YOUR TURN

- ☐ Write a c++ code that generates a distribution from 0 to 1
  - ☐ Plot bins, distribution, etc
  - ☐ Compute the various tests listed here (moment, correlation)
- ☐ Do the same for a distribution you get from random.org

```
    #include <time.h>

    #include <cstdlib>

double randDouble(double low, double high)
{
    double temp;
    /* calculate the random number & return it */
    temp = ((double) rand() / (static_cast<double>(RAND_MAX) + 1.0))* (high - low) + low;
    return temp;
}

in your code, you can use these two functions; the first one is for initializing the seed,
the second one is to get a number between 0.0 and 1.0

srand( (unsigned)time(0) );
randDouble(0.0,1.0);
```

PHY-4810
COMPUTATIONAL PHYSICS

LECTURE 5: MONTE CARLO APPLICATIONS

ANNOUNCEMENT: TA

- Make sure you talk to Jonathan if you've any problem with programming

RANDOM NUMBERS: WHAT WE LEARNED LAST WEEK

- **Computers can generate sequences of random numbers.**

- **These are in fact *pseudo* random as the determinism built in computer translates into sequences of numbers that are neither completely *uniform* nor *uncorrelated*.**

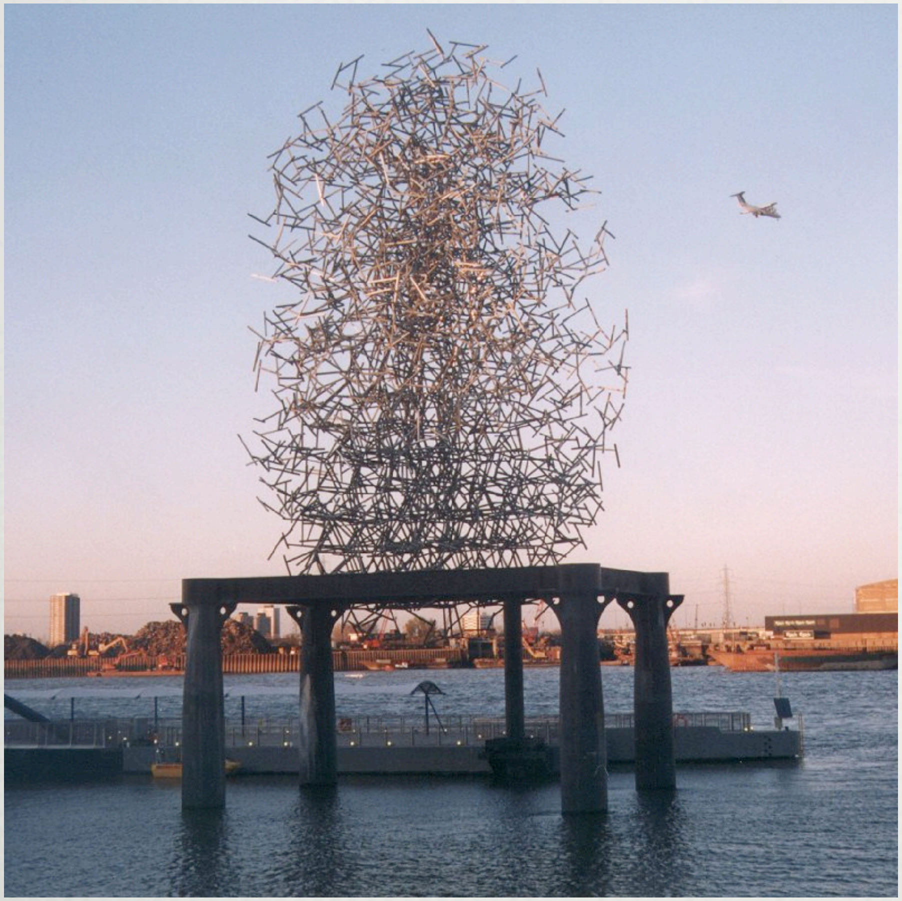
- **Today, we will explore classic applications of random numbers to three distinct fields of science.**

ON THE MENU TODAY

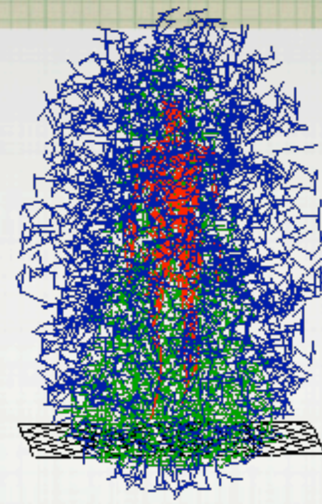
- ☐ **Monte Carlo Applications**
  - ☐ **Random Walk**
  - ☐ **Decay**
  - ☐ **Integral**
- ☐ **Error analysis (again!)**

PART 1:
RANDOM WALK IN 2D

ANTONY GORMLEY
QUANTUM CLOUD



"Quantum Cloud" is a 30 meter high x 16 meter wide x 10 meter deep elliptical cloud sculpture which stands on four cast iron caissons in the River Thames adjacent to the Millennium Dome in London



Antony Gormley, "New Works"

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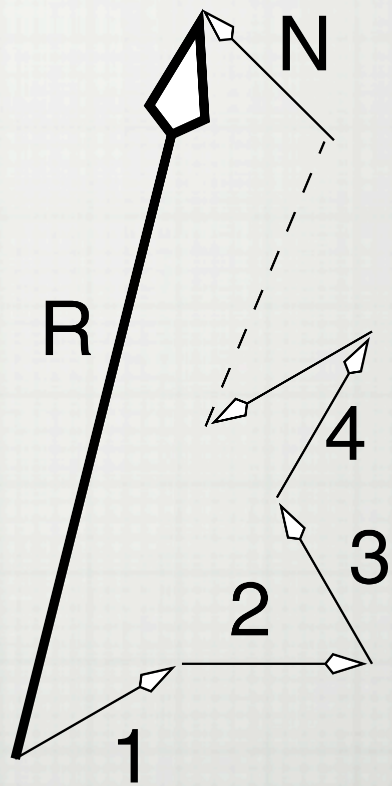
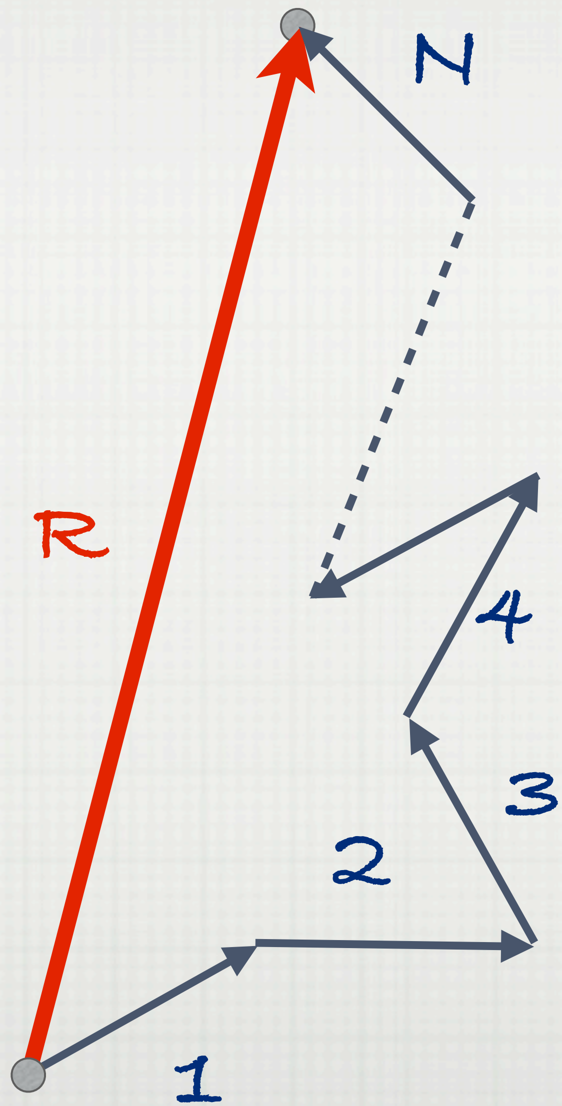
RANDOM WALK

- **Problem:** **incense smoke follows seemingly random movement. The collision of particles inside the "cloud" determines the trajectory adopted by the particles.**

- **How can we determine the number of collisions experienced by the particles to cover a distance R, if each particle moves an average distance of r_{rms} (root mean square) between collision?**





R FOR N

STEPS?

