15th EURADOS SCHOOL
Computational Methods in Dosimetry State of the Art and Emerging Developments
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# MONTE CARLO RADIATION TRANSPORT SIMULATIONS

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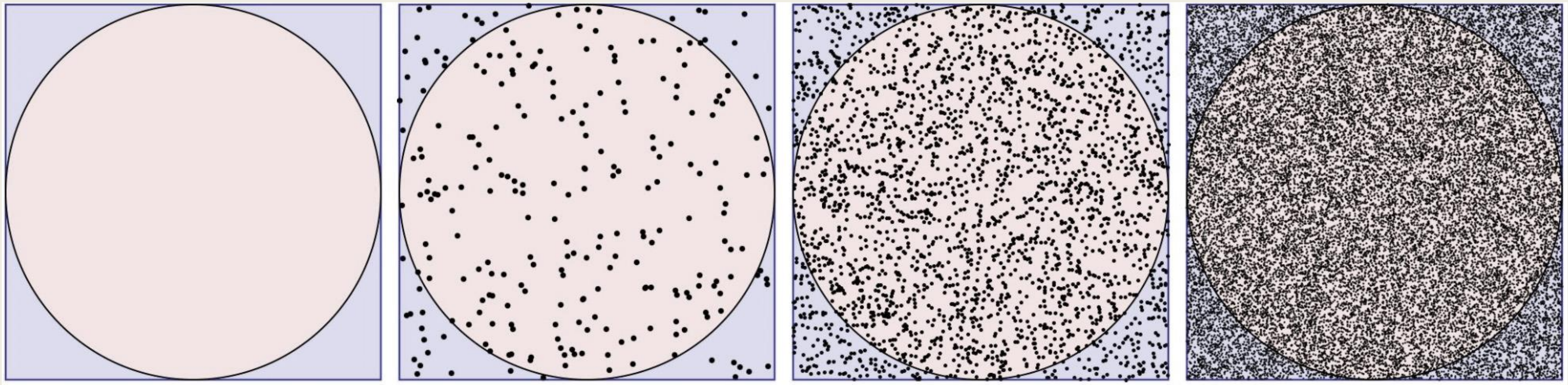
# MONTE CARLO SIMULATON or MONTE CARLO METHOD

- Monte Carlo method – general method of solving problems by using random sampling and random numbers to obtain numerical results

- Randomness is used to solve problems that can be either deterministic or random in nature



# EXAMPLE OF MONTE CARLO METHOD

- Estimating PI

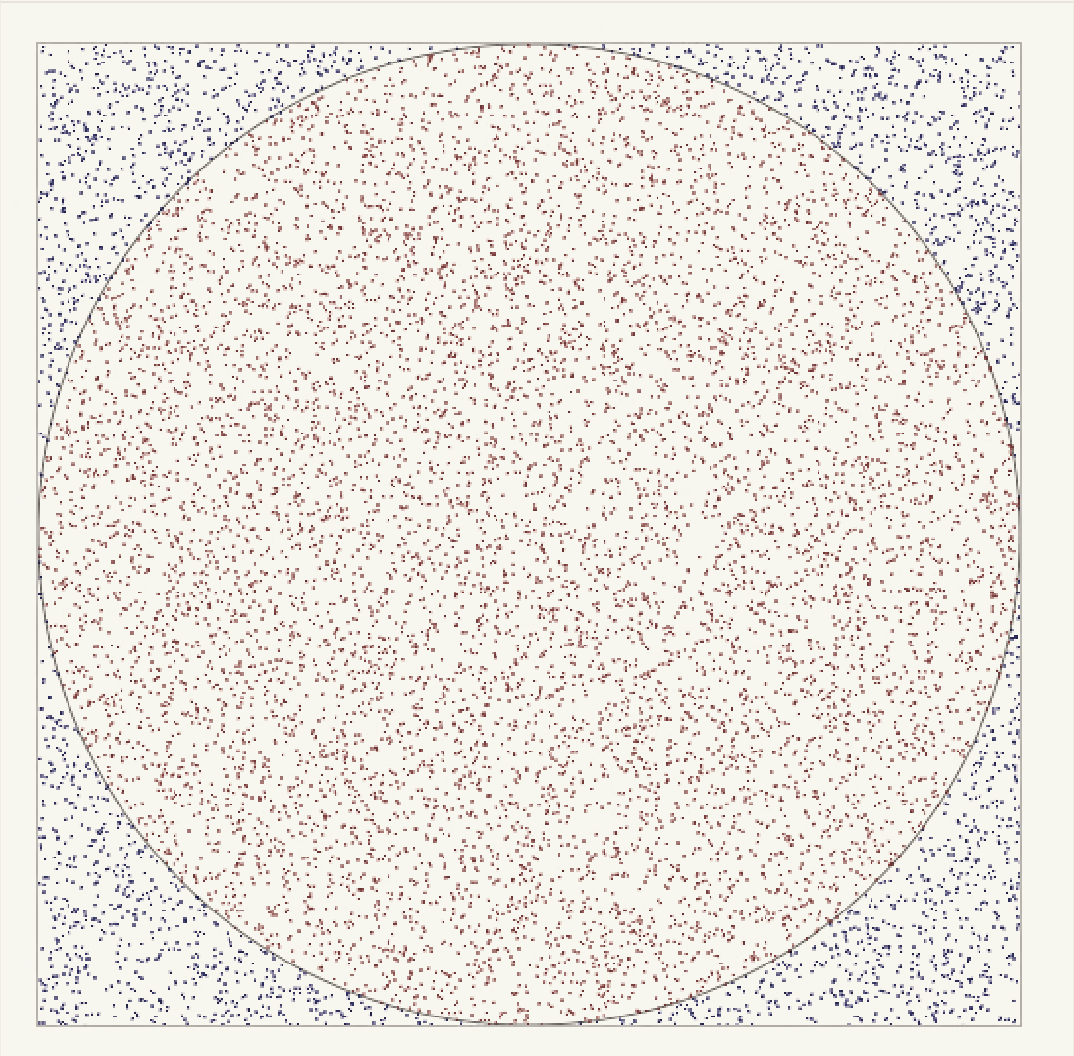
$$\frac{P_{\text{CIRCLE}}}{P_{\text{SQARE}}} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4}$$

$$\frac{P_{\text{CIRCLE}}}{P_{\text{SQARE}}} = \frac{N_{\text{POINTS INSIDE OF CIRCLE}}}{N_{\text{POINTS INSIDE OF SQARE}}}$$

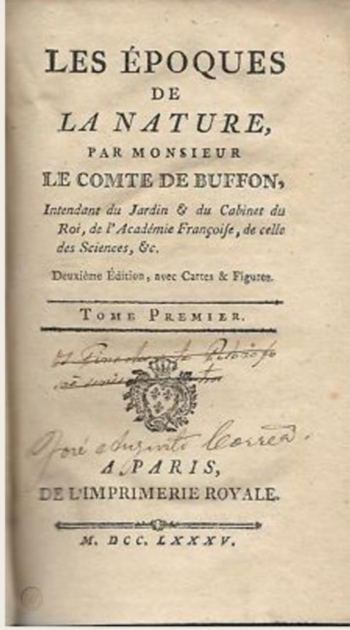
$$\pi = 4 \cdot \frac{N_{\text{POINTS INSIDE OF CIRCLE}}}{N_{\text{POINTS INSIDE OF SQARE}}}$$

Total number of points = 248100

Estimated $\pi$ = 3.14156



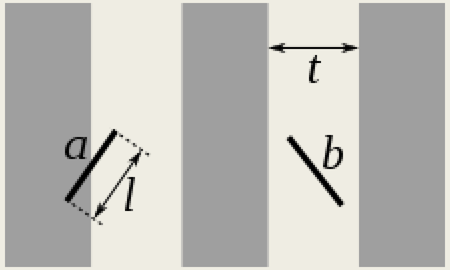
# HISTORY OF MONTE CARLO METHOD

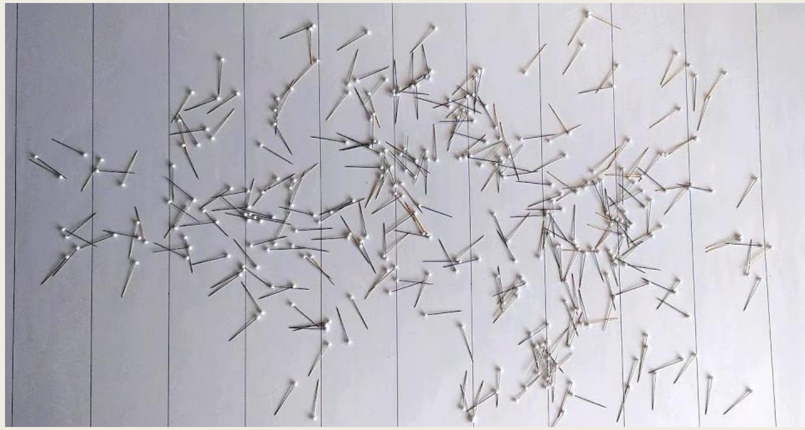

LES ÉPOQUES
DE
LA NATURE,
PAR MONSIEUR
LE COMTE DE BUFFON,
Intendant du Jardin & du Cabinet du Roi, de l'Académie Françoise, de celle des Sciences, &c.
Deuxième Édition, avec Cartes & Figures.
TOME PREMIER.
A PARIS,
DE L'IMPRIMERIE ROYALE.
M. DCC. LXXXV.

- 1777. Buffon's needle problem[1] . Comte de Buffon evaluated the probability of tossing a needle onto a sheet with strips

$$p = \frac{2}{\pi}\frac{l}{t}$$

- 1886. Laplace[2] suggested that this can be used calculate the value of π.



$l = 2t$ number of needles =314

$\pi = \frac{1}{p}$ needles crossing lines = 101

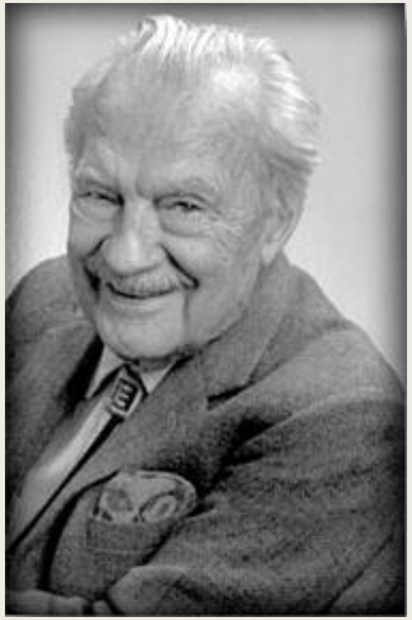
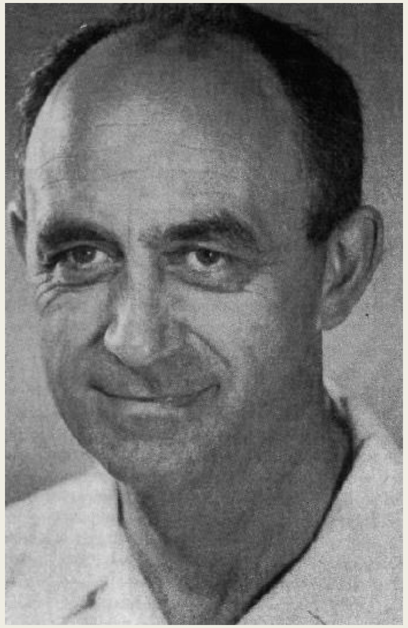
$$\pi = \frac{\text{number of needles}}{\text{needles crossing lines}} = 3.109$$

1. G. Comte de Buon. *Essai d'arithmetique morale*, volume 4. Supplement a l'Histoire Naturelle, 1777.
2. P. S. Laplace. Theorie analytique des probabilites, Livre 2. In *Oeuvres completes de Laplace*, volume 7, Part 2, pages 365 - 366. L'academie des Sciences, Paris, 1886.
3. https://www.youtube.com/watch?v=3VHp_E5FfQM
4. https://en.wikipedia.org/wiki/Buffon%27s_needle_problem

# HISTORY OF MONTE CARLO RADIATION TRANSPORT METHOD

- John von Neumann, Stanislaw Ulam and Nicholas Metropolis
- Enrico Fermi

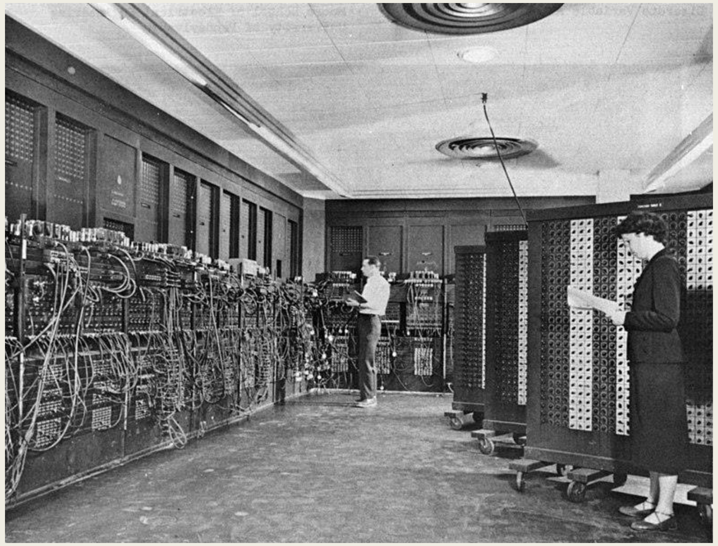


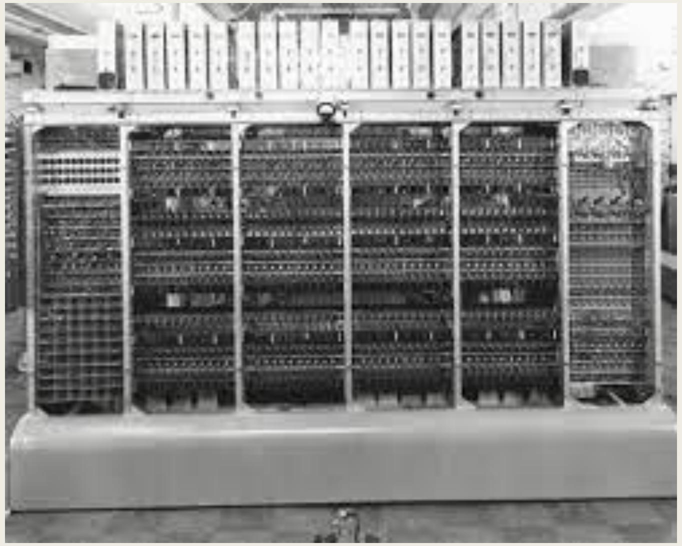



1. N. Metropolis, "The beginning of the Monte Carlo method", Los Alamos Science Special Issue 125-130 (1987)

# DEVICES USED FOR SIMULATION OF NEUTRON TRANSPORT

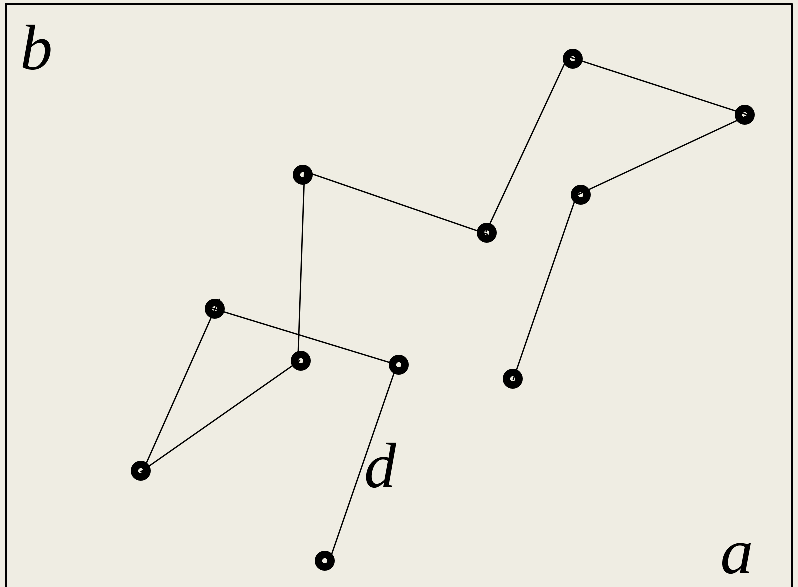
- ENIAC - Electronic Numerical Integrator And Computer
- MANIAC I (Mathematical Analyzer Numerical Integrator and Automatic Computer Model I)
- FERMIAC

