared

$$R_{rms} = \sqrt{\langle R^2(N)\rangle} \qquad (3)$$



10. Plot $R_{\rm rms}$ vs $\sqrt{N}$

11. Large N for theory OK

12. N for 2-3 place agreement?

Problem 2: Spontaneous Decay

Facts of Nature

1. Natural process (we describe)
2. Atomic & nuclear decays
3. "Spontaneous" process
   a. no external stimulate
4. Transmutation (in nucleus)
   a. U $\rightarrow$ Th + $\propto$
5. *t* when decays: random
6. Independent of:
   a. how long exist
   b. number others around

Theory:

$\mathscr{P}(t)$ = prob decay/*t*/particle

$$= -\lambda \qquad (1)$$

$\Rightarrow$ *N(t), dN/dt* $\downarrow$ with time

Simulation Problem

- Simulate various number decays
- Ever look exponential $N(t) \propto e^{-\lambda t}$?
- When look "stochastic"?
- Simulation or $e^{-\lambda t}$ more accurate?

Law of Nature: Number decay/t/# = $-\lambda$

$$\frac{\Delta N(t)}{N(t)\Delta t} = -\lambda \qquad (1)$$

$$\frac{\Delta N(t)}{\Delta t} = -\lambda N(t) \stackrel{\text{def}}{=} \text{activity} \qquad (2)$$

Method: Decay Simulation

Algorithm:

Loop through remaining nuclei

$r\_i < \lambda$? $\Rightarrow$ decays ($\lambda \propto$ rate $\uparrow \Rightarrow$ more decay)

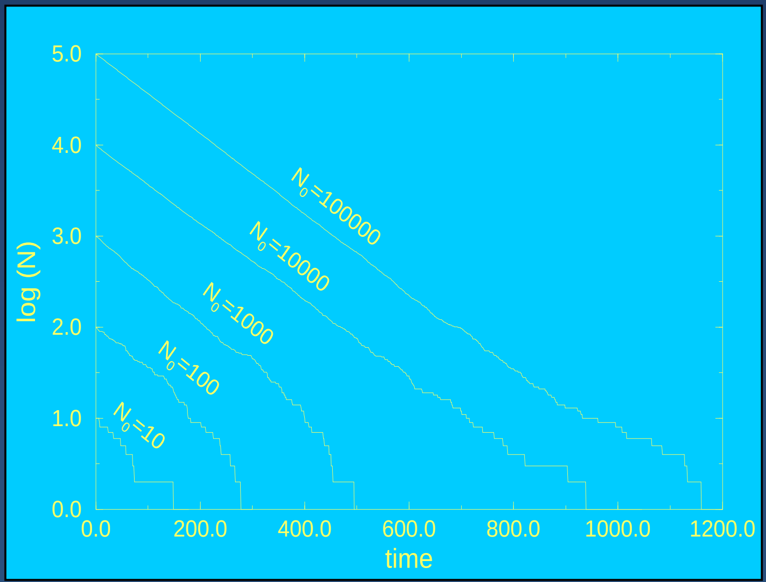
$t = t + \Delta t$

Repeat loop

Sounds like Geiger counter?

Java applet

```
while N > 0
  DeltaN = 0
  for i = 1..N
     if (r_i < lambda) DeltaN = DeltaN +1
  t = t +1
  N = N - DeltaN
  Output t, DeltaN, N
```



Model: Continuous Decay

If $N \rightarrow \infty$, & $\Delta N \rightarrow 0$, & $\Delta t \rightarrow 0$

$$\frac{\Delta N(t)}{\Delta t} \longrightarrow \frac{dN(t)}{dt} = -\lambda N(t) \tag{1}$$

Can integrate differential equation

$$N(t) = N(0)e^{-\lambda t} = N(0)e^{-t/\tau} \tag{2}$$

$$\Rightarrow \lambda = \frac{1}{\tau} \tag{3}$$

$$\frac{dN}{dt}(t) = -\lambda N(0)e^{-\lambda t} = \frac{dN}{dt}(0)e^{-\lambda t} \tag{4}$$

Exponential decay = approx to simulation

Nature: small N & stochastic