ASSUMPTIONS

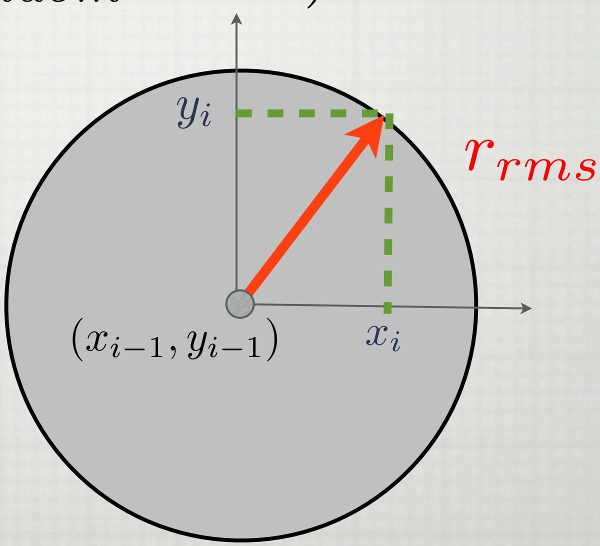
- 2D walk; each step length (r_{rms} is constant, not its direction)
- At each step, *x* an *y* vary according to a pair of random numbers

$$x_{\text{random}} \in [0, 1] \qquad \Delta_x = (x_{random} - 0.5)$$

$$y_{\text{random}} \in [0, 1] \qquad \Delta_y = (y_{random} - 0.5)$$

$$x_i = x_{i-1} + r_{rms} \frac{\Delta_x}{\sqrt{\Delta_x^2 + \Delta_y^2}}$$

$$y_i = y_{i-1} + r_{rms} \frac{\Delta_y}{\sqrt{\Delta_x^2 + \Delta_y^2}}$$



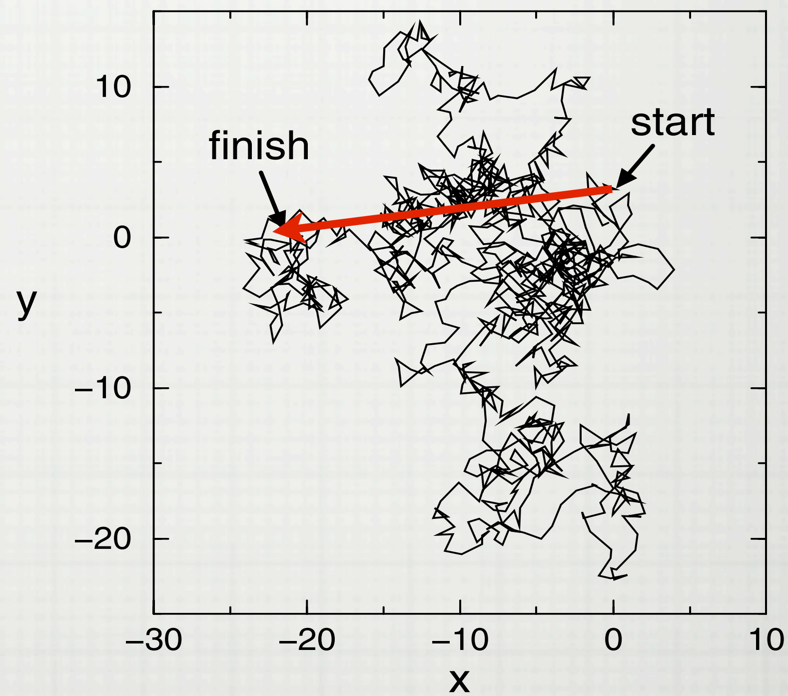
ANALYSIS

- The total distance covered is then

$$R_i = R_{i-1} + \sqrt{x_i^2 + y_i^2}$$

- **The radial distance is:**

$$R^2 = (x_N - x_0)^2 + (y_N - y_0)^2$$

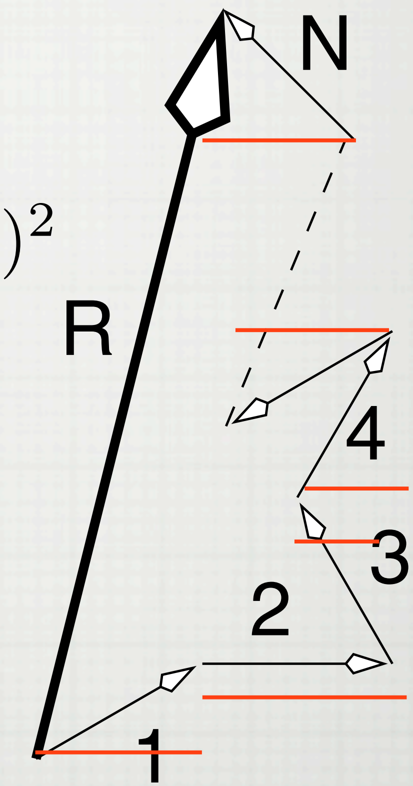


BEFORE CALCULATING...

- **In a truly random system, we can compute R as:**

$$R^2 = (\sum_i^N (x_i - x_{i-1}))^2 + (\sum_i^N (y_i - y_{i-1}))^2$$

$$R^2 = (\sum_i^N \delta x_i)^2 + (\sum_i^N \delta y_i)^2$$



$$R^2 = \delta x_1^2 + \delta x_2^2 + \delta x_3^2 + \cdots + 2\delta x_1 \delta x_2 + 2\delta x_1 \delta x_3 + \ldots \delta y_1^2 + \delta y_2^2 + \delta y_3^2 + \cdots + 2\delta y_1 \delta y_2 + 2\delta y_1 \delta y_3 + \ldots$$