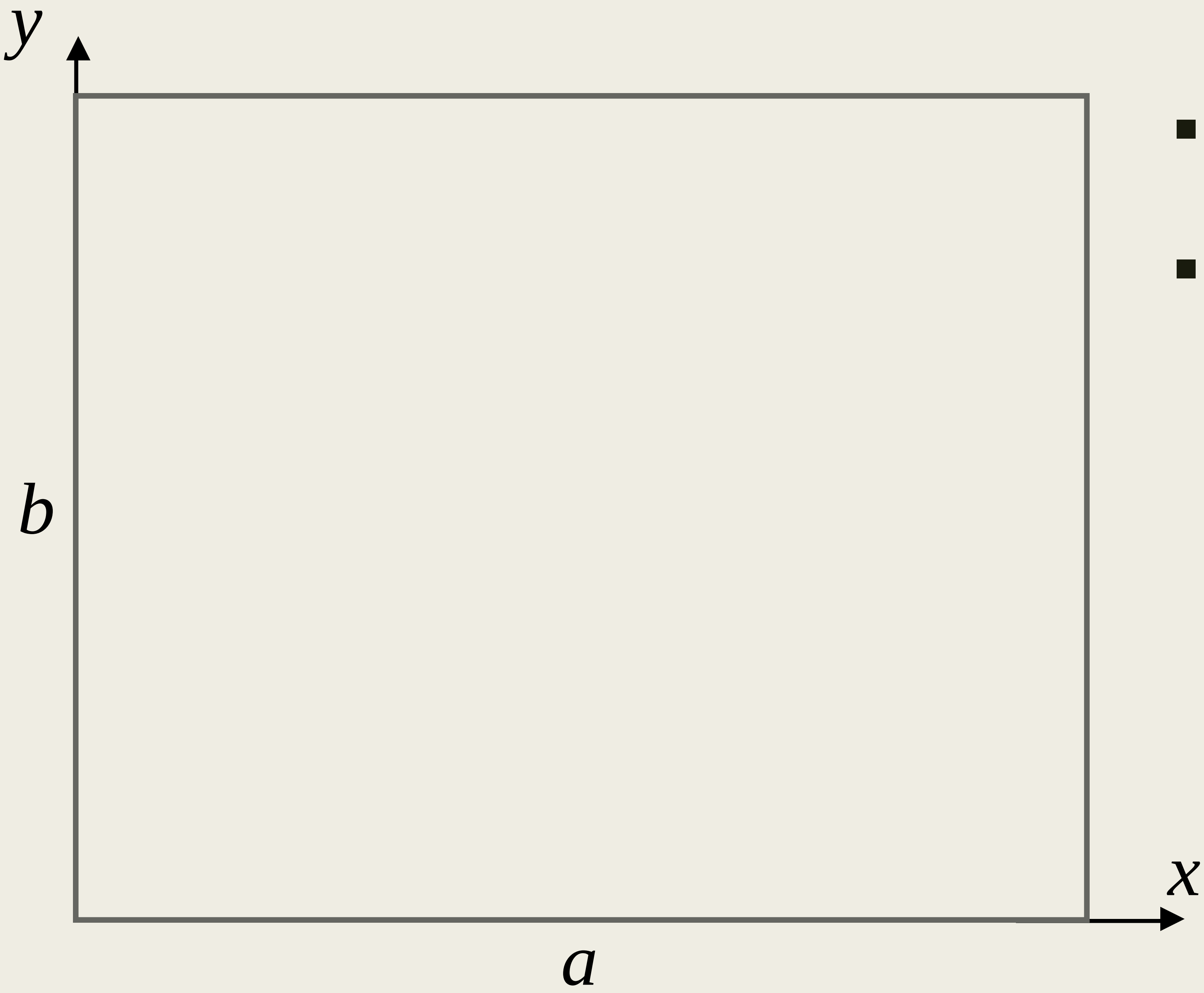




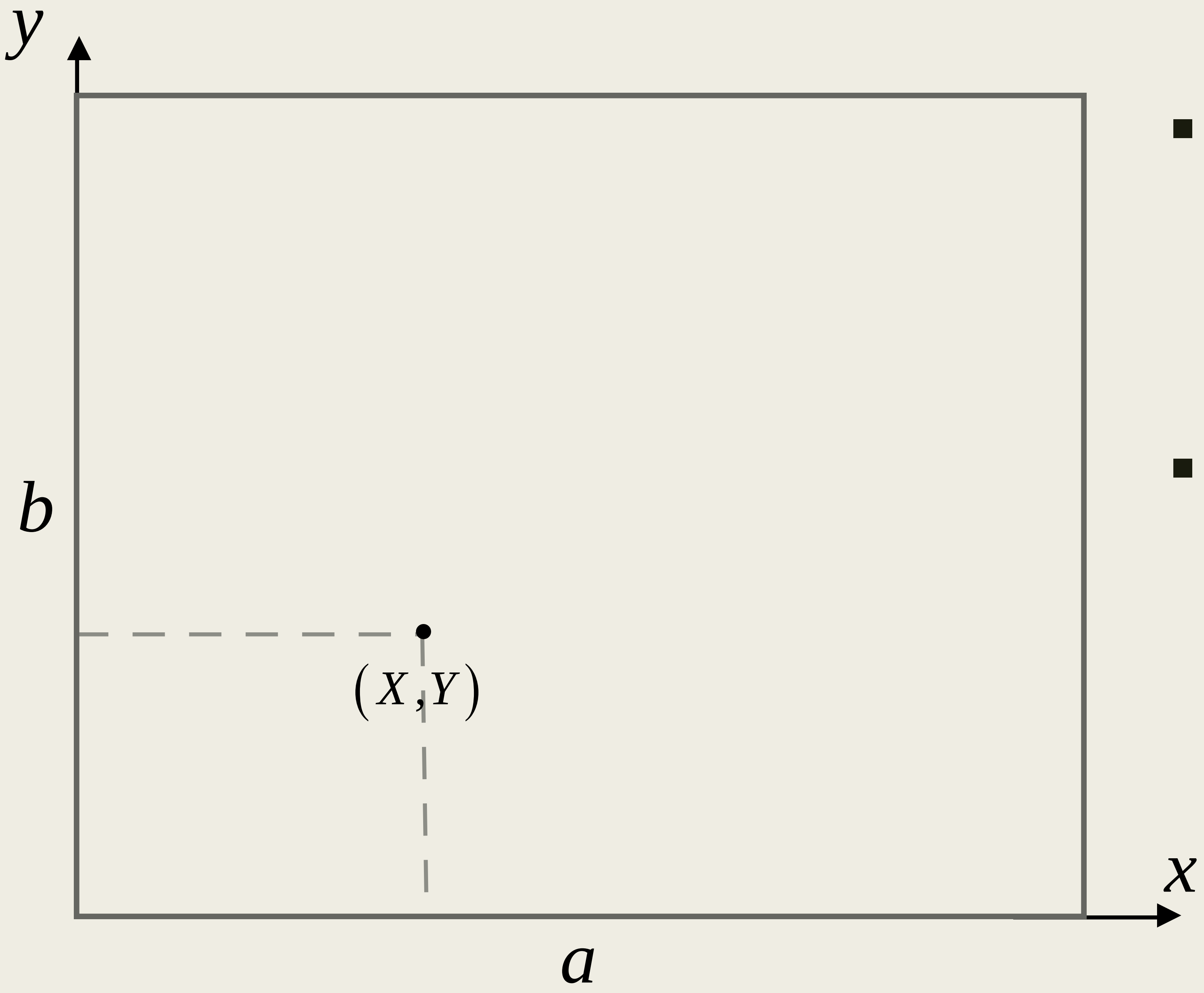
# INSIGHT IN RADIATION TRANSPORT

- Let us start from simple example – **two-dimensional movement** of Brownian like particle inside of rectangle with dimensions $a \times b$
- More simplification – free path between any two collision is fixed; particle at the point of collision exhibit only random change of direction
- Starting point of particle is unknown and should be randomly chosen



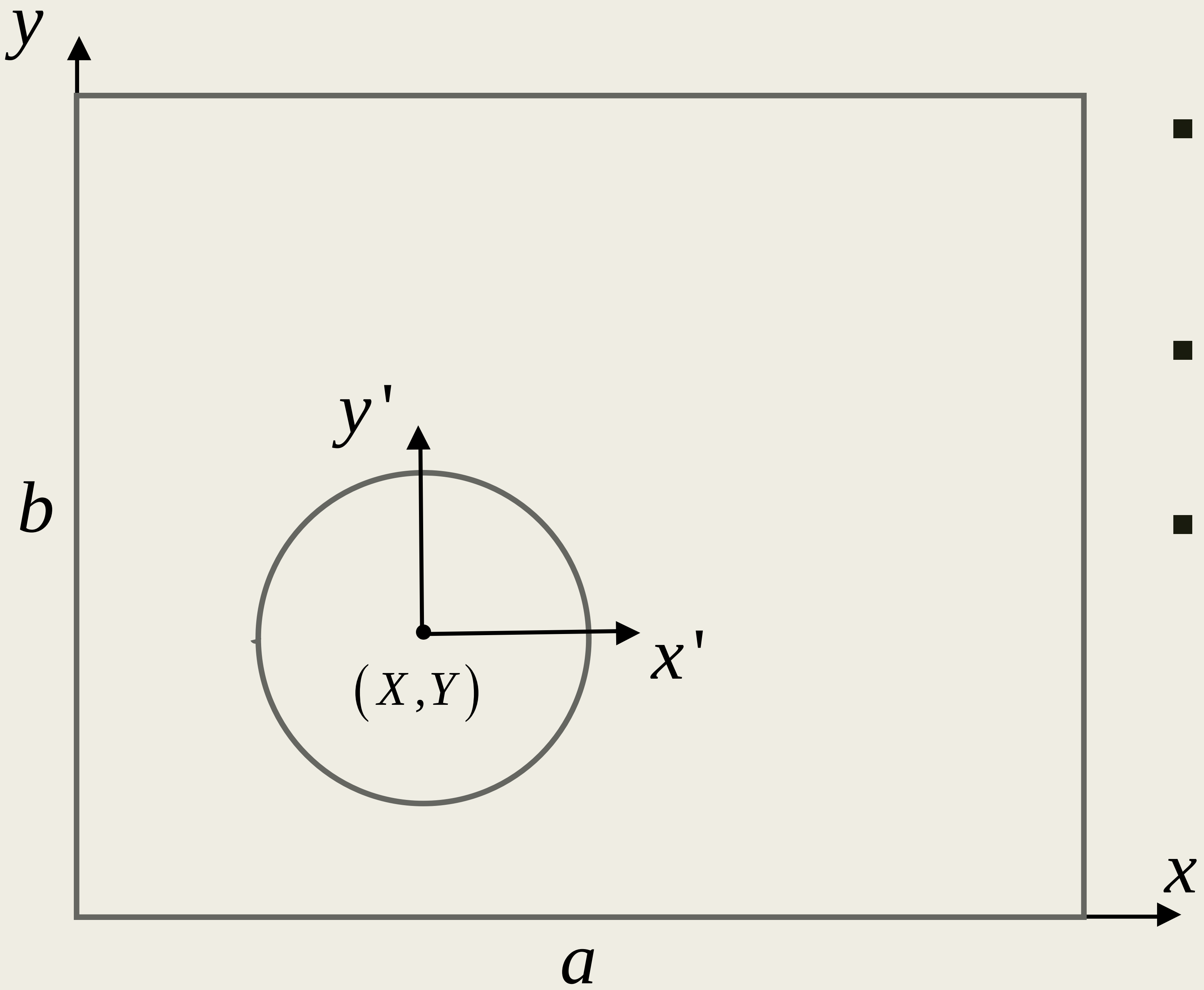



- Define coordinate system
- For this problem it is natural to use Cartesian coordinate system



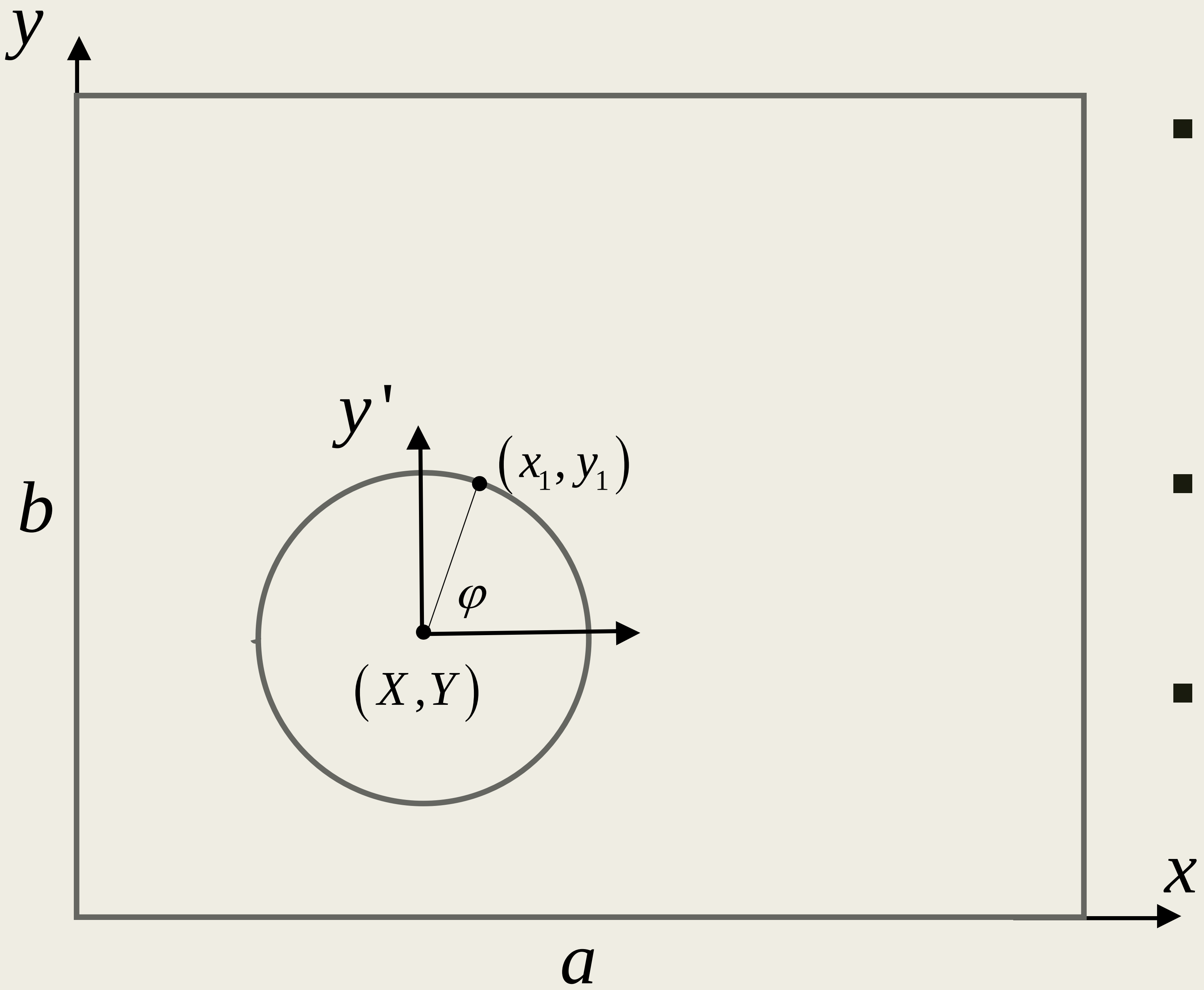

- Need for random number generator
  - let **rand** *returns random number in interval* [0, 1]

- **STEP 1**
  - *X*=*a****rand**
  - *Y*=*b****rand**




- **STEP 2**
  - move particle in arbitrary direction with step length ***d***
- **Problem!**
  - How to chose arbitrary direction?
- Draw circle with radius ***d*** with center in starting point

