Monte Carlo Simulation

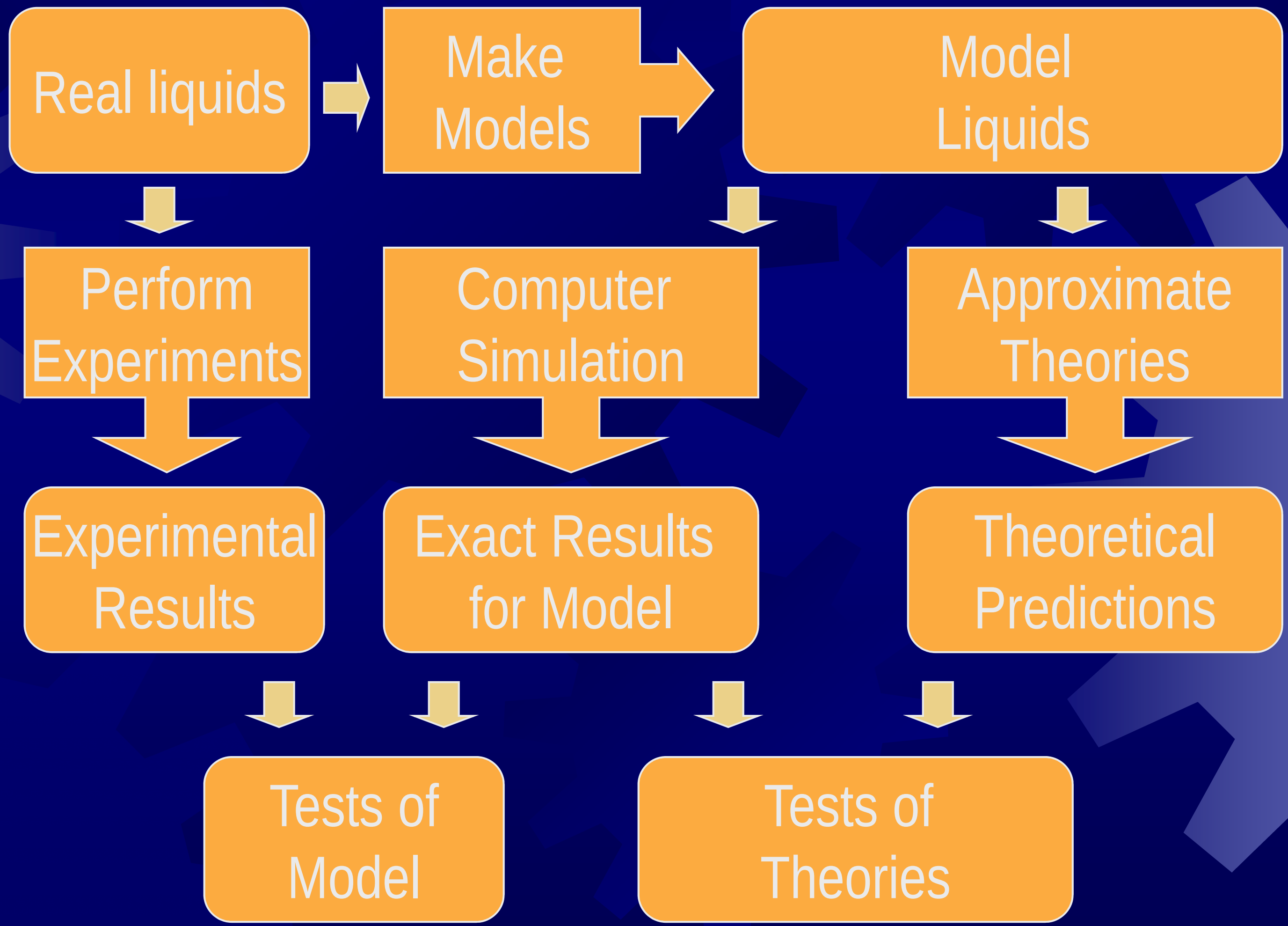
Ju Ho Lee

Thermodynamics and Properties Lab, Korea University

What is Simulation?