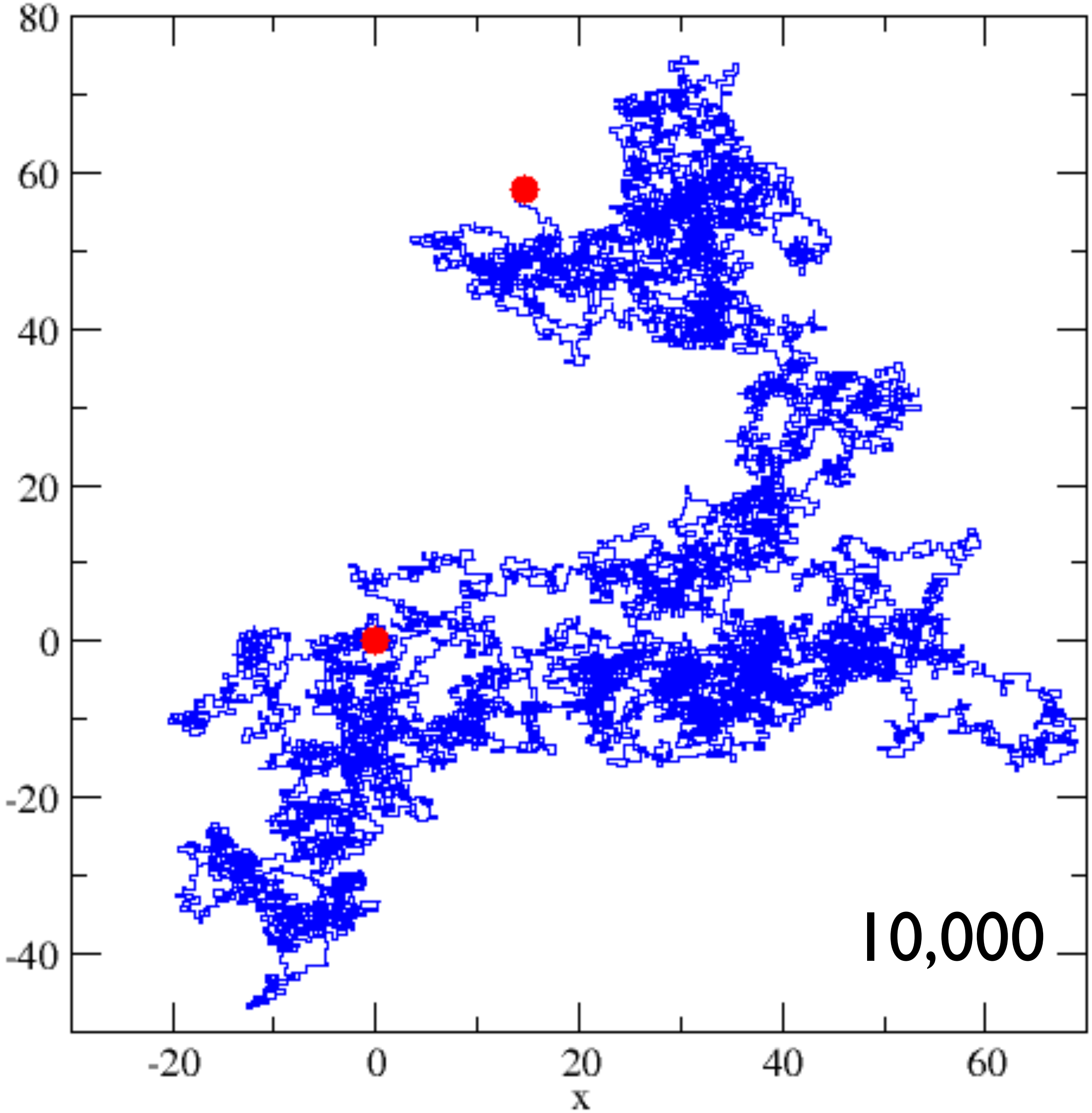
$$R^2 = \delta x_1^2 + \delta x_2^2 + \delta x_3^2 + \cdots + 2\delta x_1 \delta x_2 + 2\delta x_1 \delta x_3 + \ldots \delta y_1^2 + \delta y_2^2 + \delta y_3^2 + \cdots + 2\delta y_1 \delta y_2 + 2\delta y_1 \delta y_3 + \ldots$$

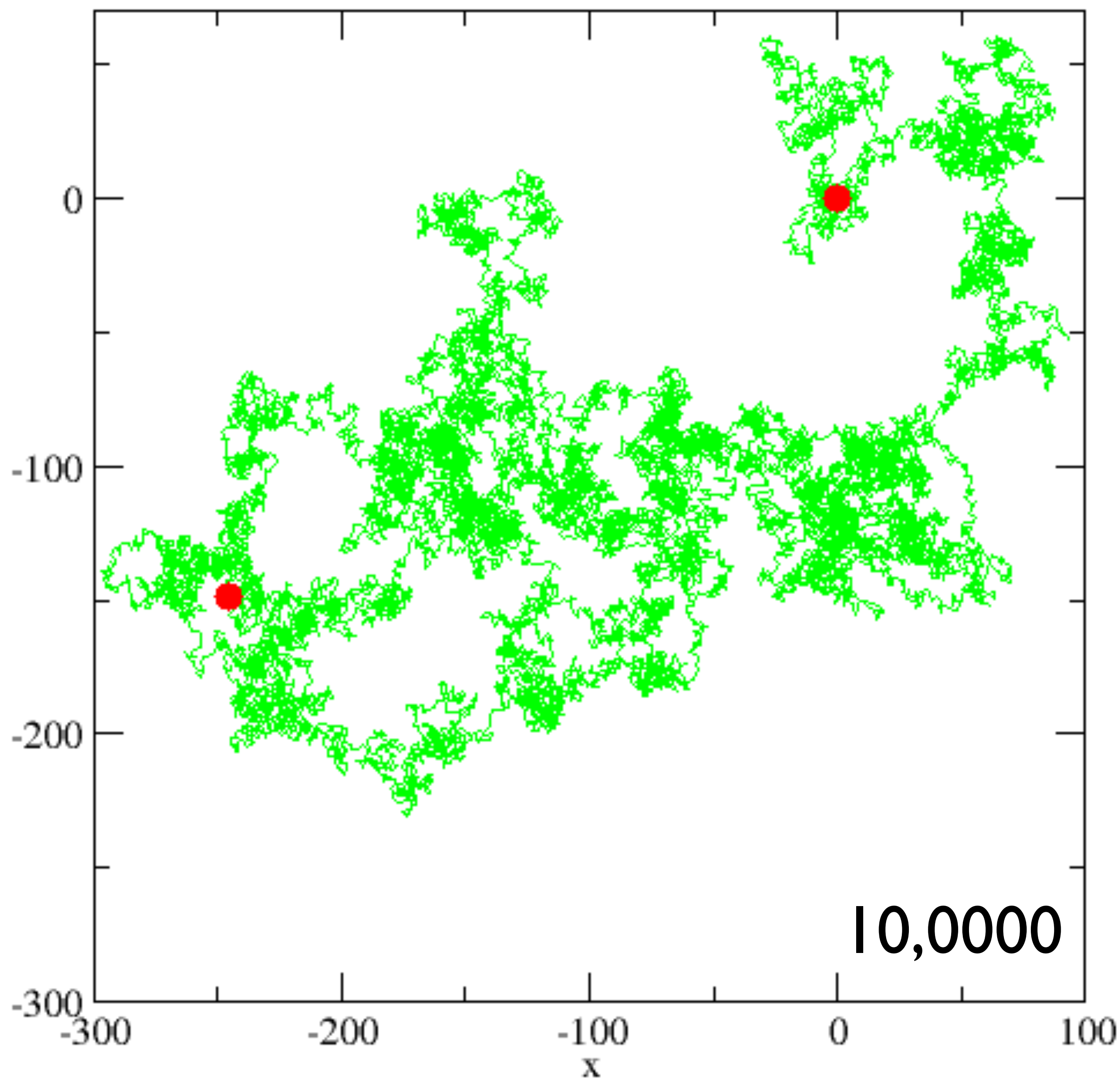
- **If true randomness:**
  - **Each cross-term should cancel!**
  - **Therefore:**