$$x'^2 + y'^2 = d^2$$




- **Polar coordinates**
  - Introduce new coordinate system

$$x' = \rho' \cos\varphi,\ y' = \rho \sin\varphi$$

$$\rho' = d,\ \varphi \in [0, 2\pi]$$

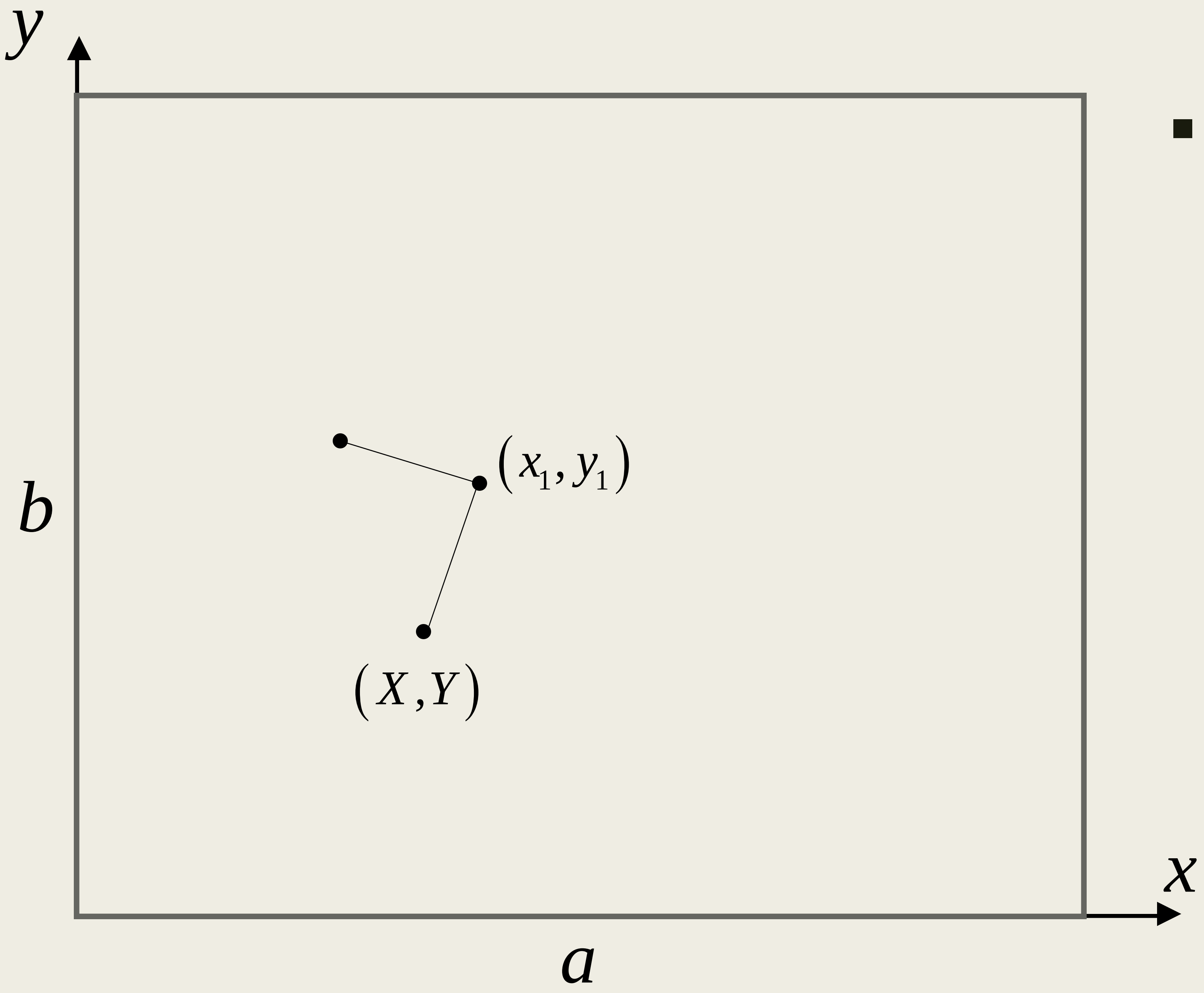
- **Generate random angle**

$$\varphi = 2\pi \cdot \text{rand}$$

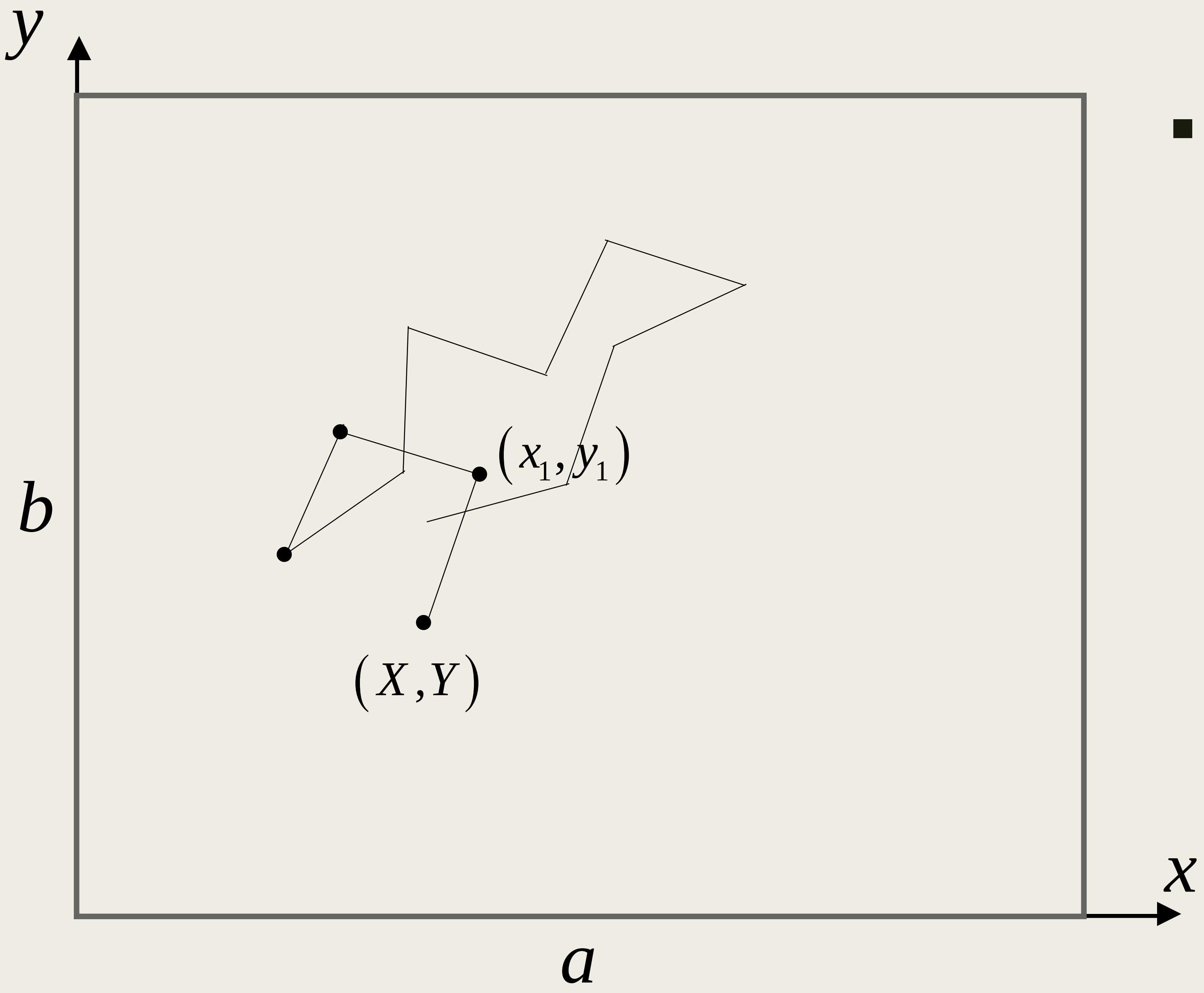
- **Calculate next point and move particle to that point**

$$x_1 = x + d\cos\varphi$$

$$y_1 = y + d\sin\varphi$$




- **STEP 3**
  - Repeat procedure




- Cycle Repetitions

# PROBABILITY THEORY CONTINIOUS VARIABLES

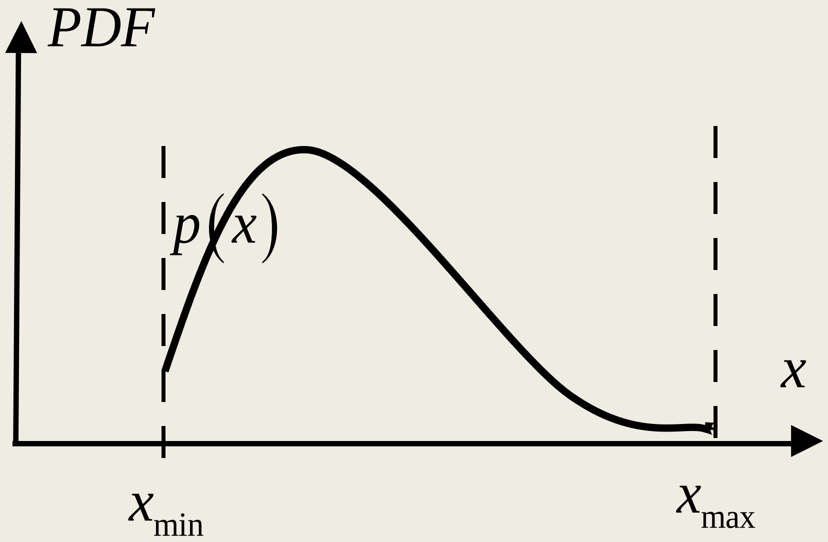
- **Random variable** – variable which value is obtained from repeatable process and its values can not be predicted with certainty (e.g. counting quanta from radioactive source)
- *x* – continuous random variable which takes values in the interval [$x_{min}$, $x_{max}$]

$$P\{x \mid x_1 < x < x_1 + dx\} = p(x_1)\,dx$$

- Probability

$$P\{x \mid x_1 < x < x_1 + dx\} = \lim_{N \to \infty} \frac{n}{N}$$

- *n* – number of values of x that falls into interval [$x_1$, $x_1$+dx]
- *N* – number of generated *x* values



# Probability Density Function - PDF

- Properties of PDF $p(x) \geq 0 \int_{x_{min}}^{x_{max}} p(x)dx = 1$
- Mean $\langle x \rangle = \int_{x_{min}}^{x_{max}} x \cdot p(x)dx$
- Standard deviation

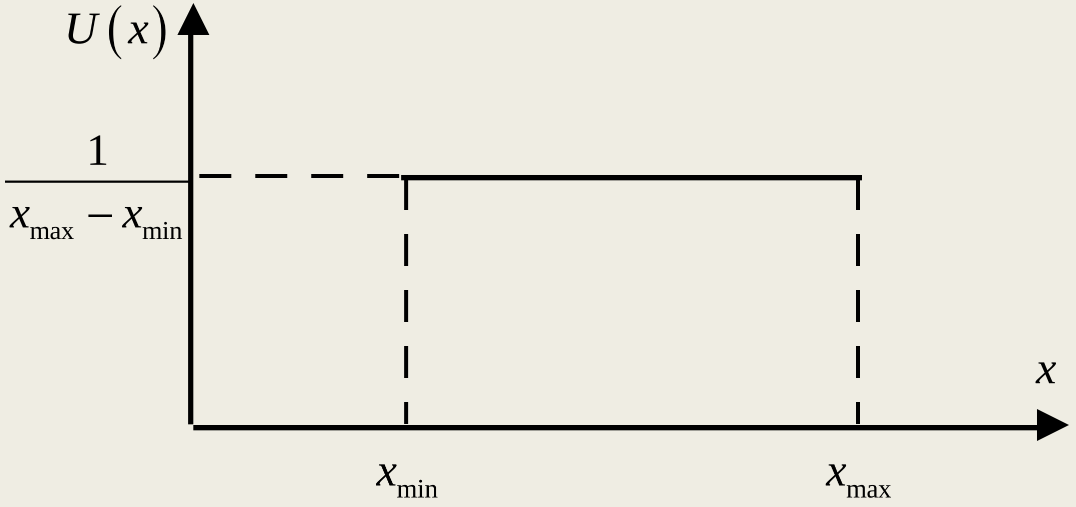
$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$\langle x^2 \rangle = \int_{x_{min}}^{x_{max}} x^2 \cdot p(x)dx$$

- Uniform distribution

$$U(x); \quad x \in [x_{min}, x_{max}]$$

$$U(x) = \begin{cases} 1/(x_{max} - x_{min}) & x_{min} \leq x \leq x_{max} \\ 0 & x < x_{min} \wedge x > x_{max} \end{cases}$$



# Cumulative Distribution - CD

- Cumulative distribution is defined as $CD(x) = \int_{x_{\min}}^{x} p(x)dx$

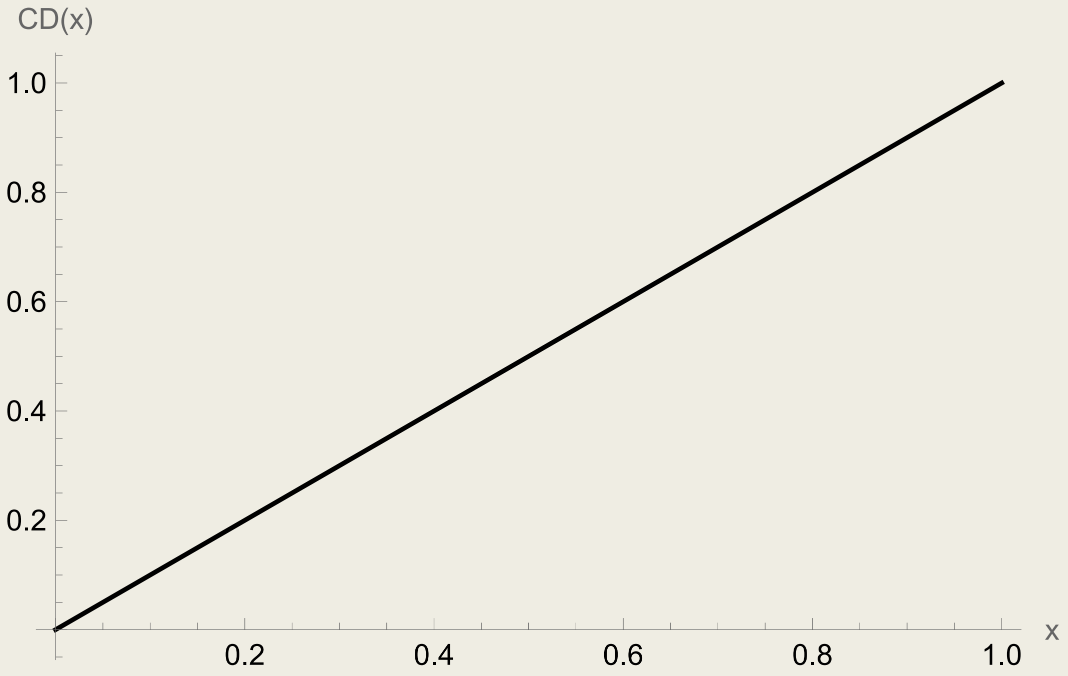
$$P(x \mid a < x < b) = \int_a^b p(x)dx = CD(b) - CD(a)$$

$$p(x) = \frac{dCD(x)}{dx}$$

- For uniform distribution

$$U(x) = \begin{cases} 1 & 0 \le x \le 1 \\ 0 & x < 0 \wedge x > 1 \end{cases}$$

$$CDU(x) = x,\ x \in [0, 1]$$



# Method of Random Sampling Inverse function method

- Let us introduce new variable *ξ, where x* -> *ξ* as $\xi = f(x)$
- We derived new PDF, where $p_\xi(\xi)d\xi = p(x)dx$
- If we chose $\xi = CD(x), \xi \in [0,1]$

$$p_\xi(\xi) = p(x)\frac{dx}{d\xi} = p(x)\left(\frac{d\xi}{dx}\right)^{-1}$$

$$p_\xi(\xi) = p(x)\left(\frac{d\xi}{dx}\right)^{-1} = p(x)\left(\frac{dCD(x)}{dx}\right)^{-1}$$

- Since $p(x) = \frac{dCD(x)}{dx}$
- We derive

$$p_\xi(\xi) = p(x)(p(x))^{-1} = 1$$

- **IMPORTANT**
  - ***ξ*** **is uniformly distributed on interval [0, 1]**

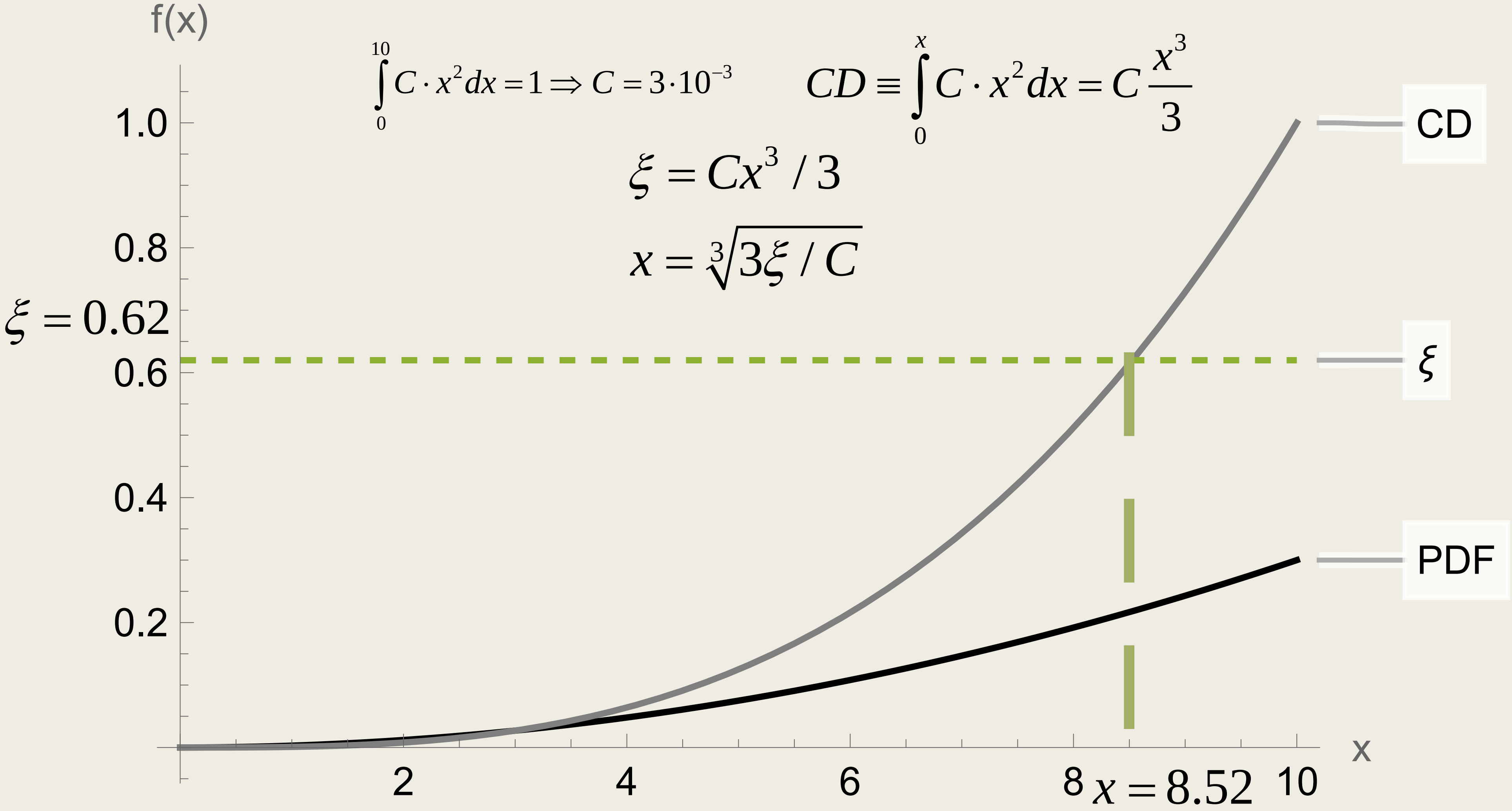
# EXAMPLE $PDF \equiv C \cdot x^2,\ x \in [0, 10]$

$$\int_0^{10} C \cdot x^2 dx = 1 \Rightarrow C = 3 \cdot 10^{-3}$$

$$CD \equiv \int_0^x C \cdot x^2 dx = C\frac{x^3}{3}$$

$$\xi = Cx^3 / 3$$

$$x = \sqrt[3]{3\xi / C}$$



# Inverse function method EXAMPLES

$$\xi = CD(x) = \int_{x_{\min}}^{x} p(x)dx$$

- Uniform distribution

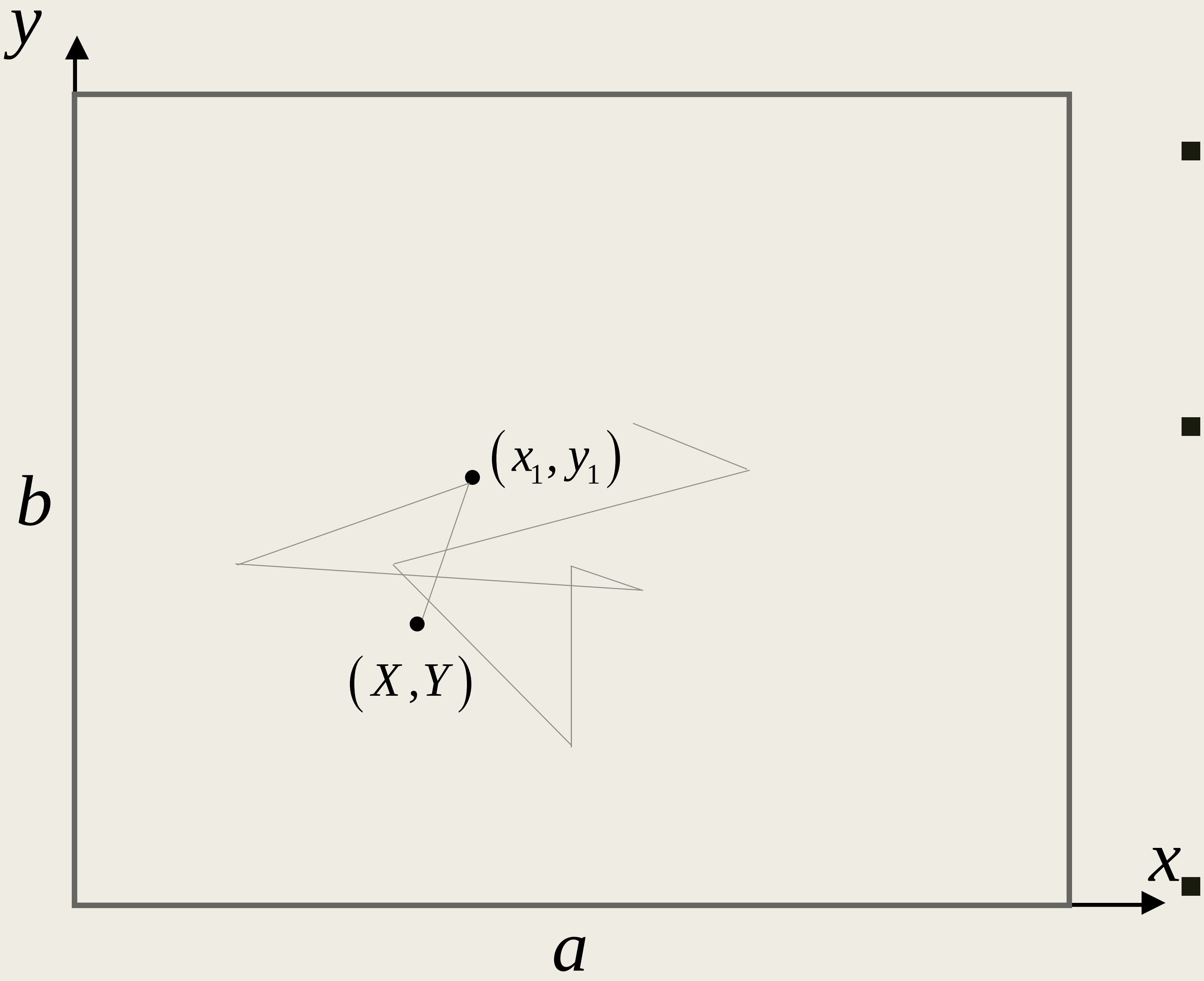
$$U_{a,b}(x) = \frac{1}{b-a} \qquad x = a + \xi(b-a)$$

- Exponential distribution

$$p(x) = \frac{1}{\lambda} e^{-\frac{x}{\lambda}}, \; x \geq 0$$

$$x = -\lambda \ln(1-\xi) \equiv -\lambda \ln(\xi)$$

- Exponential distribution is the PDF of the free path of particle between interaction events
- λ is mean free path
- **Now our example with two-dimensional random movement of Brownian particle can be more realistic (we know how to sample free path)**




- Free path

$$d = -\lambda \ln(\xi)$$

$$\xi = \text{rand}$$

- To sample free path, we need to know mean free path λ

$$\varphi = 2\pi \cdot \text{rand}$$

$$x_1 = X + d\cos\varphi$$

$$y_1 = Y + d\sin\varphi$$

- WE STILL DO NOT KNOW HOW TO CREATE **rand** FUNCTION

# Rejection sampling method

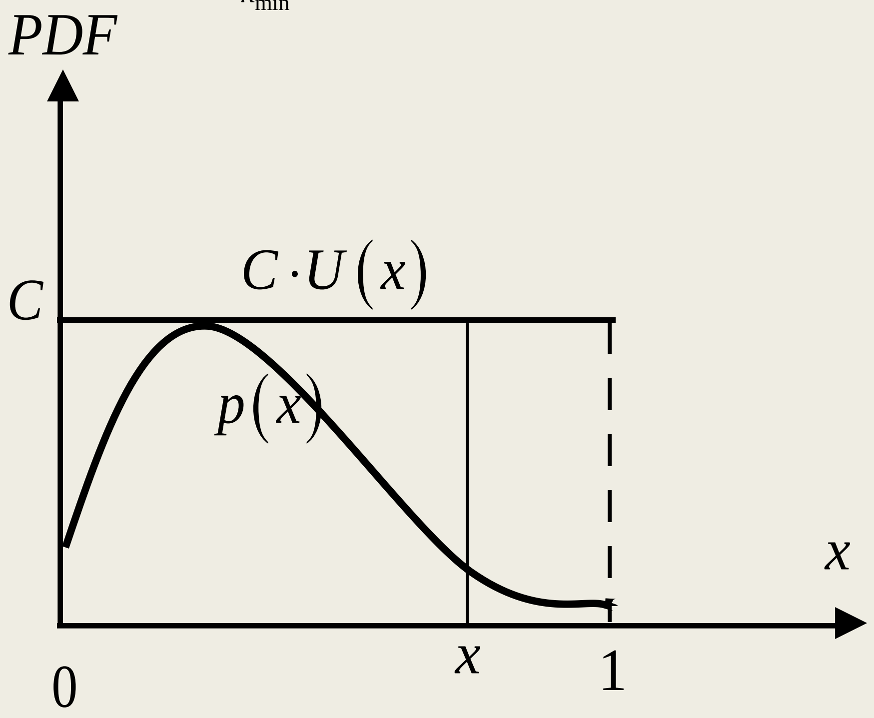
- Inverse transformation method is based on functional dependance between variables ξ and x
- In some cases, this function is unknown analytically or integral $\xi = \int_{x_{\min}}^{x} p(x)dx$ cannot be solved
- Sample x from arbitrary known PDF

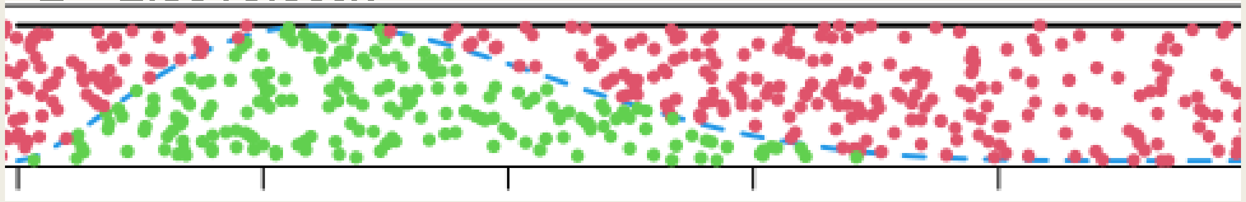
e.g. $U(x)$

- Sample random variable from $U(x)$

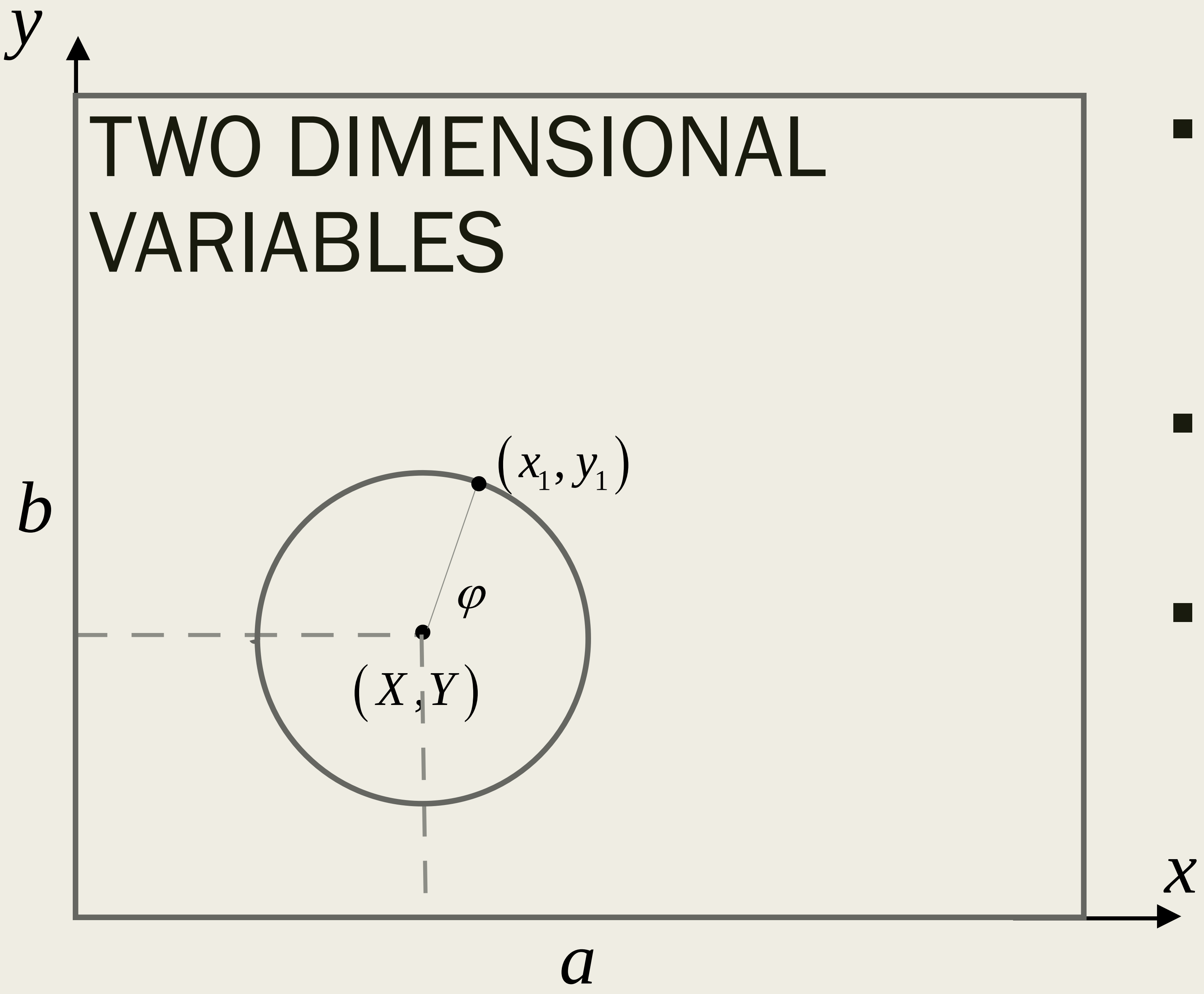
$$x = \text{rand}$$

- Sample new random number $\xi = \text{rand}$
- **If C·ξ<p(x) accept x**
- **Else reject x**



# TWO DIMENSIONAL VARIABLES




- Random number generator
  - **rand** *returns random number in interval* [0, 1]

- **STEP 1**
  - *X=a****rand***
  - *Y=b****rand***
- **STEP 2**

$$\varphi = 2\pi \cdot \text{rand}$$

$$x_1 = x + d\cos\varphi$$
$$y_1 = y + d\sin\varphi$$

# TWO DIMENSIONAL VARIABLES POINT ON THE SPHERE

- In theory of radiation transport direction of motion of particle can be described with unit vector

$$\vec{d} = (u,v,w) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

- Probability for point to have coordinates on unit sphere is

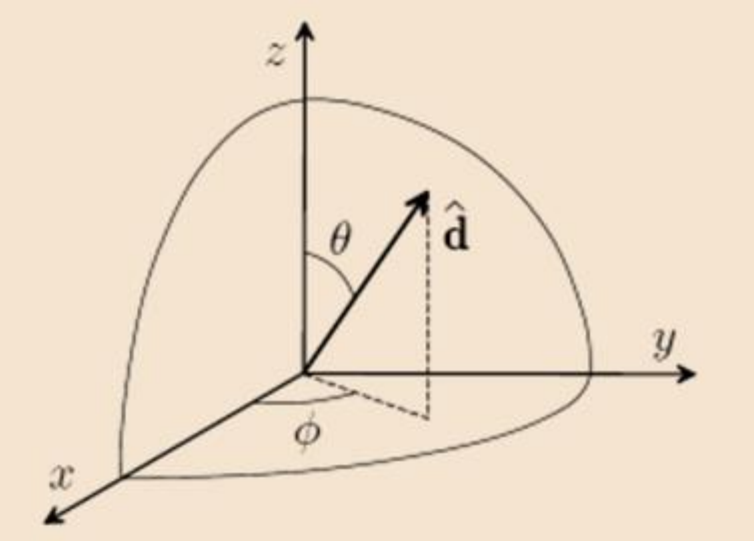
$$p(\theta,\phi)\,d\theta d\phi = \frac{ds}{S} = \frac{\sin\theta d\theta d\phi}{4\pi}$$

$$p(\theta,\phi) = \frac{\sin\theta}{2}\frac{1}{2\pi} = p_\theta(\theta)\,p_\phi(\phi)$$

$$p_\theta(\theta) = \frac{\sin\theta}{2}$$

$$p_\phi(\phi) = \frac{1}{2\pi}$$

$$\xi = \int_{x_{\min}}^{x} p(x)dx$$




1. F. Salvat et al, PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon transport , Workshop proceedings, Barcelona, Spain 2011

- By inverse method we get

$$\theta = \arccos\left(1-2\xi_1\right) \qquad \phi = 2\pi\xi_2$$

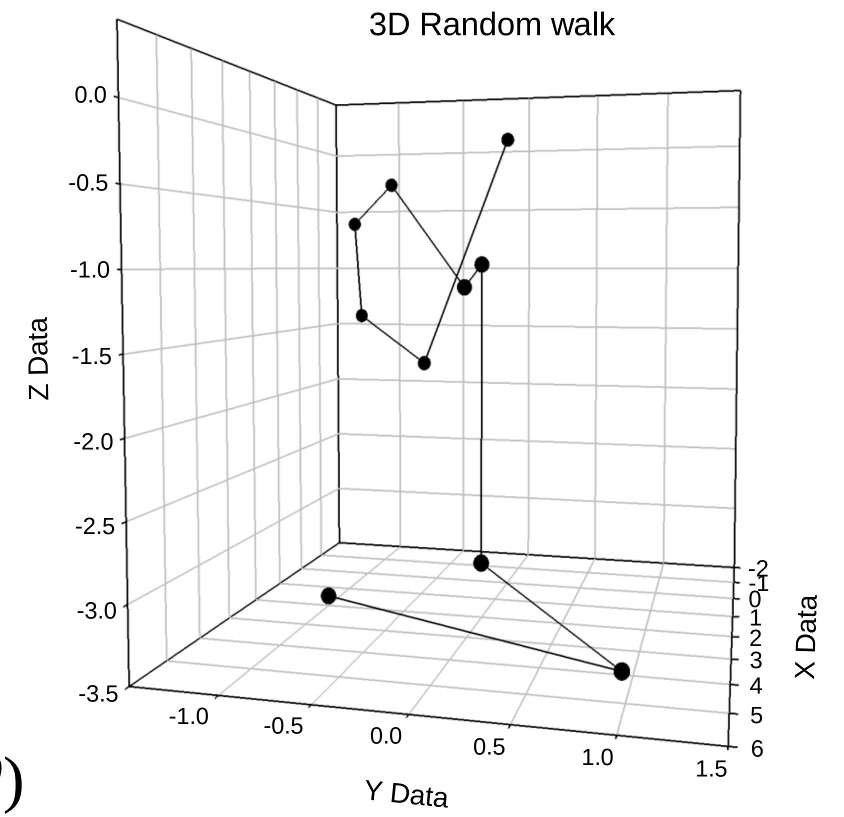
- Now we can move particle in arbitrary direction in space for randomly sampled free path. If starting point is $(x_0, y_0, z_0)$

$$\vec{d} = (u,v,w) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

final point is $(x_0 + x, y_0 + y, z_0 + z)$

where $(x,y,z) = (d\sin\theta\cos\phi, d\sin\theta\sin\phi, d\cos\theta)$

$$d = -\lambda\ln\left(\xi_3\right)$$




Example with Mathematica code

```
lam=1;
x[0]=0;
y[0]=0;
z[0]=0;
```

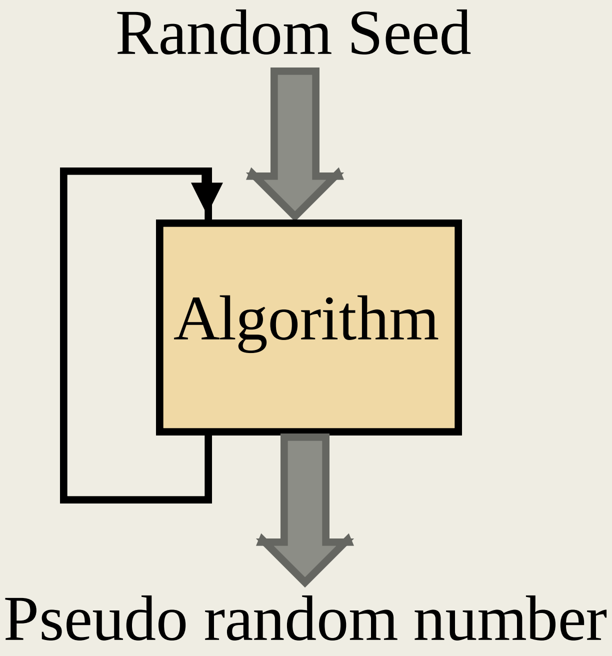
```
Do[
 d=-lam*Log[RandomReal[]];
 Theta=ArcCos[1-2*RandomReal[]];
 Phi=2*π*RandomReal[];
 x[I]=x[I-1]+d*Sin[Theta]*Cos[Phi];
 y[I]=y[I-1]+d*Sin[Theta]*Sin[Phi];
 z[I]=z[I-1]+d*Cos[Theta];
 ,{I,1,10}]
```

```
Table[{x[I],y[I],z[I]},{I,0,10}]
{{0,0,0},{0.856794,-0.488536,-1.72351},{-1.04082,-1.17474,-1.40488},{-0.758415,-1.18502,-0.631209},
{-0.82377,-0.915295,-0.307849},{3.11599,0.415882,-0.901731},{3.52462,0.0407051,-1.11712},
{3.27205,0.117112,-0.970174},{4.49777,0.22331,-2.79603},{5.10449,0.985619,-3.29611},
{4.59319,-0.614773,-3.05726}}
```

# RANDOM NUMBERS

- First step of Monte Carlo simulations are numerical sampling of relevant variables from specified PDF.
- Random sampling algorithms are based on the use of RANDOM NUMBERS uniformly distributed in the interval [0, 1]
- TRUE random numbers cannot be generated from algorithm process, they should be sampled from some true random physical process
- For the computer based simulations PSEUDO RANDOM numbers are in use

# PSEUDO RANDOM NUMBERS




- Pseudo random numbers are not true random numbers,

  since they are generated using algorithm
- Even do they are not true random numbers, if you are given with sequence of pseudo random numbers, it should past randomness tests
- QUOTE from N. METROPOLIS[1]

"How are the various decisions made? To start with, the computer must have a source of uniformly distributed psuedo-random numbers.
A much used algorithm for generating such numbers is the so-called von Neumann "middle-square digits." Here, an arbitrary n-digit integer is squared, creating a 2n-digit product. A new integer is formed by extracting the middle n-digits from the product."

$$123456^2 = 15\,\mathbf{241\,383}\,936 \qquad 241\,383^2 = 58\,\mathbf{265\,752}\,689\,\ldots$$