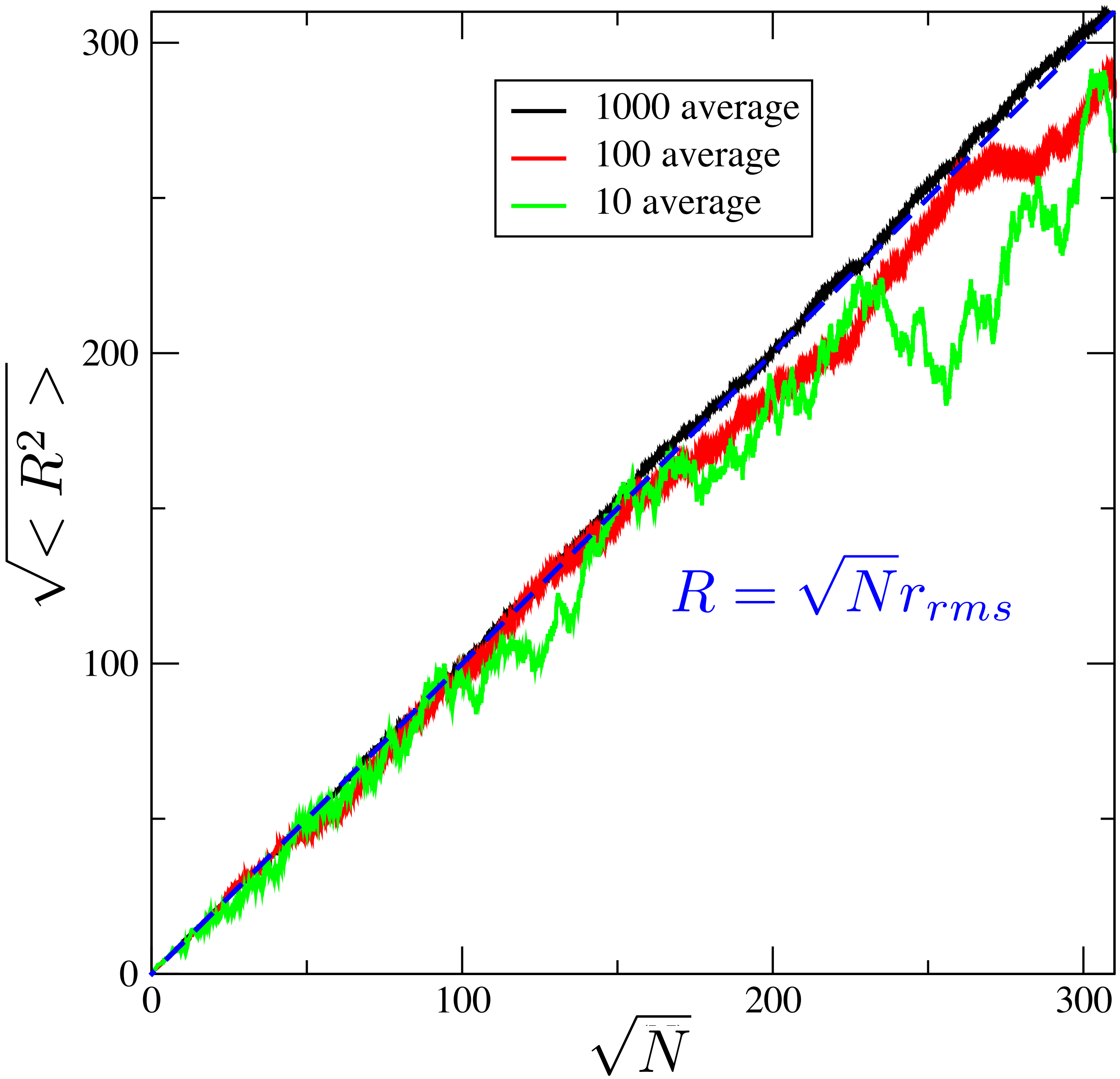
$$R^2 = \delta x_1^2 + \delta x_2^2 + \delta x_3^2 + \ldots \delta y_1^2 + \delta y_2^2 + \delta y_3^2 + \ldots$$

$$\boxed{R^2 = N \times r_{rms}^2}$$

$$\boxed{R = \sqrt{N} r_{rms}}$$


80
60
40
20
0
-20
-40
-20
0
20
40
60
x
10,000


0
-100
-200
-300
-300
-200
-100
0
100
x
10,0000

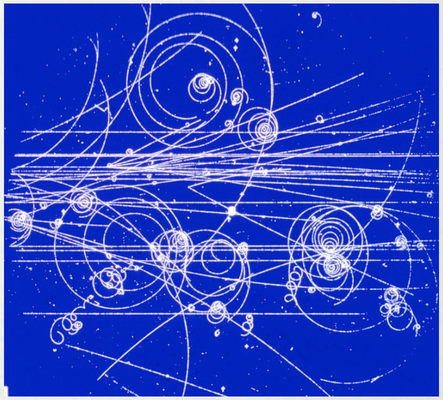


Here, average means that I repeated the experiment, 10, 100, and 1000 times

PART 2:
RADIOACTIVE DECAY

INTRODUCTION

- **How does a small number of radioactive particles decay?**



- **In particular, when does radioactive decay look exponential and when does it look stochastic (that is, determined by chance).**

- **The exponential decay law is only valid for large number of particles**

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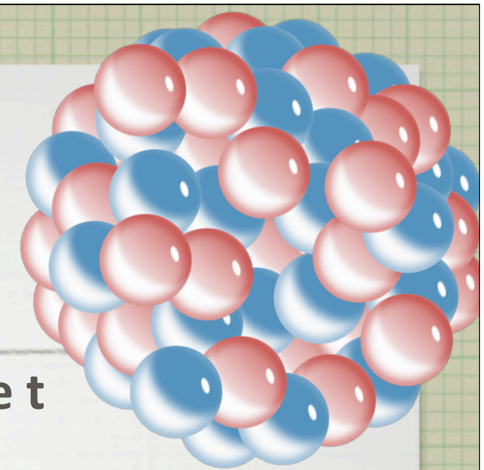
RADIOACTIVE DECAY

- <u>Spontaneous decay</u> is a natural process in which a particle, with no external stimulation, and at one instant in time, decays into other particles.
- Because the exact moment when any one particle decays is random, it does not matter how long the particle has been around or what is happening to the other particles.
- In other words, the probability P of any one particle decaying per unit time is a constant, and when that particle decays, it is gone forever.
- Of course, as the number of particles decreases with time, so will the number of decays. Nonetheless, the probability of any one particle decaying in some time interval is always the same constant as long as the particle still exists.

THEORY



- Suppose we have a sample of N(t) radioactive nuclei at time t
- Consider a time interval (Δt) and suppose ΔN particles decay during that time
- The probability of any one particle to decay per unit time is a constant
  - The decay probability per particle is ΔN/N
  - Probability of decay per unit time: ΔN/N/Δt
  - ΔN/N/Δt=-λ (negative because the number of particle decreases, i.e. ΔN is positive for a decay)

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

SOLUTION

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

- If the number N of particles is very large and the observation time Δt is very small, we have