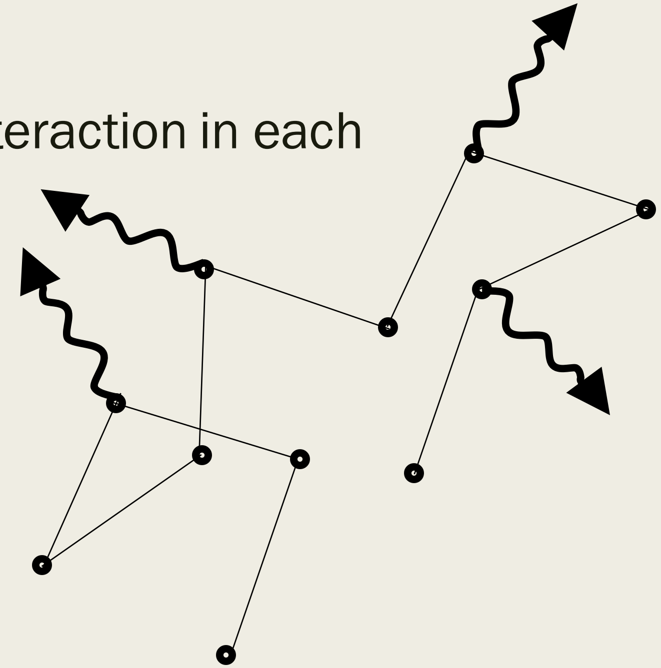
1. N. Metropolis, "The beginning of the Monte Carlo method", Los Alamos Science Special Issue 125-130 (1987)

```
C  ***********************************************************************
C                          FUNCTION RAND
C  ***********************************************************************
      FUNCTION RAND(DUMMY)
C
C  This is an adapted version of subroutine RANECU written by F. James
C  (Comput. Phys. Commun. 60 (1990) 329-344), which has been modified to
C  give a single random number at each call.
C
C  The 'seeds' ISEED1 and ISEED2 must be initialised in the main program
C  and transferred through the named common block /RSEED/.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER*4 (I-N)
      PARAMETER (USCALE=1.0D0/2.147483563D9)
      COMMON/RSEED/ISEED1,ISEED2
C
      I1=ISEED1/53668
      ISEED1=40014*(ISEED1-I1*53668)-I1*12211
      IF(ISEED1.LT.0) ISEED1=ISEED1+2147483563
C
      I2=ISEED2/52774
      ISEED2=40692*(ISEED2-I2*52774)-I2*3791
      IF(ISEED2.LT.0) ISEED2=ISEED2+2147483399
C
      IZ=ISEED1-ISEED2
      IF(IZ.LT.1) IZ=IZ+2147483562
      RAND=IZ*USCALE
C
      RETURN
      END
```

1. F. Salvat et al, PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon transport , Workshop proceedings, Barcelona, Spain 2011

# SIMULATION OF RADIATION TRANSPORT
# Detailed methods – Track structure codes

- All interaction events are simulated in chronological succession – event by event
- Set of all events is often called history of one particle
- In opposite of Brownian particle, radiation quanta can exhibit interaction in each event
- In interactions secondary particles can be created

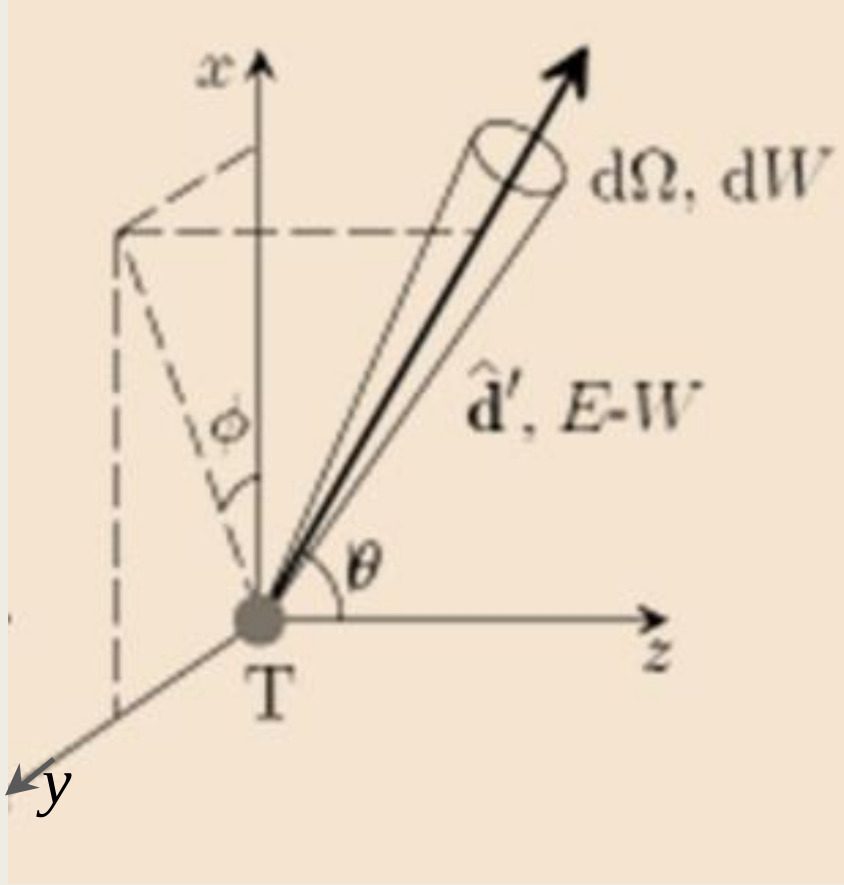


# INTERACTION MODELING - CROSSECTTIONS

- Radiation interact with medium through various competing mechanisms. Each interaction event is associated with appropriate differential cross section DFS

- Double deferential cross section - $\sigma(\Omega, W) = \frac{d^2\sigma}{d\Omega dW}$

- Total cross section $\sigma = \int_W \int_\Omega \sigma(\Omega, W) d\Omega dW$




1. F. Salvat et al, PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon transport , Workshop proceedings, Barcelona, Spain 2011

# MEAN FREE PATH AND SCATTERING MODEL

- Total cross section $\sigma$ can be related to mean free path $\lambda$ for given medium

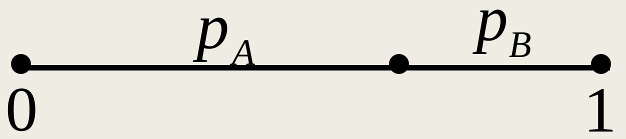
$$N = N_{\mathrm{A}} \frac{\rho}{A_{\mathrm{M}}} \qquad A_{\mathrm{M}} = n_i A_i \qquad \lambda = \frac{1}{N\sigma}$$

- Suppose that particle can interact via two independent mechanisms A, and B

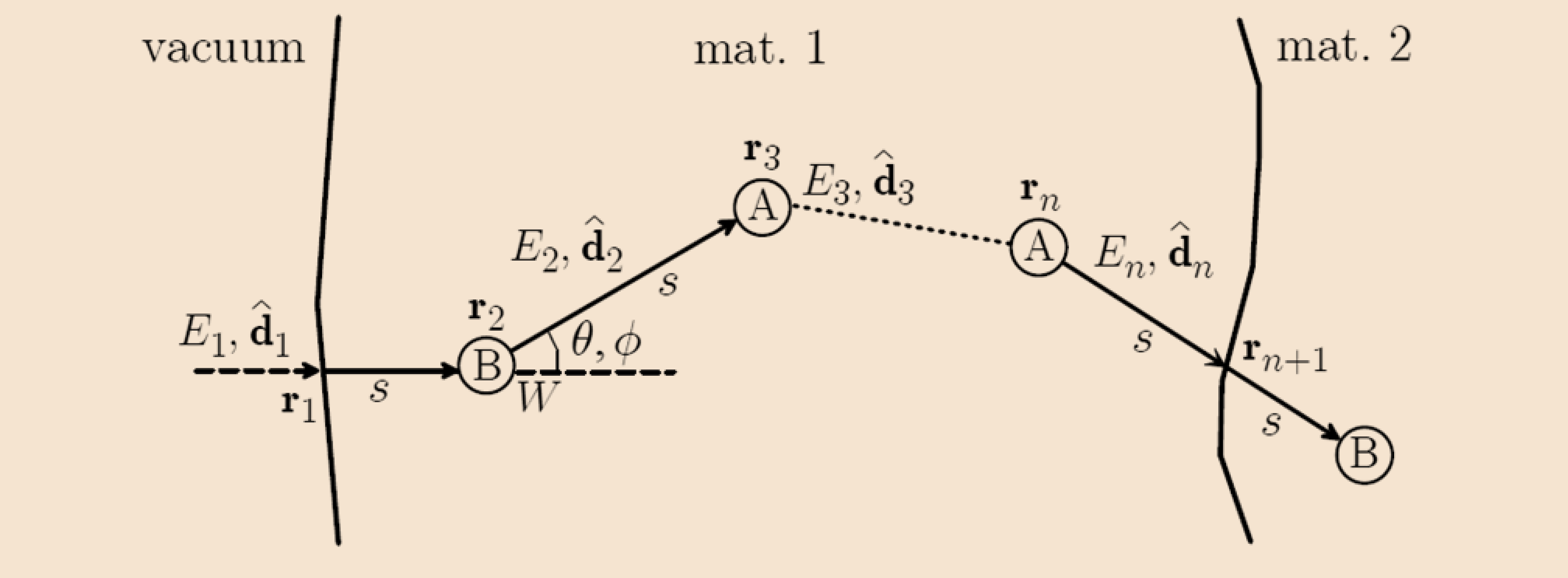
$$\frac{d^2\sigma_A}{d\Omega dW} \qquad \frac{d^2\sigma_B}{d\Omega dW} \qquad \sigma_T = \sigma_A + \sigma_B$$

$$\lambda_T = \frac{1}{N\sigma_T} \qquad \lambda_A = \frac{1}{N\sigma_A} \qquad \lambda_B = \frac{1}{N\sigma_B} \qquad \frac{1}{\lambda_T} = \frac{1}{\lambda_A} + \frac{1}{\lambda_B}$$

$$p_A = \frac{\sigma_A}{\sigma_T} \qquad p_B = \frac{\sigma_B}{\sigma_T}$$



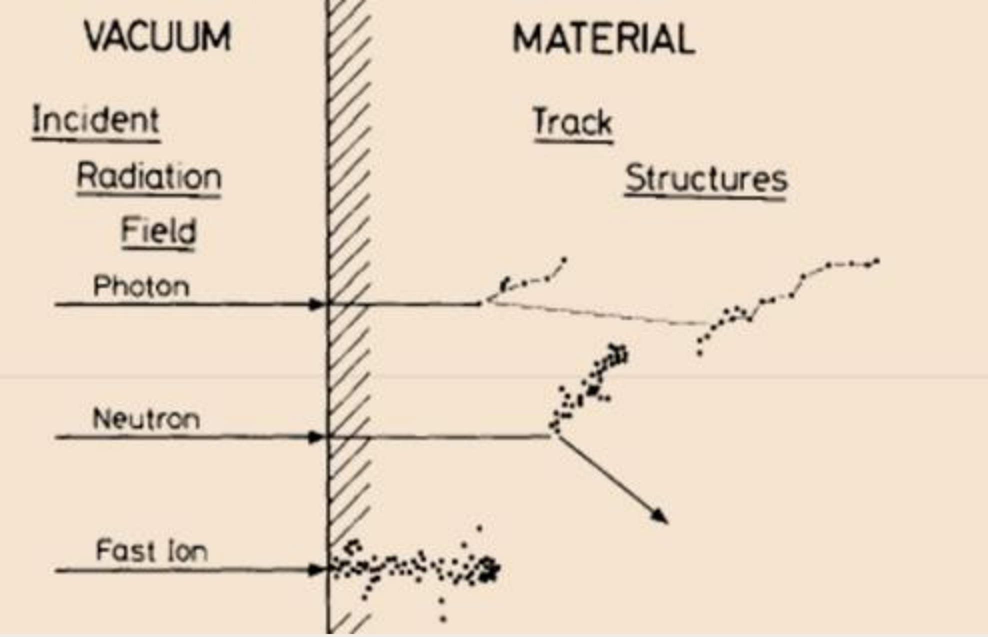
# GNERATION OF RANDOM TRACK – Markov process




- Generation of random tracks using detailed simulation

1. F. Salvat et al, PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon transport , Workshop proceedings, Barcelona, Spain 2011

# SECONDARY PARTICLES



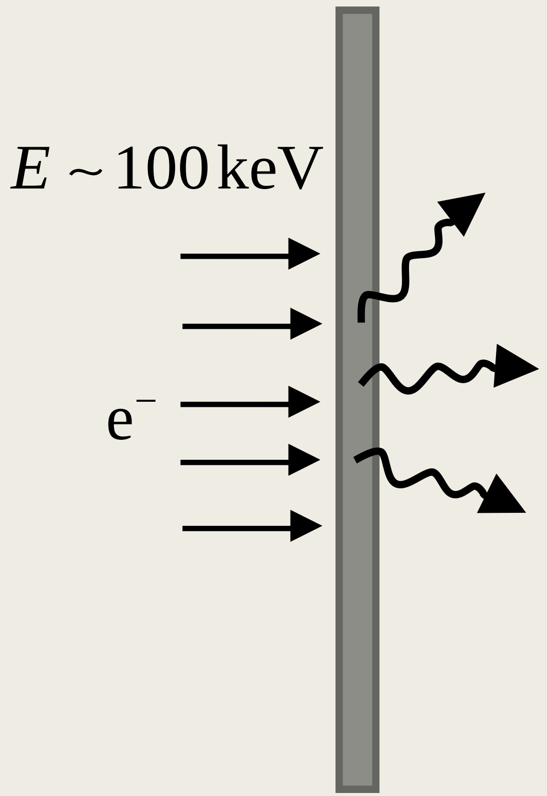

- In collision event secondary particles can be created
  - photons, electrons, delta rays, …
- In Detail Simulation generated secondary particles are scored, their properties are stored in appropriate variables
- Secondary particles are simulated after simulation of primary particle (the one that generated secondaries) and are treated in same manner as primary one

# VARIANCE REDUCTION METHODS

- Statistical uncertainty of relevant quantities calculated using Monte Carlo method can be reduced, without increasing number of histories and enlarging computation time using VARIANCE REDUCTION METHODS
- This is done by optimizing particular problem, and Variance Reduction methods are problem dependent
- Lowering statistical uncertainty of relevant quantity is at expense of uncertainties of other quantities

# VARIANCE REDUCTION METHODS
# Interaction forcing

- In cases of low interaction probability, variance can be high, since that events happens very really
- Example – 100 keV electrons imparted on thin foil. Radiate events are much less probable than elastic and inelastic scattering
- If we want to calculate Bremsstrahlung photon spectrum great deal of histories in needed because of low probability of radiative events



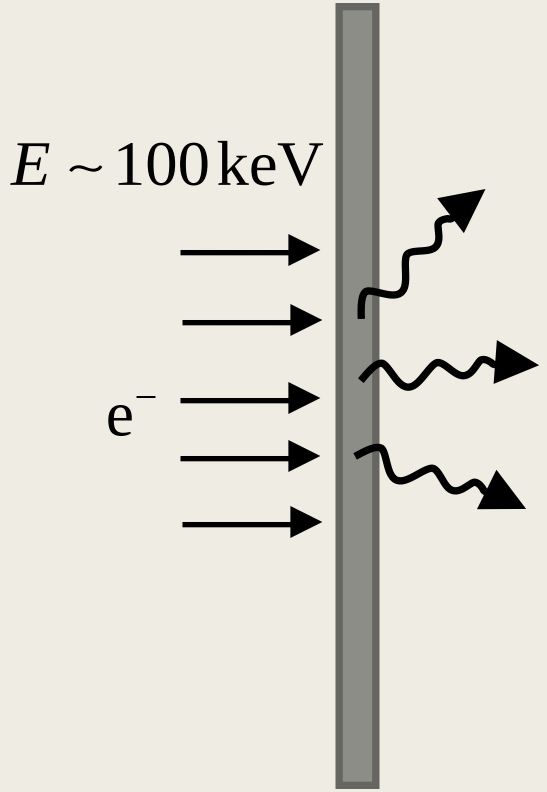
# VARIANCE REDUCTION METHODS
## Interaction forcing

- Variance Reduction of Bremsstrahlung photon spectrum – force radiative events to happened more frequently

$\lambda_{\mathrm{A}} \to \lambda_{\mathrm{A},f}$ replace mean free path with shorter one

$F = \dfrac{\lambda_{\mathrm{A}}}{\lambda_{\mathrm{A},f}} > 1$ interaction probability increases for factor *F*

- By increasing interaction probability simulation is biased. Un biasing requires introducing of weighting factors



# VARIANCE REDUCTION METHODS
# Interaction forcing

- Associate weighting factors for primary particle

$$\omega = 1$$

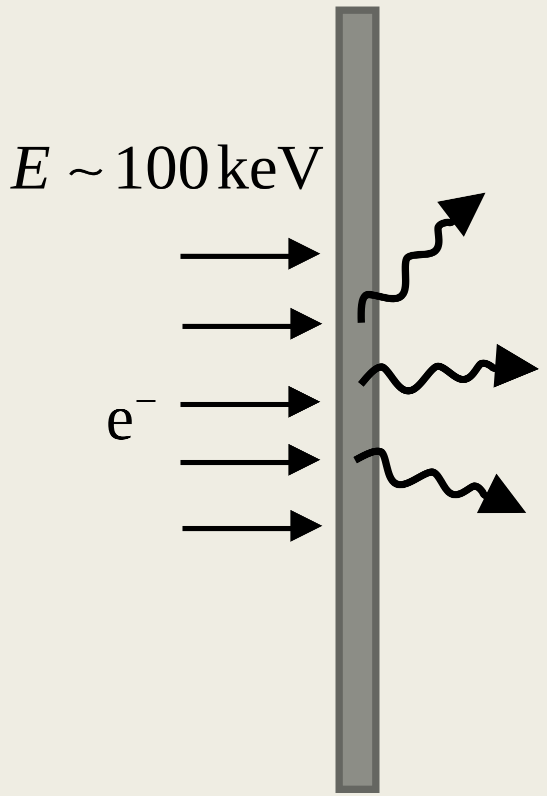
- Prediction of secondary particles is alerted by interaction forcing. Associate weighting factors for secondary particles

$$\omega_s = \frac{\omega}{F}$$

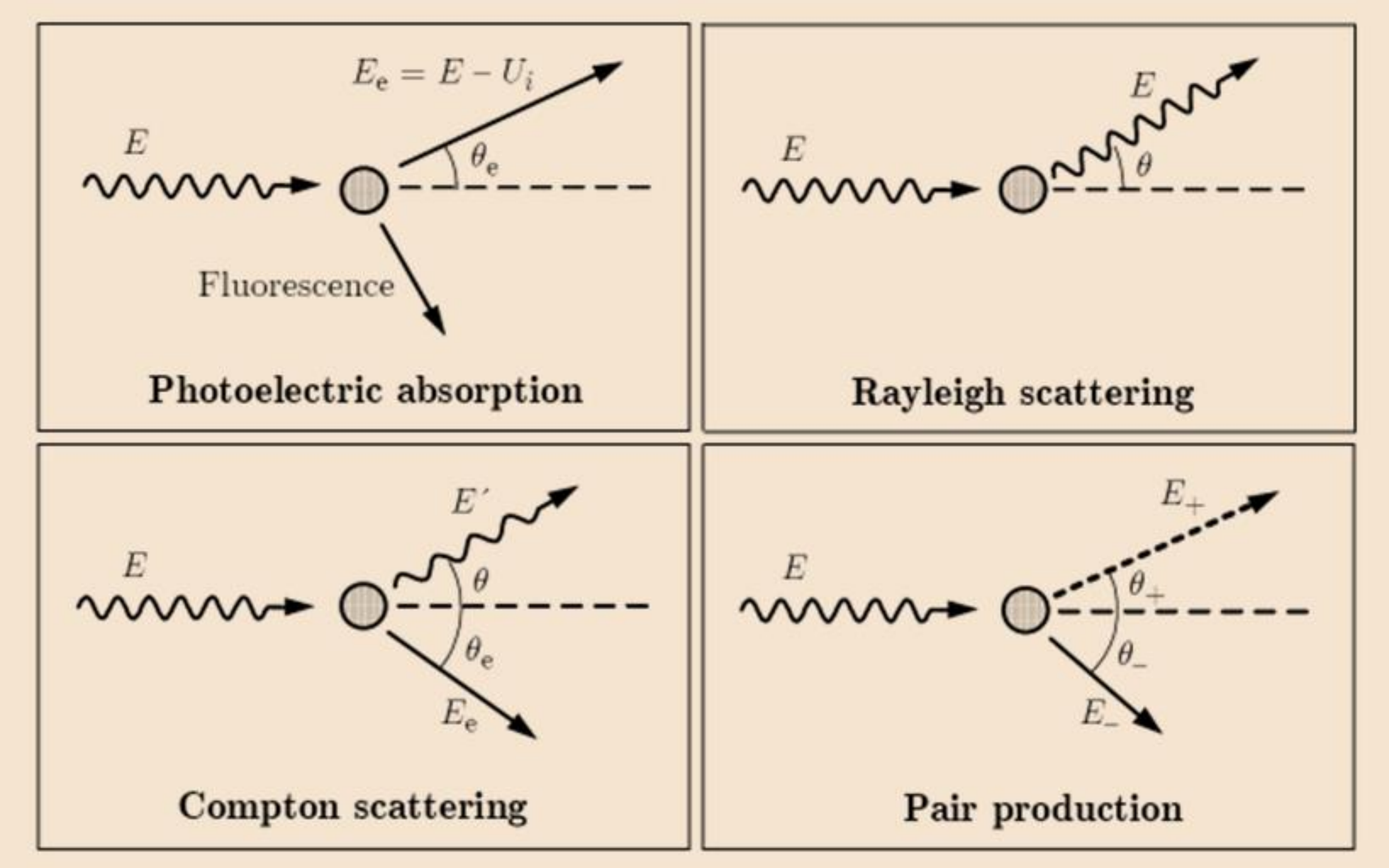
- Give weight to e.g. deposited energy if it is calculated from interaction forcing particles

$$\omega_E = \frac{\omega}{F}$$

- Interaction forcing reduce variance for some calculation, but increase for others and can insert bias in simulation



# PHOTON INTERACTIONS

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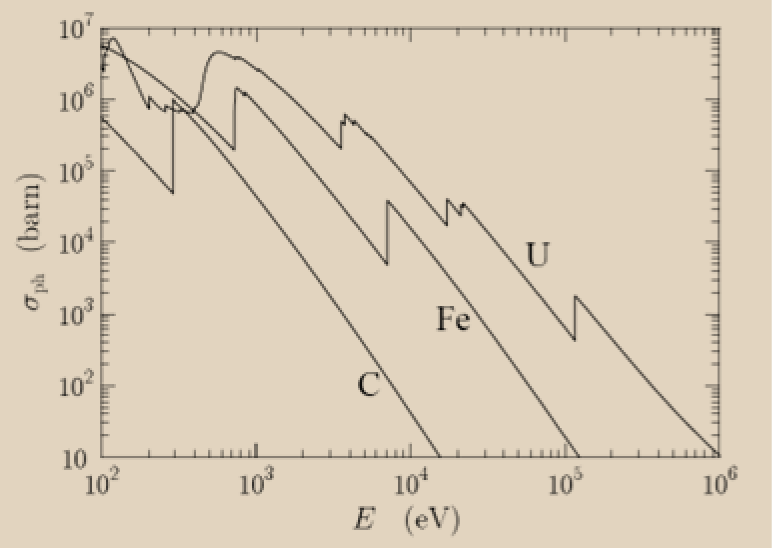
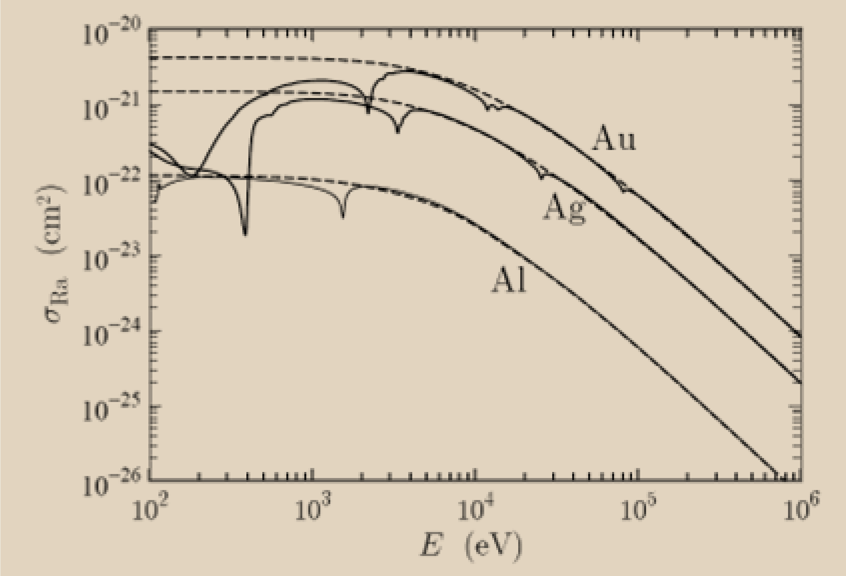
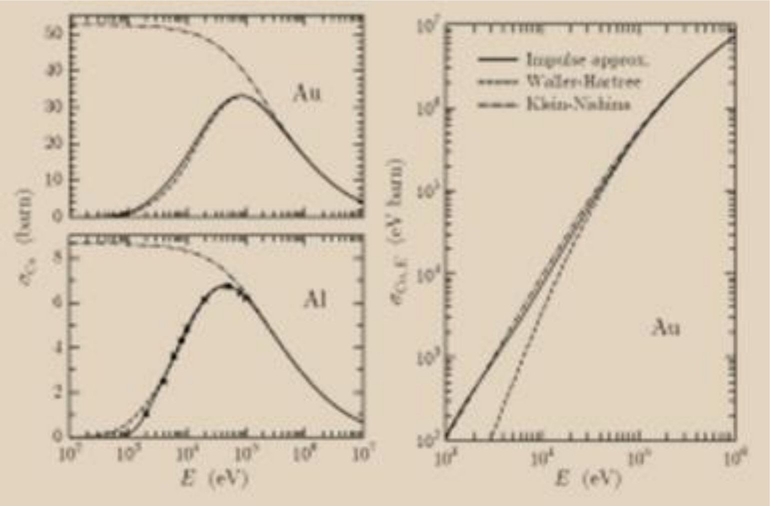
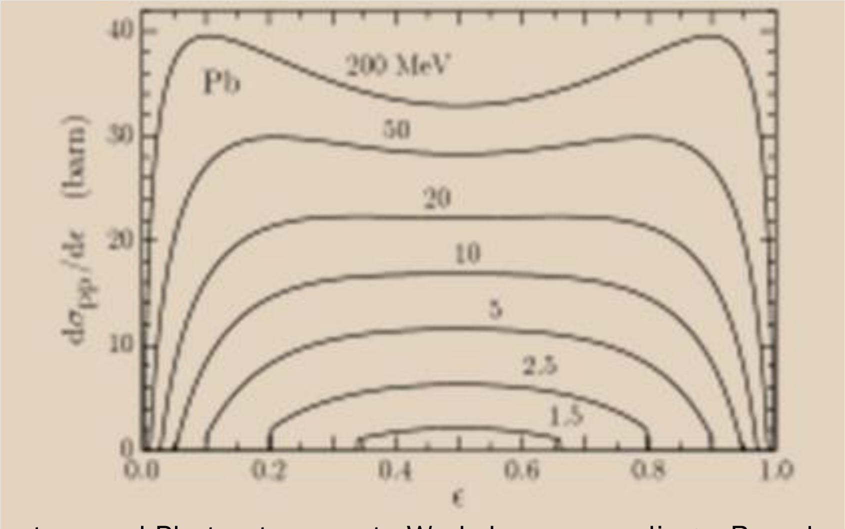
# PHOTON CROSS SECTION

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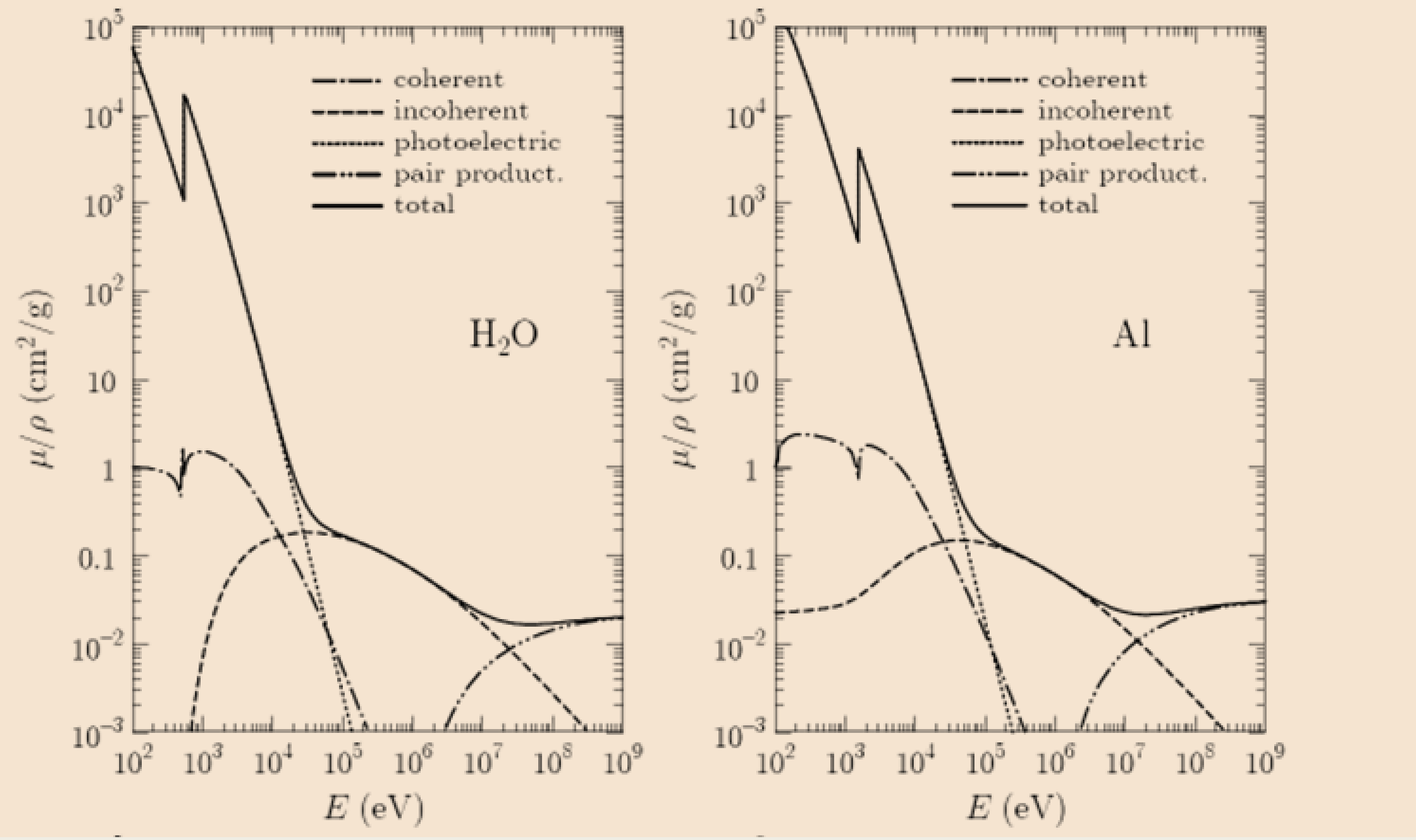
# ATTENUATION COEFFICIENTS

$$\frac{\mu}{\rho} = \frac{N_{\mathrm{A}}}{A_{\mathrm{M}}}\left(\sigma_{\mathrm{Ra}} + \sigma_{\mathrm{Co}} + \sigma_{\mathrm{ph}} + \sigma_{\mathrm{pp}}\right)$$

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# ATTENUATION COEFFICIENTS

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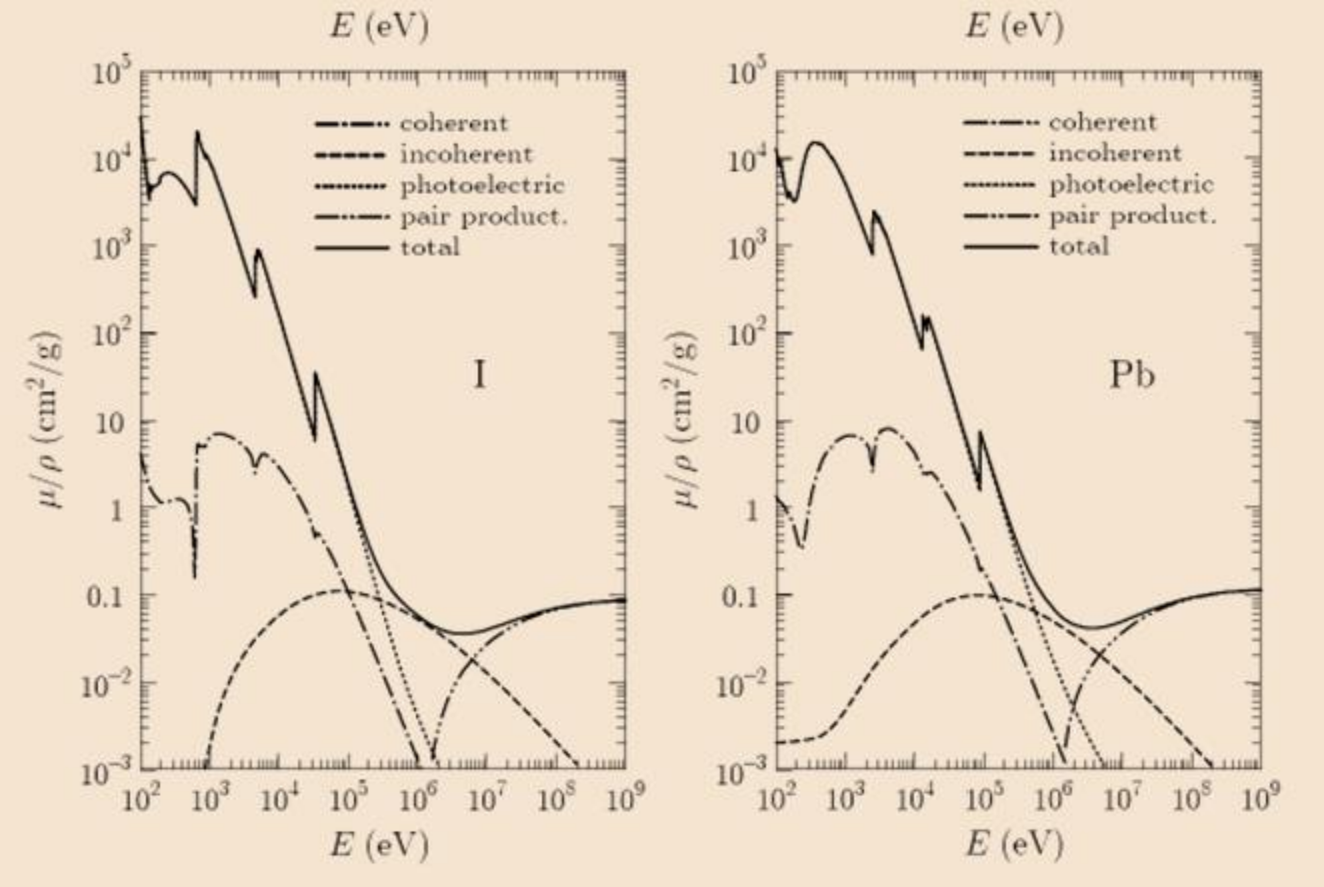