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

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

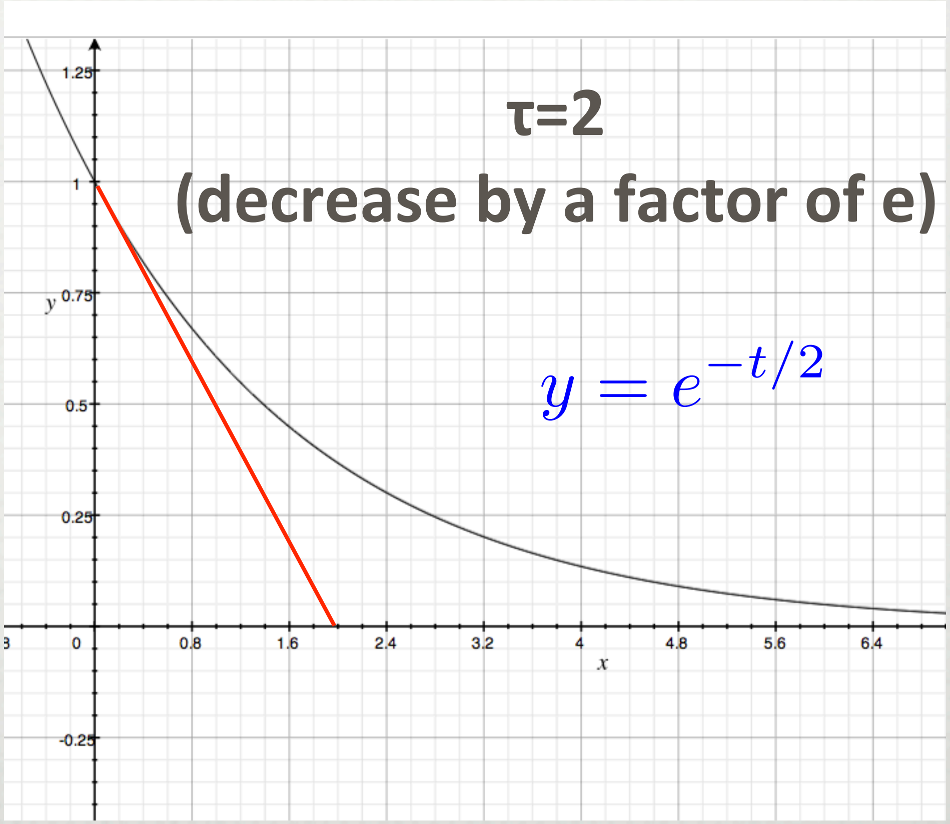
- And the solution is $\frac{dN}{dt}(t) = -\lambda N(0)e^{-\lambda t} = \frac{dN}{dt}(0)e^{-\lambda t}$

DISCUSSION

- We have an exponential decay with a decay rate related to the inverse of the lifetime

$$\lambda = \frac{1}{\tau}$$

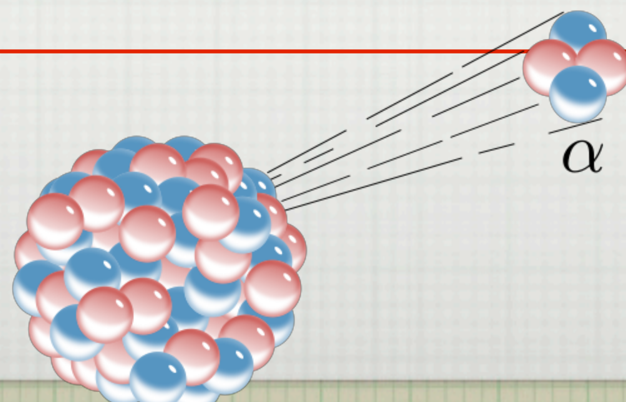
$$N(t) = N(0)e^{-\lambda t} = N(0)e^{-t/\tau}$$



NUMERICAL APPROACH

- During each time period, we have to impose that a given nucleus decays with probability **λ**, independent of time **t** and number of existing particle at that time **$N(t)$**

- In practice, we "roll a die" (i.e. pick a number between 0.0 and 1.0)
  - For each nucleus
  - If the number is smaller than **λ**, then we remove that nucleus and update **$N(t)$**



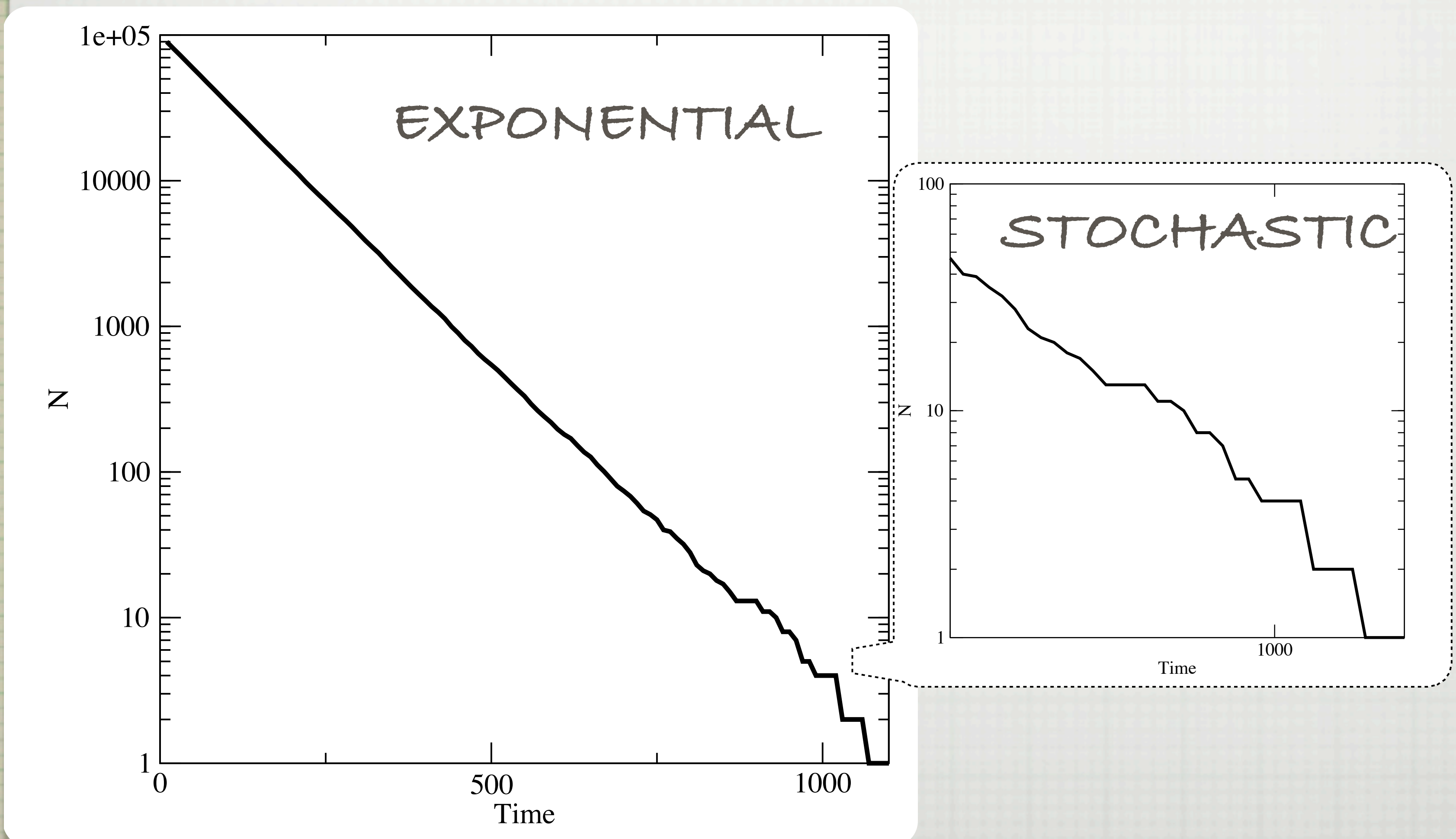
C++

```
 srand((unsigned)time(0) );

dx=0.0;

number=max;
while(number>0){
    t++;
    loop=number;
    for (i=0;i<number;i++){
       if(randDouble(0,1.0)<lambda) loop--;
    }
    number=loop;
    PI1 << (float) t/lambda << " " << number << endl;
    if(number==0) break;
    }
PI1.close();
}
```

RESULT: λ=0.1

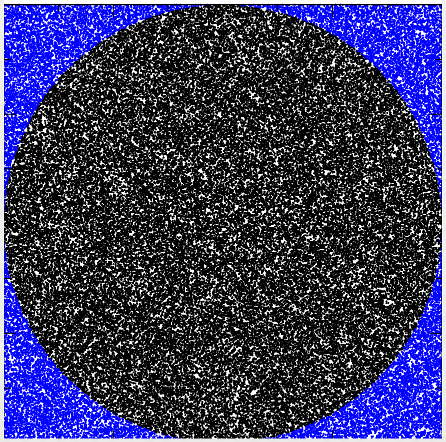


PART 3: INTEGRATION

DO YOU REMEMBER INTEGRATION METHODS?

NUMERICAL INTEGRATION USING SAMPLING: MOTIVATION

- **Example 1: See the Pi evaluation explained at last lecture. We find a ratio of two surfaces to compute one of the two (the other one being known)**



$$4 \times \frac{n_{in}}{n_{tot}} \approx 4 \times \frac{\pi R^2}{(2R)^2} = \pi$$

$$4 \times \frac{n_{in}}{n_{tot}} = 3.143$$

NUMERICAL INTEGRATION USING SAMPLING: MOTIVATION

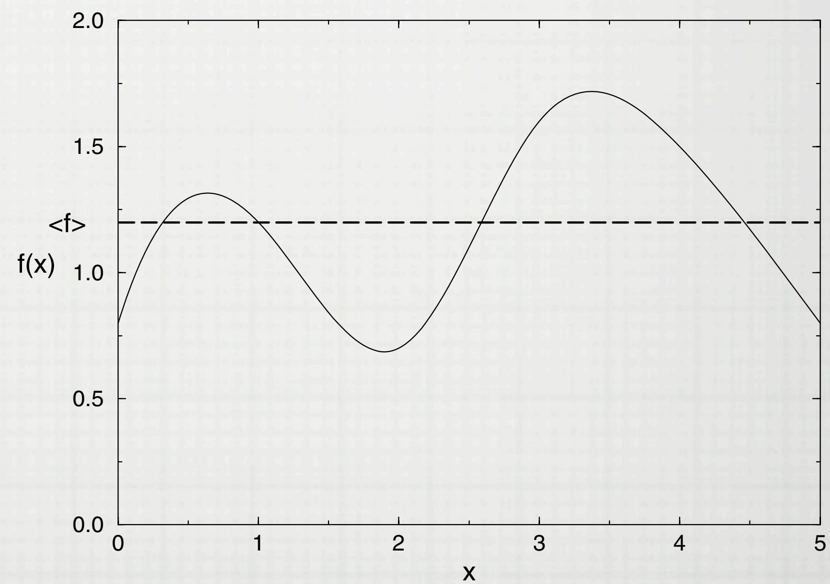
- **Example 2: High dimensional integral. Suppose you have a function with, say, 36 variables (*e.g. wave-function of a 12 electron system*) [example of a 12 electron system?!?]**
  - **If you use 64 points for each integral, you need $64^{36} = 2^{42}$ function evaluations!**
  - **If you can calculate the function once in 1s, you need 10^{64} years**
  - **How can we calculate a multidimensional integral?**

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dx_1 dx_2 dx_3 dx_4 dx_5 f(x_1, x_2, x_3, x_4, x_5)$$

MEAN-VALUE THEOREM: INTEGRATION

- **Mean value theorem:** $$I = \int_a^b dx f(x) = (b-a)\langle f \rangle$$

- **We can use the Monte-Carlo approach to evaluate the mean value of the function**



- **We sample the range [a,b] using N random numbers:**

$$\langle f \rangle \simeq \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

- **The Integral becomes:**

$$\boxed{\int_a^b dx\, f(x) \simeq (b-a)\frac{1}{N}\sum_{i=1}^{N} f(x_i) = (b-a)\langle f \rangle}$$

MULTIDIMENSIONAL MEAN-VALUE INTEGRATION

- **Two-dimensional:**

$$\int_a^b dx \int_c^d dy\, f(x,y) \simeq (b-a)(d-c)\frac{1}{N}\sum_i^N f(\mathbf{x}_i) = (b-a)(d-c)\langle f \rangle$$

- **Error: the error is statistical and decreases as $N^{-1/2}$. This is true in 1D or any dimension.**
  - **Of course, for a fixed N, the number of points used to integrate in each dimension is N/D (D being the dimensionality).**
  - **Example: if you use 1000 points to integrate a 10-dimensional integral, you use 1000/10=100 points per integral**