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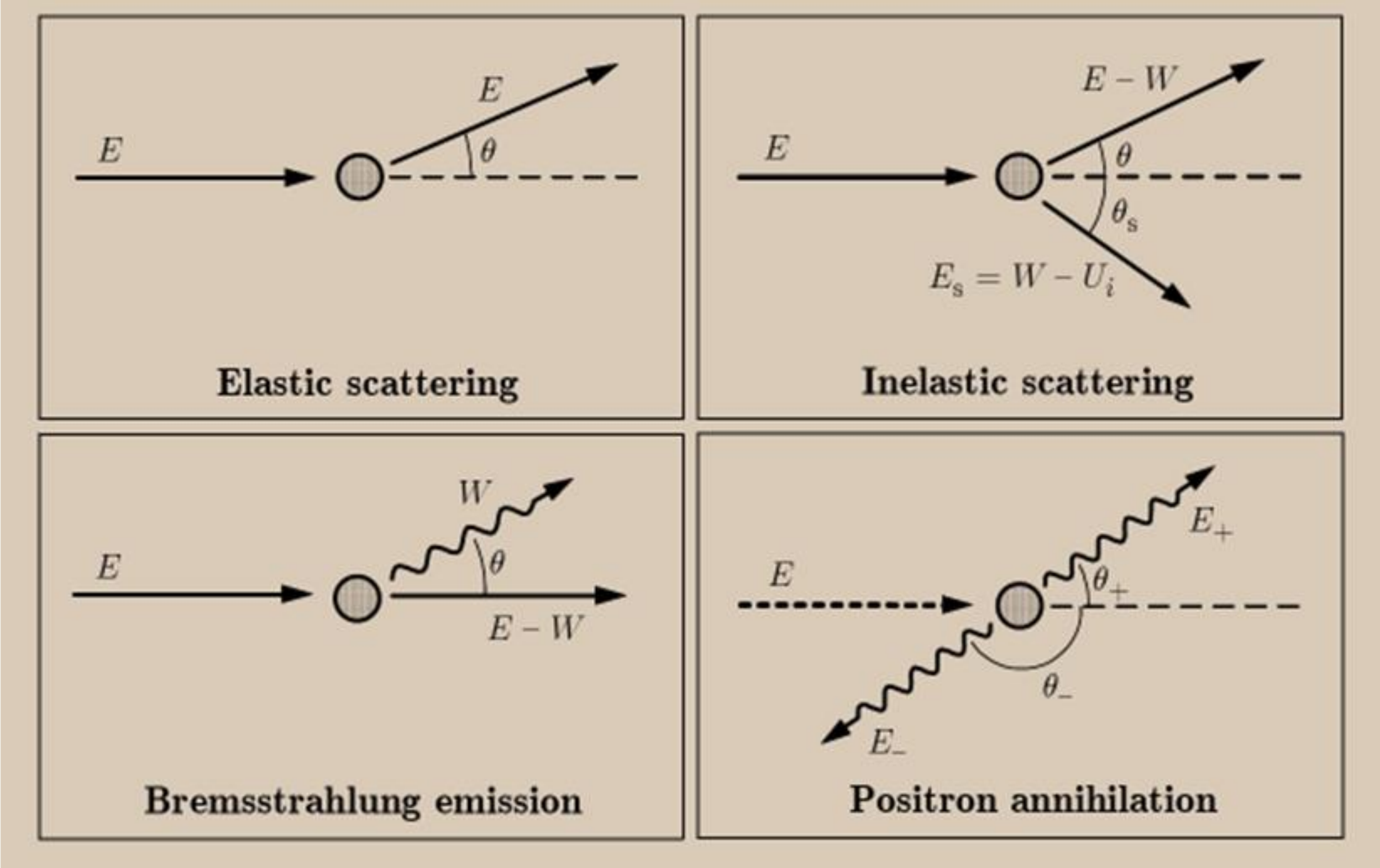
# ELECTRON AND POSITRON INTERACTION

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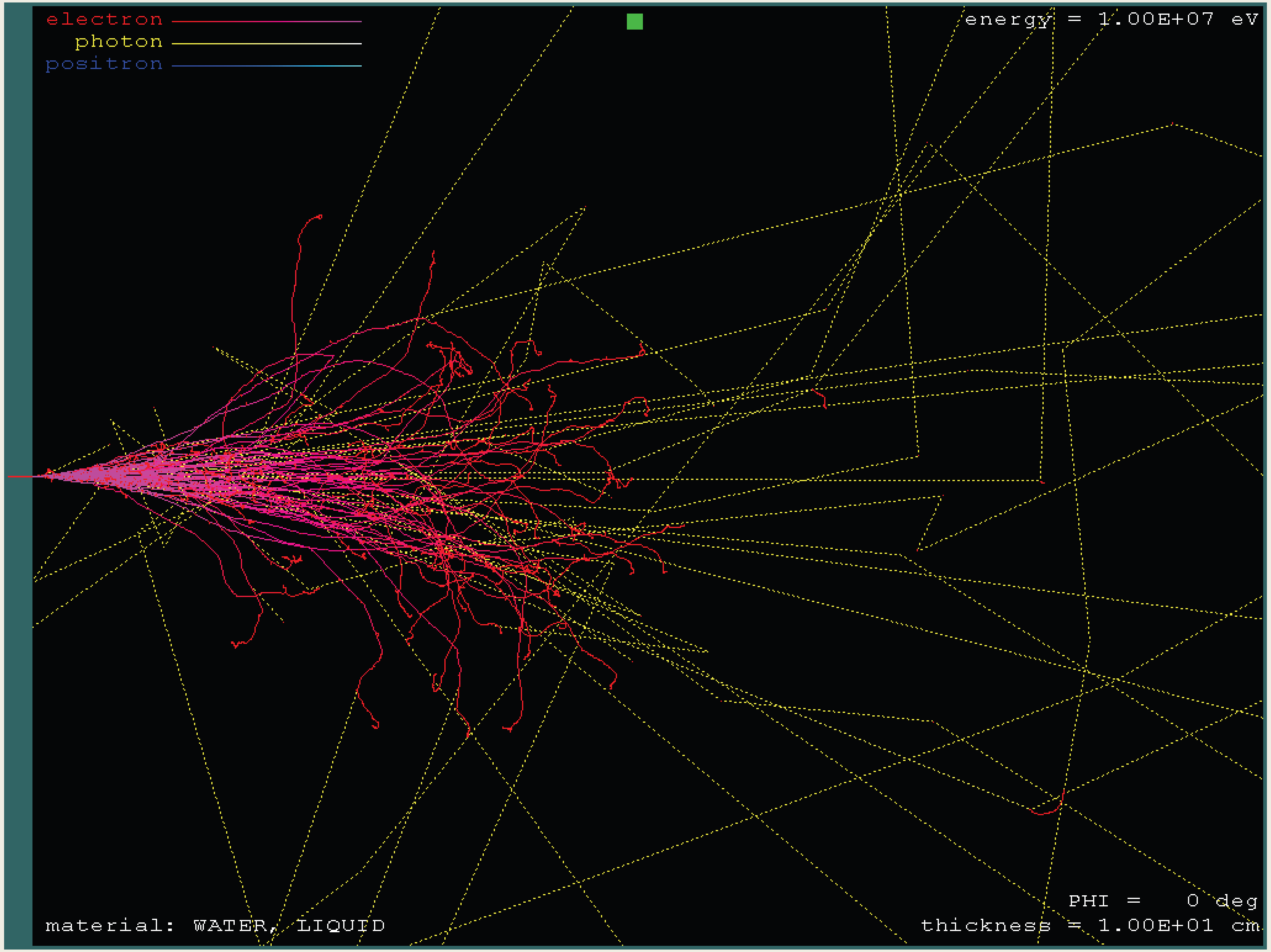
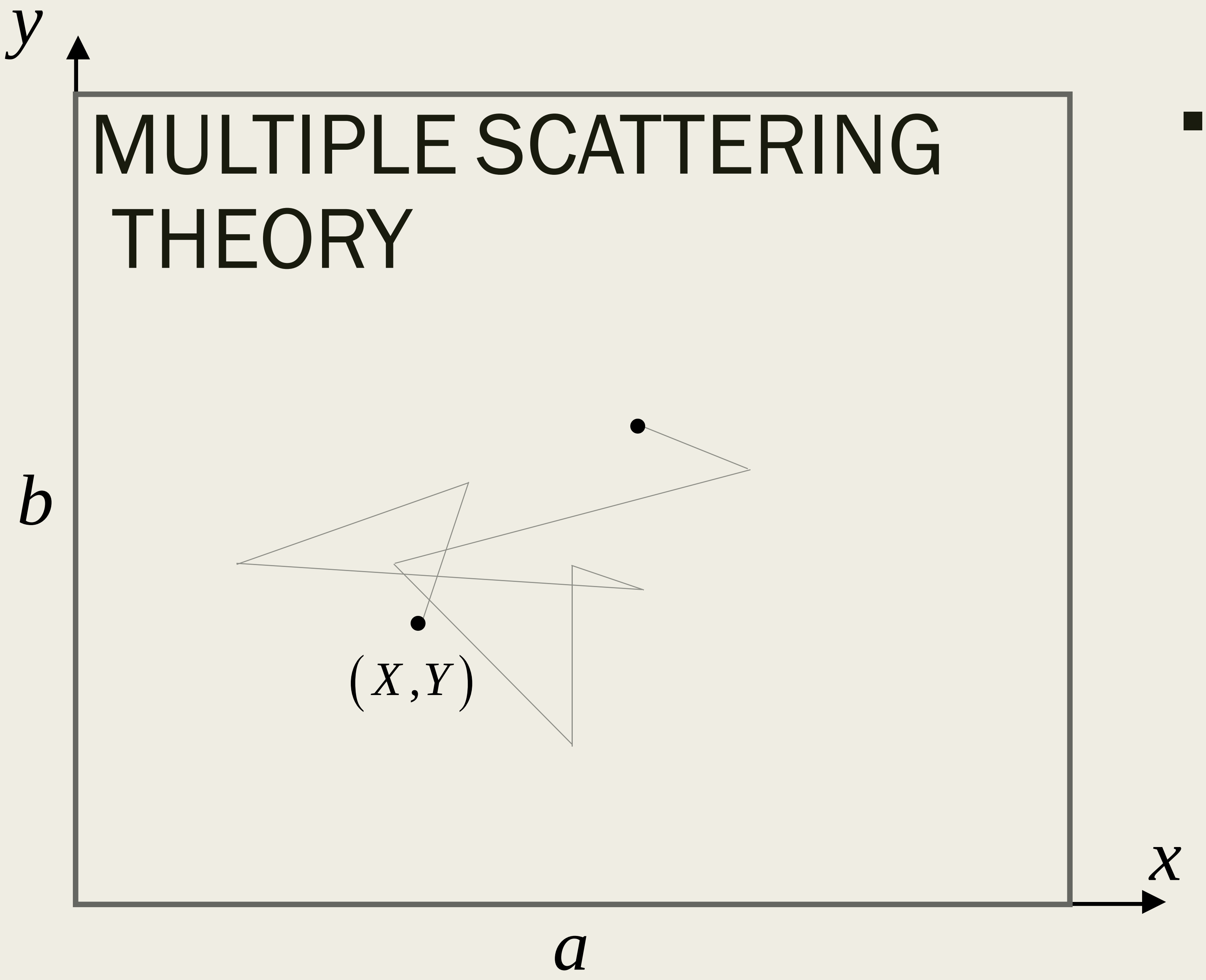
# Visualization of track structure

- Electron
- Liquid water
- 10 MeV
- Bunch of 50 electrons

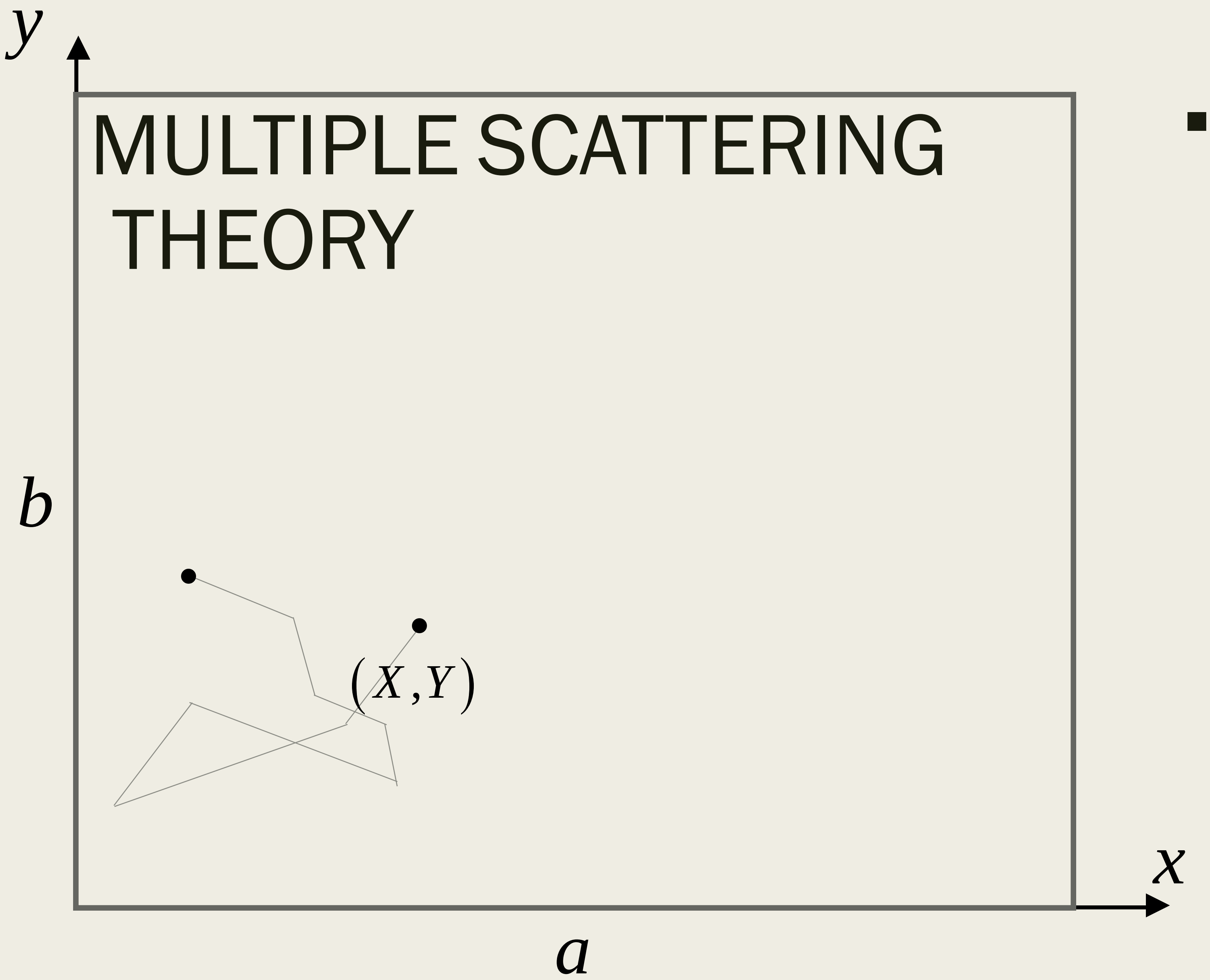


# MULTIPLE SCATTERING THEORY



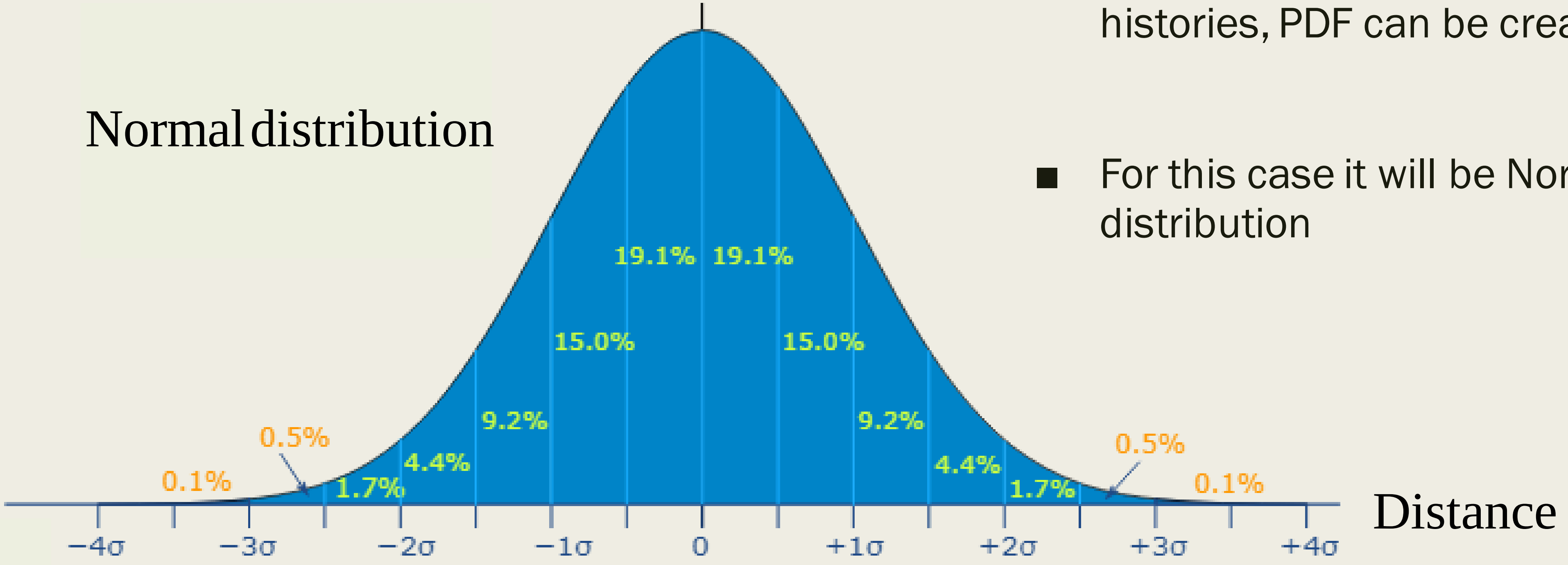

- Let us simulate 8 random free paths

# MULTIPLE SCATTERING THEORY



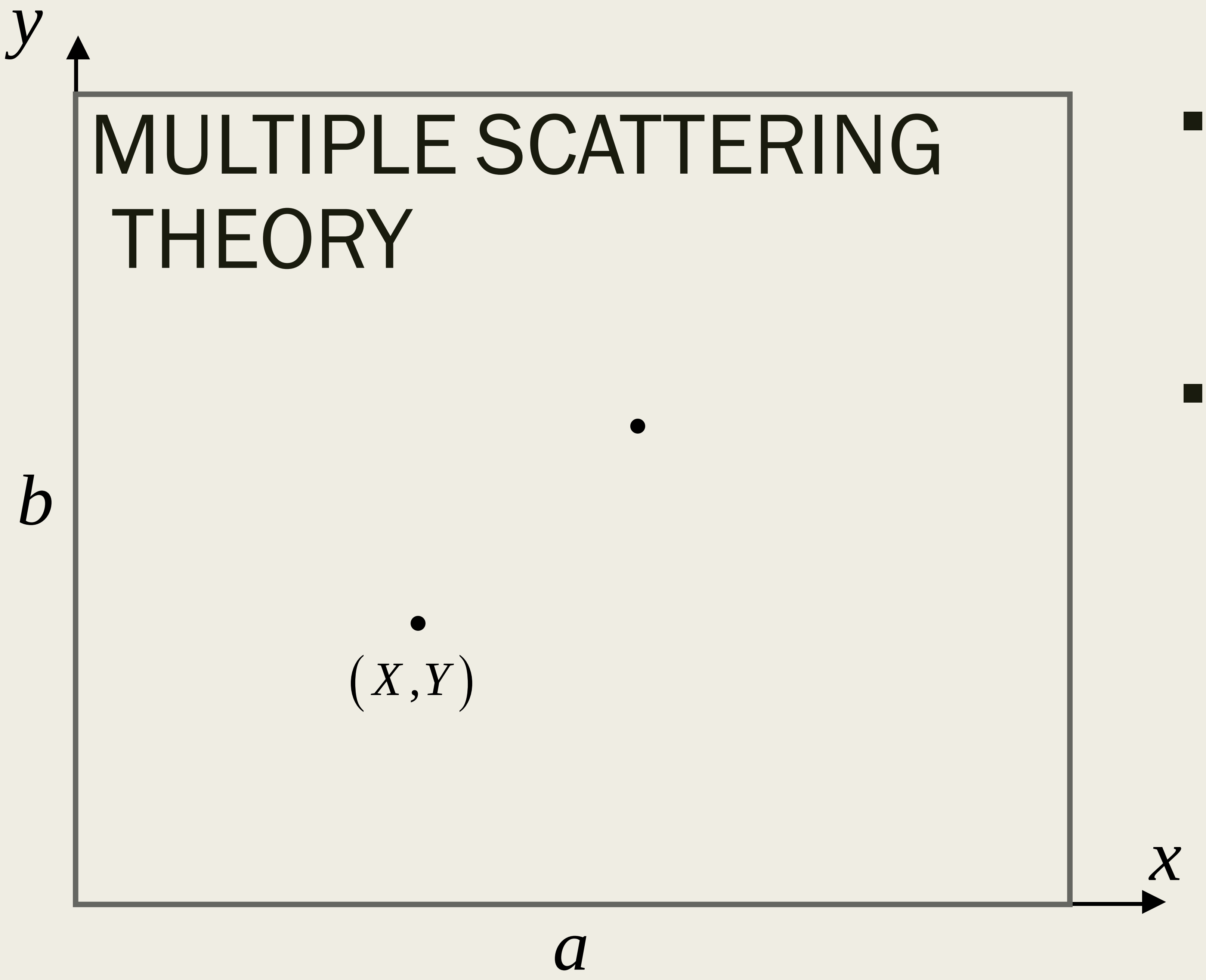

- Repeat simulation and you will get another history

# MULTIPLE SCATTERING THEORY



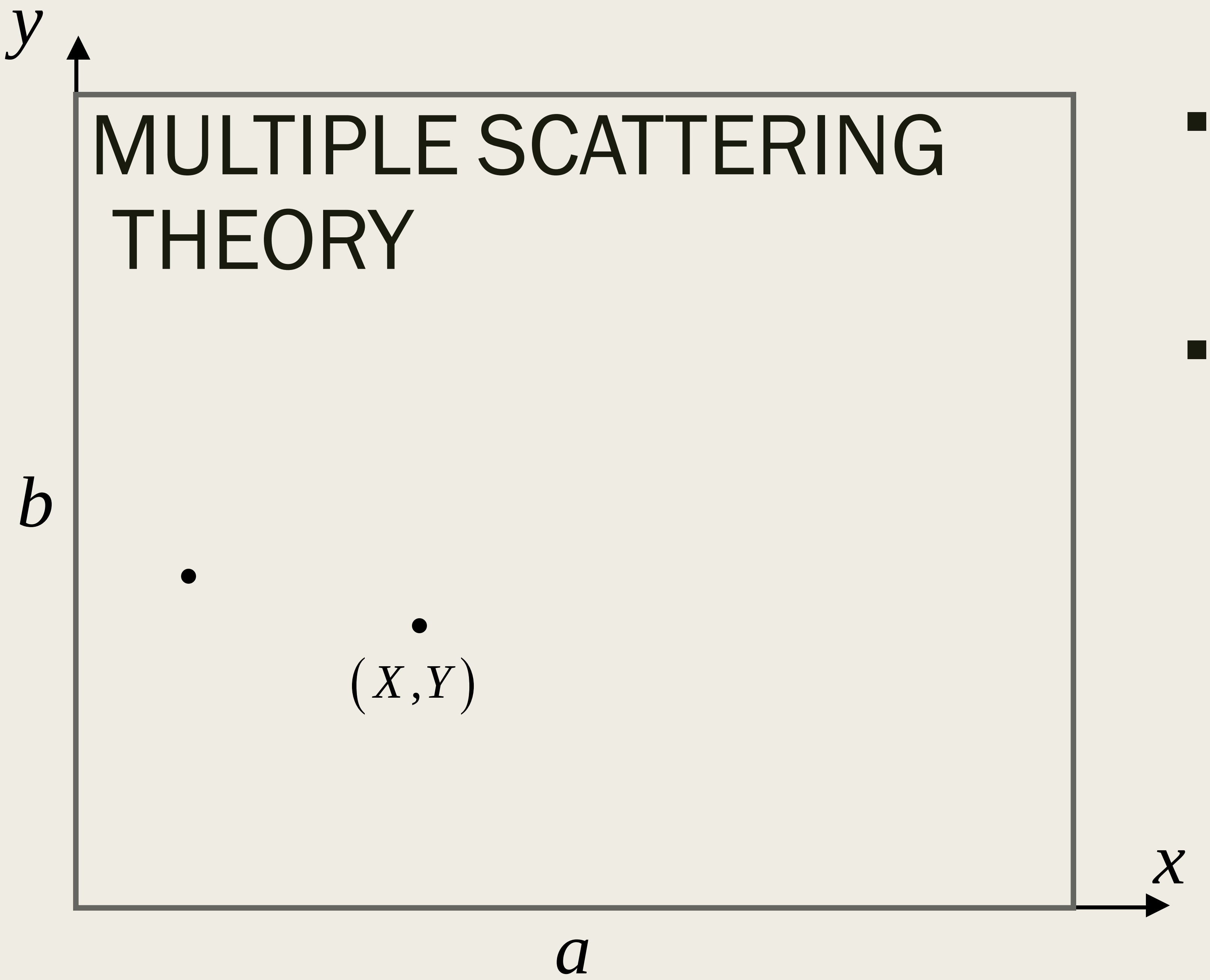

- From great number of histories, PDF can be created
- For this case it will be Normal distribution

# MULTIPLE SCATTERING THEORY



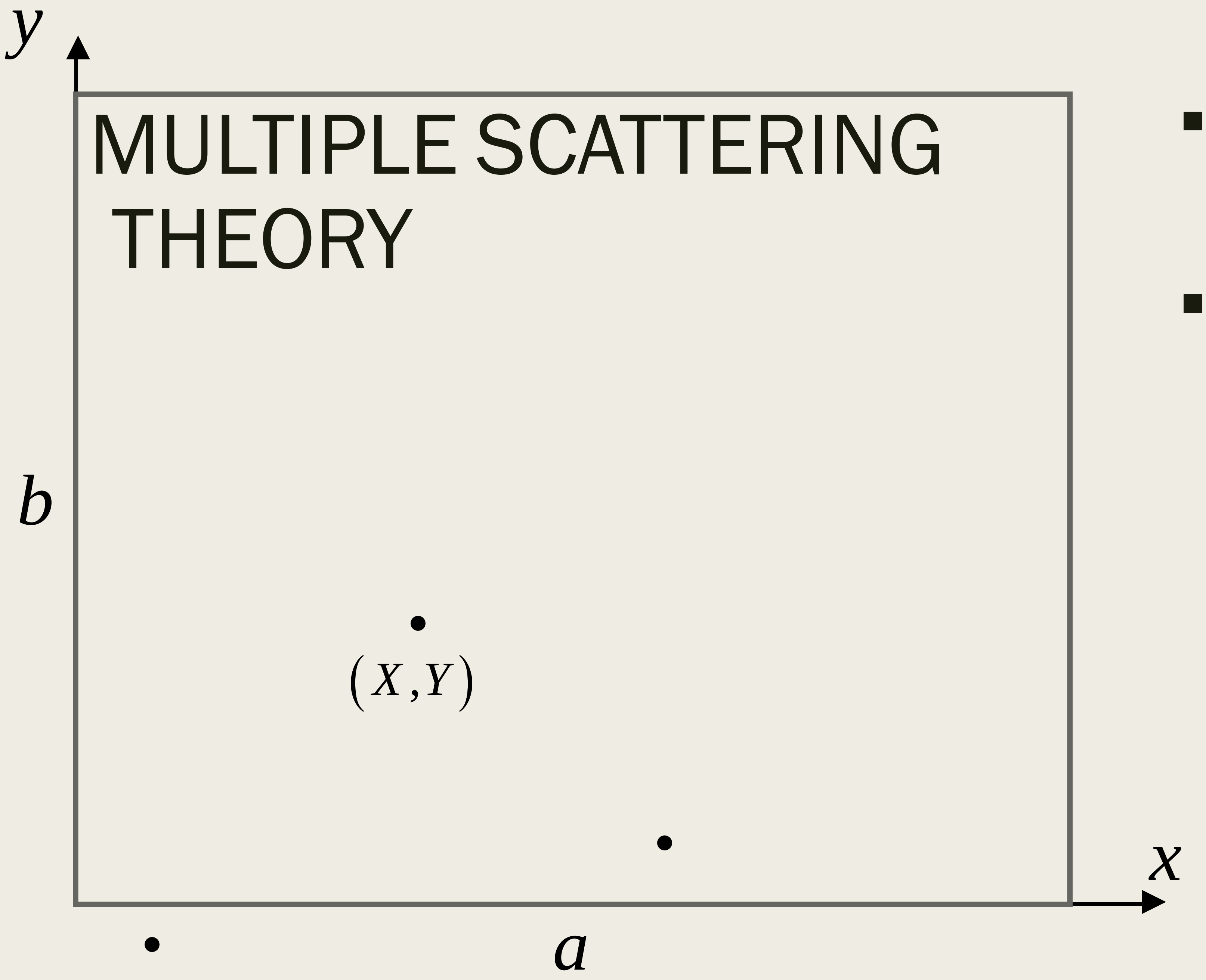

- Generate final point after movement of 8 free paths from PDF –Normal distribution
- 8 free paths are condensed and can be simulated in one step

# MULTIPLE SCATTERING THEORY



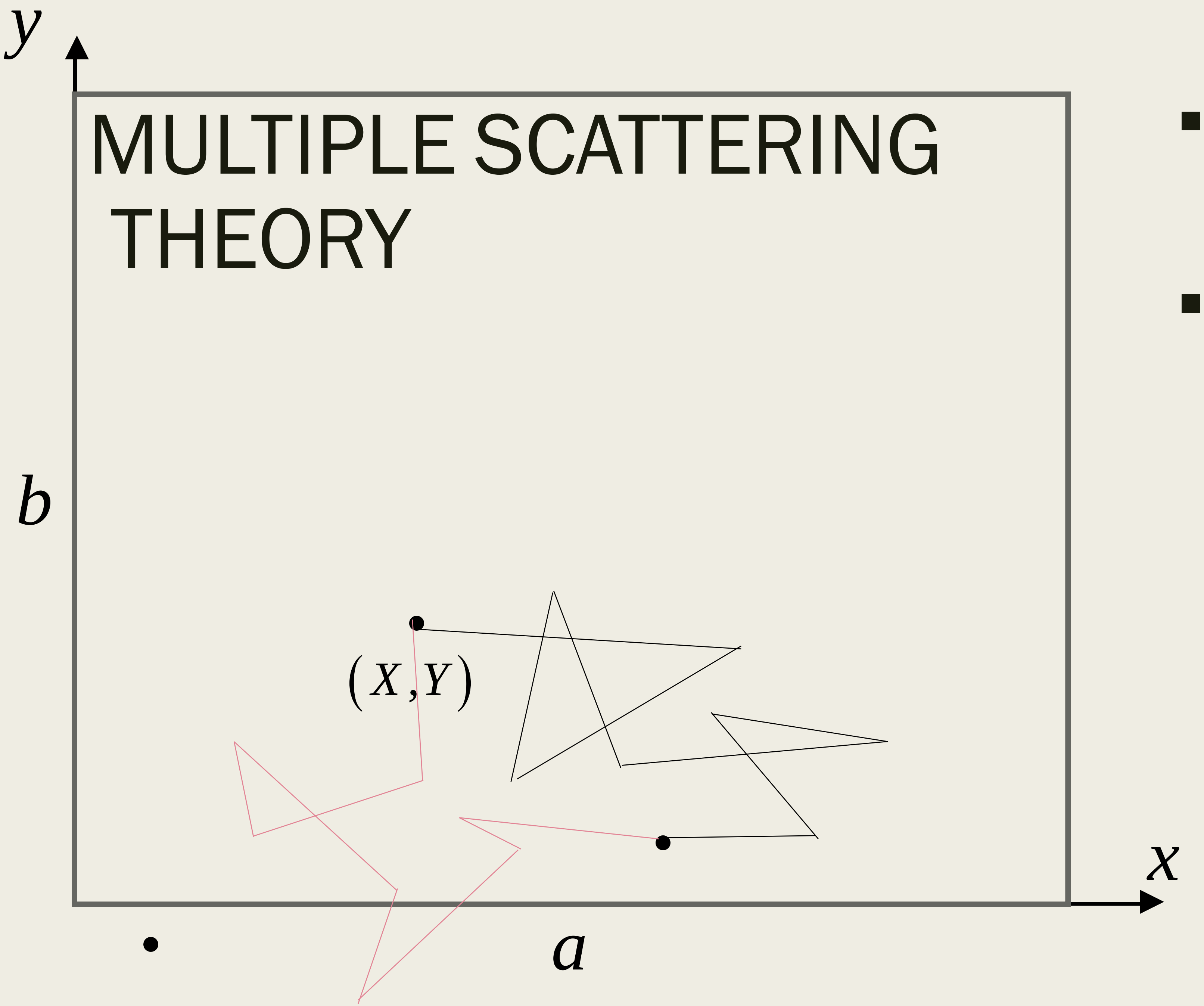

- If you repeat simulation new end point will be obtained. This is not detail simulation
- **In this way histories of particles are condensed – Multiple Scattering Theory**

# MULTIPLE SCATTERING THEORY




- There Is lose of information's when condensing histories
- If you want to check weather particle left the box, using condensed histories, you can get wrong answer

# MULTIPLE SCATTERING THEORY




- There Is lose of information's when condensing histories
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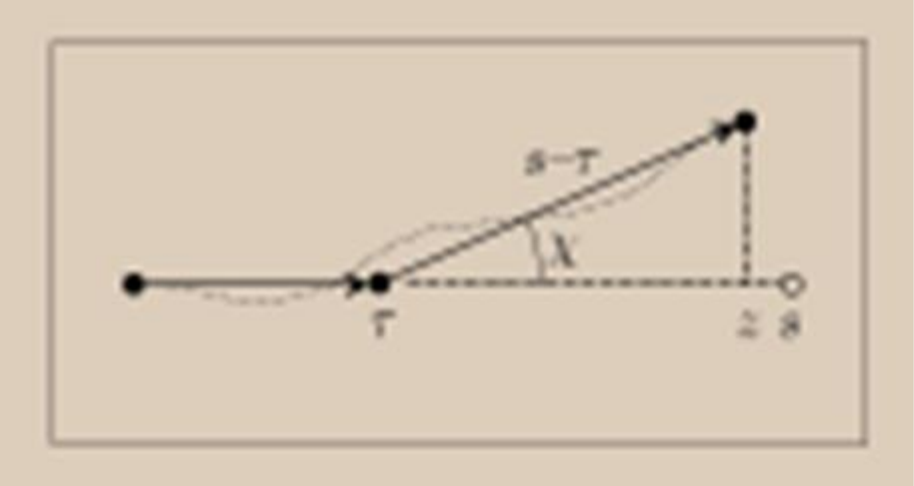
# MULTIPLE SCATTERING THEORY

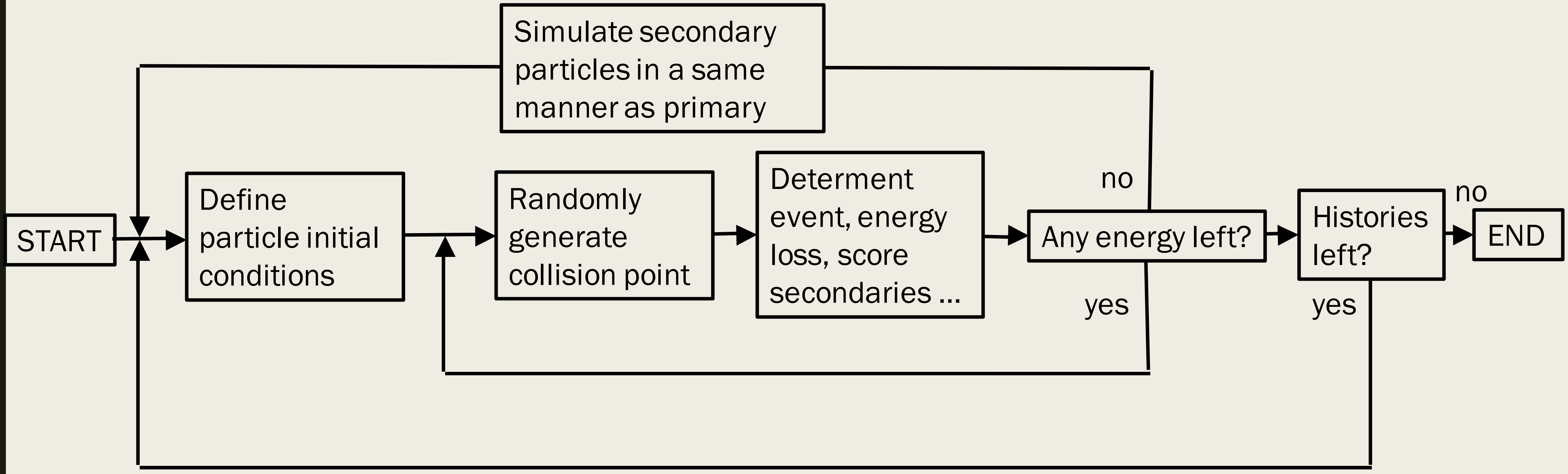
- The multiple scattering theory implemented in condensed simulations are approximate and may lead to systematic errors

- For charged particles, Multiple scattering theory is need, rather than choice
- Large number of interactions per small track length – detailed simulation is time consuming, even impossible to perform

- Molière's Theory of Multiple Scattering



# BASIC STRUCTURE OF MONTE CARLO TRANSPORT CODE



# THANK YOU FOR YOUR ATTENTION