MORE ON ERRORS

- **Analysis indicates that:**

$$I \approx V < f > \pm V \sqrt{\frac{< f^2 > - < f >^2}{N}}$$

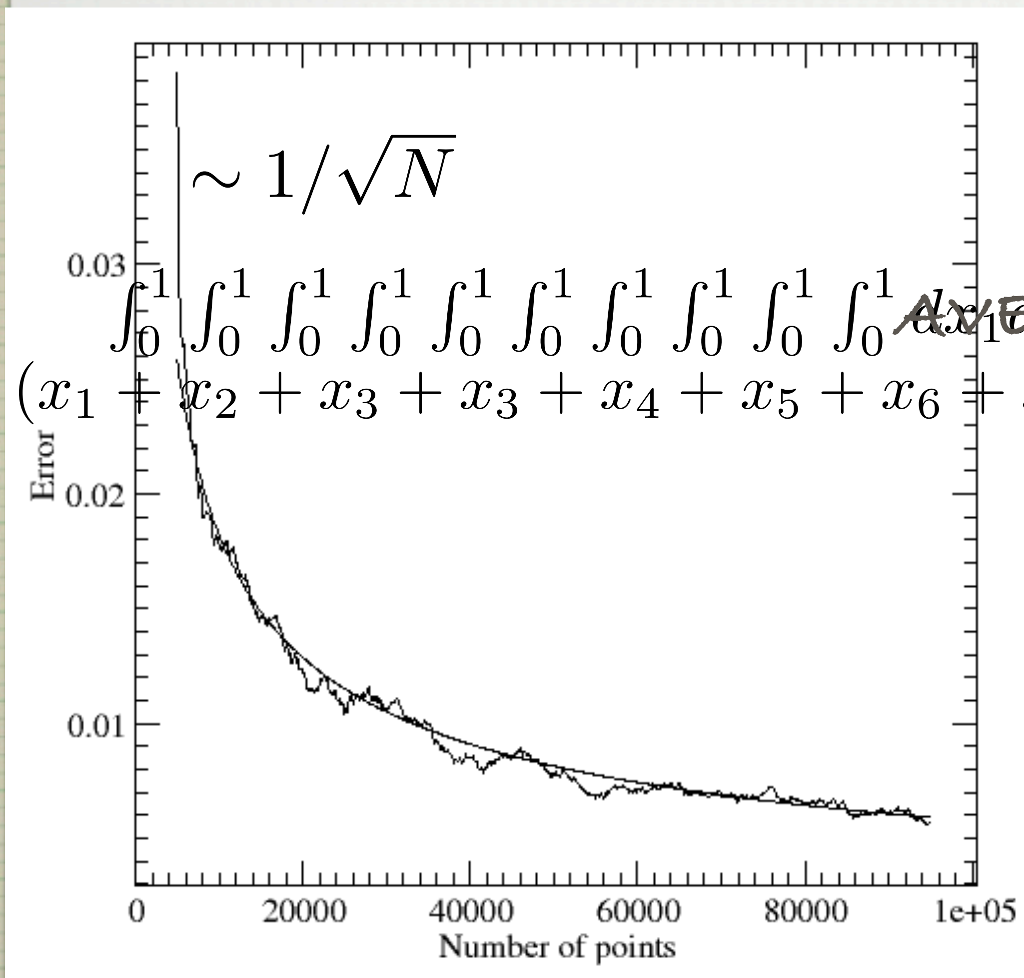
- **Where** $< f^2 > - < f >^2$

  is the function's variance

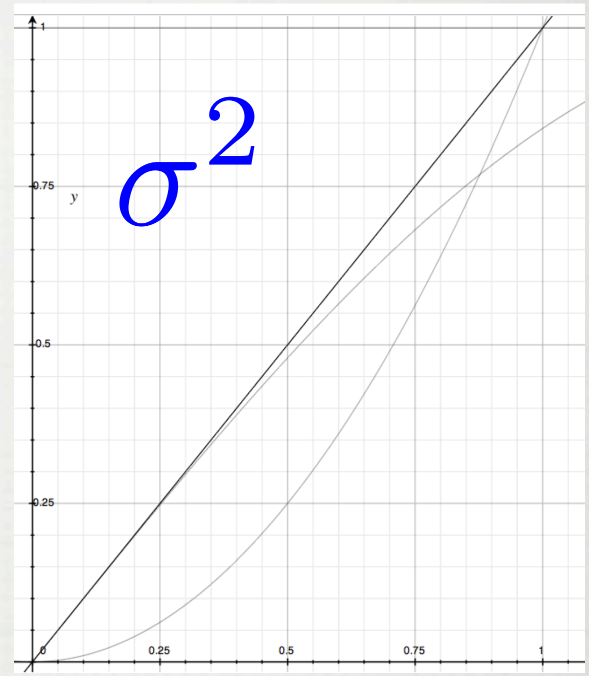
- **In other words: the larger the variance, the worst the error**

$$\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1\int_0^1 dx_1 dx_2 dx_3 dx_4 dx_5 dx_6 dx_7 dx_8 dx_9 dx_{10}$$
$$(x_1 + x_2 + x_3 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 + x_9 + x_{10})^2$$

AVERAGED OVER 16 TRIALS



EXAMPLE: STANDARD DEVIATION IN [0,1]



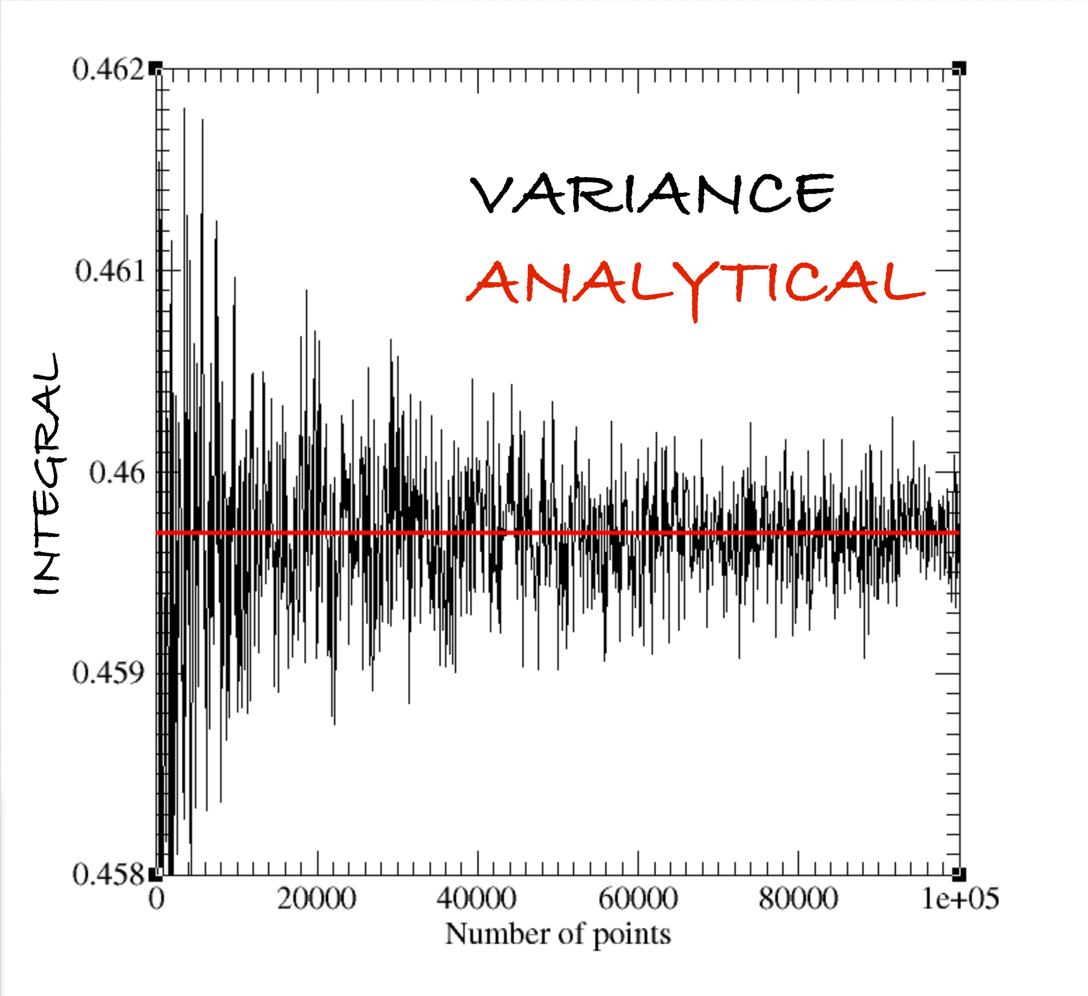
$$f = 1 \to \sigma =< f^2 > - < f >^2 = 0$$

$$f = x \to \sigma =< f^2 > - < f >^2 = 0.08$$

$$f = x^2 \to \sigma =< f^2 > - < f >^2 = 5/36 = 0.14$$

$$f = \sin x \to \sigma = (1/2 - 1/4 \sin 2 - (1 - \cos 1)^2 = 0.063$$

$$\int_0^1 dx \sin x = 1 - \cos(1) = .45969769$$



$$\sigma^2 = 0.061$$

REDUCING VARIANCE

- Find g such that

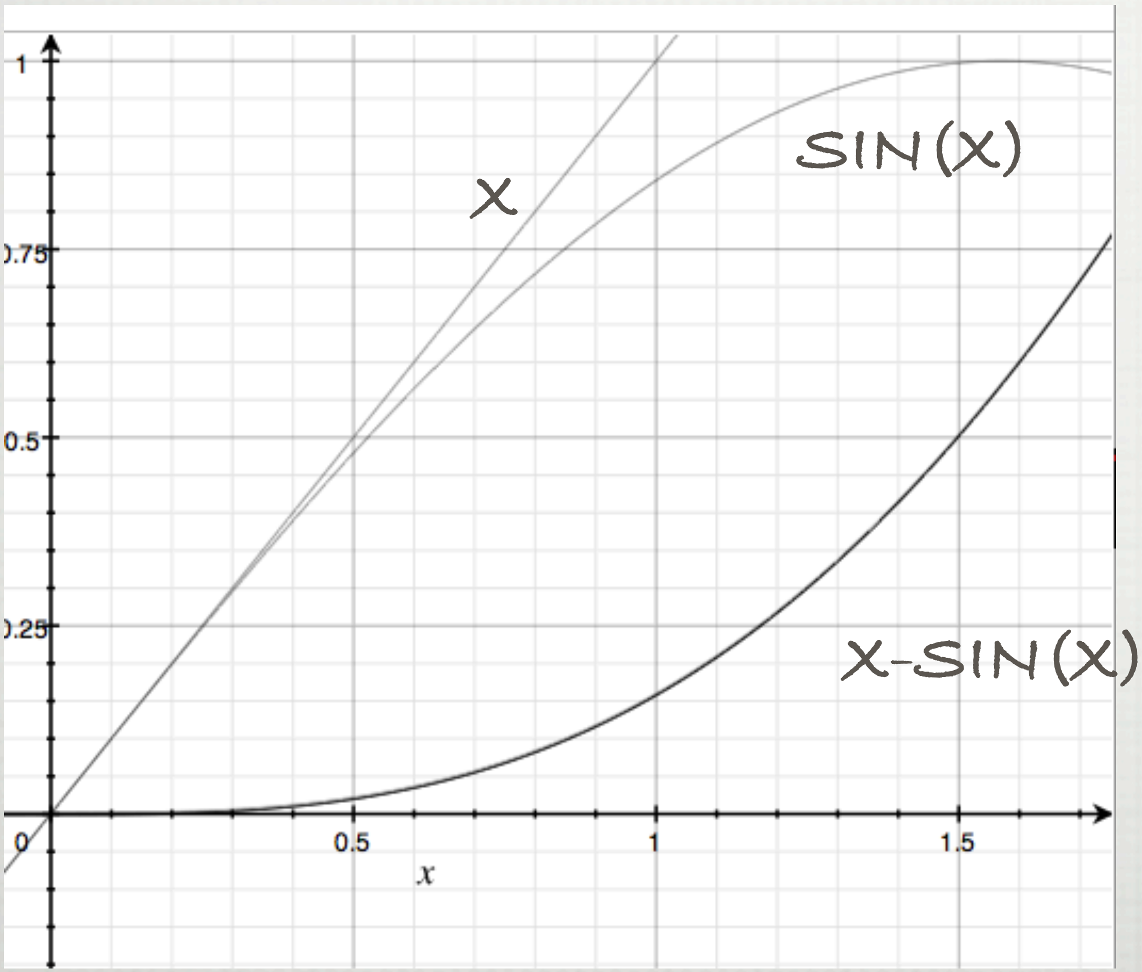
$$|f(x) - g(x)| \leq \epsilon \qquad \int_a^b dx\, g(x) = J$$

- The solution is then given by

$$\int_a^b dx\, f(x) = \int_a^b dx\, \{f(x) - g(x)\} + J$$

- The art is to find f(x)-g(x) with reduces variance compared to f(x)

REDUCING VARIANCE



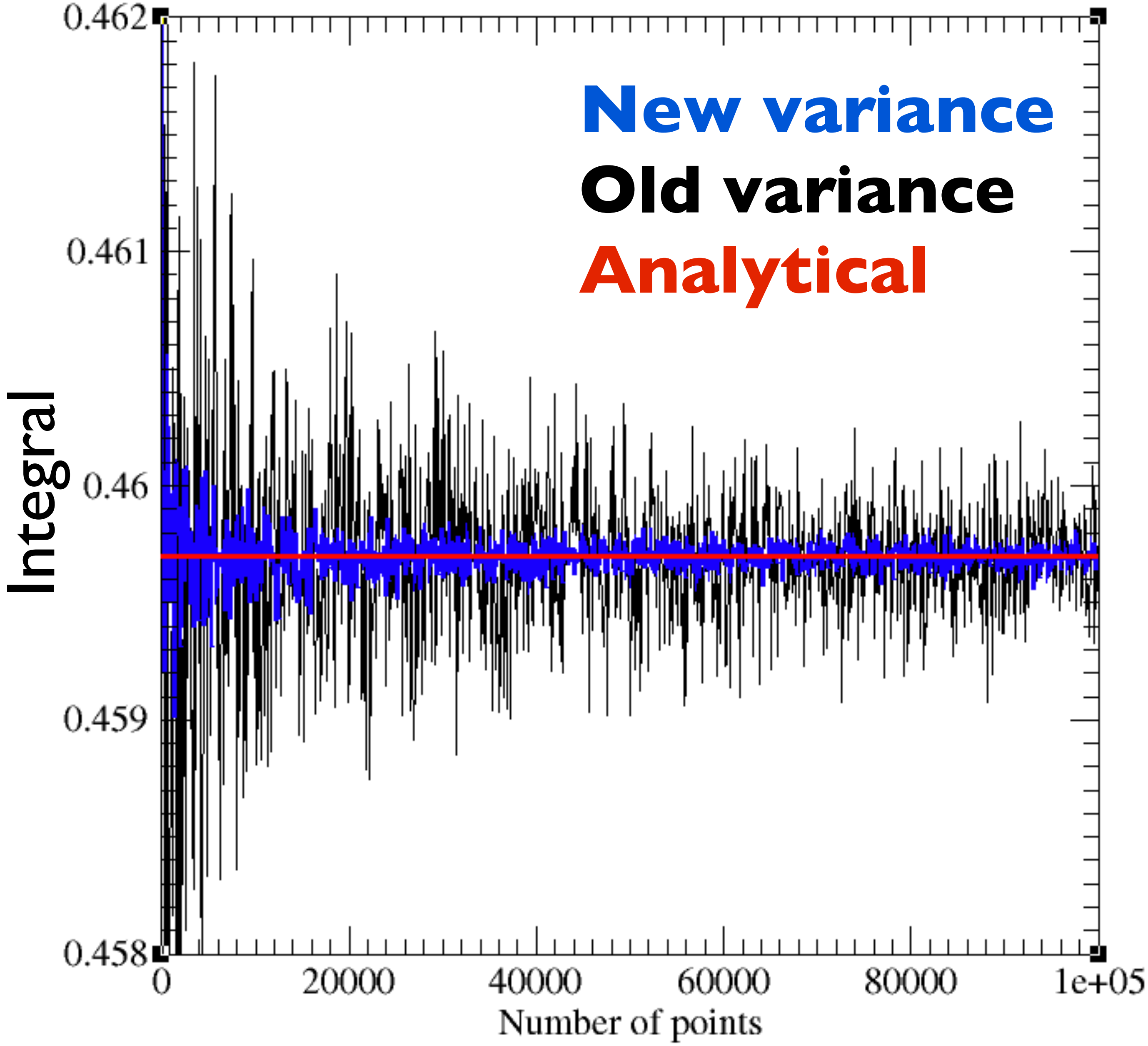
$$\sigma^2_{\sin} = 0.061$$

$$\sigma^2_{x-\sin} = 0.002$$

HOW DOES IT WORK?

$$\int_0^1 dx \sin x = \int_0^1 dx(\sin x - x) + \int_0^1 dx(x)$$

$$\int_0^1 dx \sin x = I_{numerical} + \frac{1}{2}$$



New variance
Old variance
Analytical
Integral
0.462
0.461
0.46
0.459
0.458
0
20000
40000
60000
80000
1e+05
Number of points

OTHER SCHEMES: IMPORTANCE SAMPLING

- A second method to improve Monte Carlo integration is called importance sampling because it lets us sample the integrand in the most important regions.

- It derives from expressing the integral in the form

$$I = \int_a^b dx\, f(x) = \int_a^b dx\, w(x) \frac{f(x)}{w(x)}$$

$$I = \left\langle \frac{f}{w} \right\rangle \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \qquad \int_a^b dx\, w(x) = 1 \qquad (w(x) > 0)$$

SUMMARY

- Random numbers are very important and can be used successfully to model nature's phenomena
- We learned about
  - Random Walk (importance in diffusion phenomena)
  - Natural Decay (exponential versus stochastic)
  - Integration
- HW2 (presented on Friday)