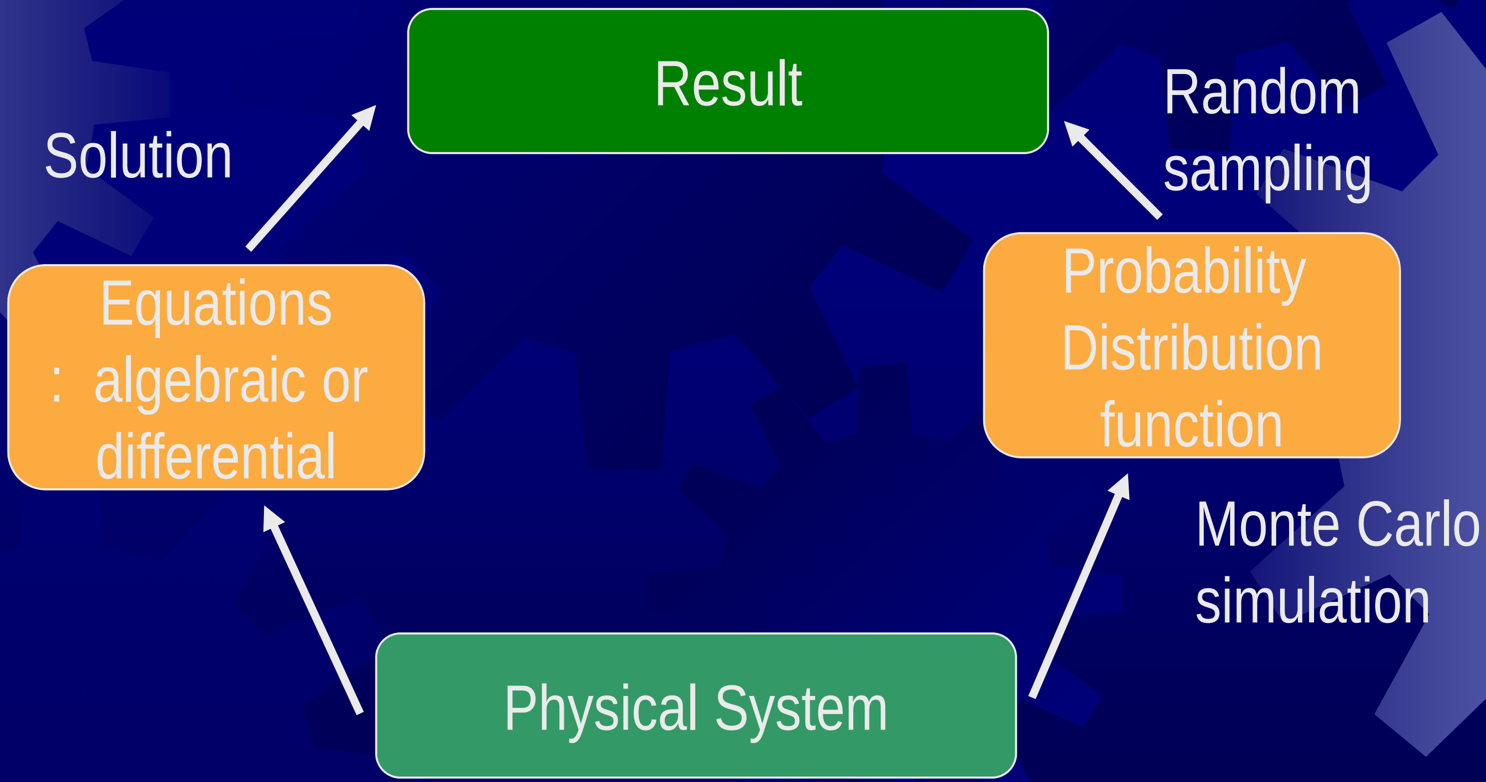
- 복잡한 문제를 해석하기 위하여 모델에 의한 실험, 또는 사회현상 등을 해결하는 데서 실제와 비슷한 상태를 수식 등으로 만들어 모의적(模擬的)으로 연산(演算)을 되풀이하여 그 특성을 파악하는 일.
- Computer Simulation : Roles of the experiment designed to test theory

Computer Simulation, Experiments and Theory



Monte Carlo Simulation

- Monte Carlo
  Similarity of statistical simulation to game of chance



Primary components of MCS

- **Probability distribution functions(pdf)**
  Description of physical system
- **Random number generator**
- **Sampling rule**
  Prescription for sampling from the specified **pdf**
- **Scoring(or tallying)** : accumulation of outcomes
- **Error estimation**
- **Variance reduction techniques**
  methods for reducing the variance
- **Parallelization and vectorization**
  Algorithms to implement efficiently

Terminology

- Experiment

  physical or mathematical process
- Outcomes

  result of experiment
- Sample space

  collection of all possible outcomes
- Trial

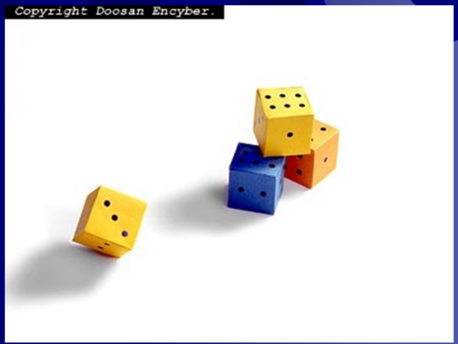
  one realization of the experiment
- Event

  a consequence of the outcome of the experiment

illustration

Example :

Observing the top face of the die



- Outcomes : six faces
- Sample space : consists of six outcomes
- Events

  E1 : top face is an even number

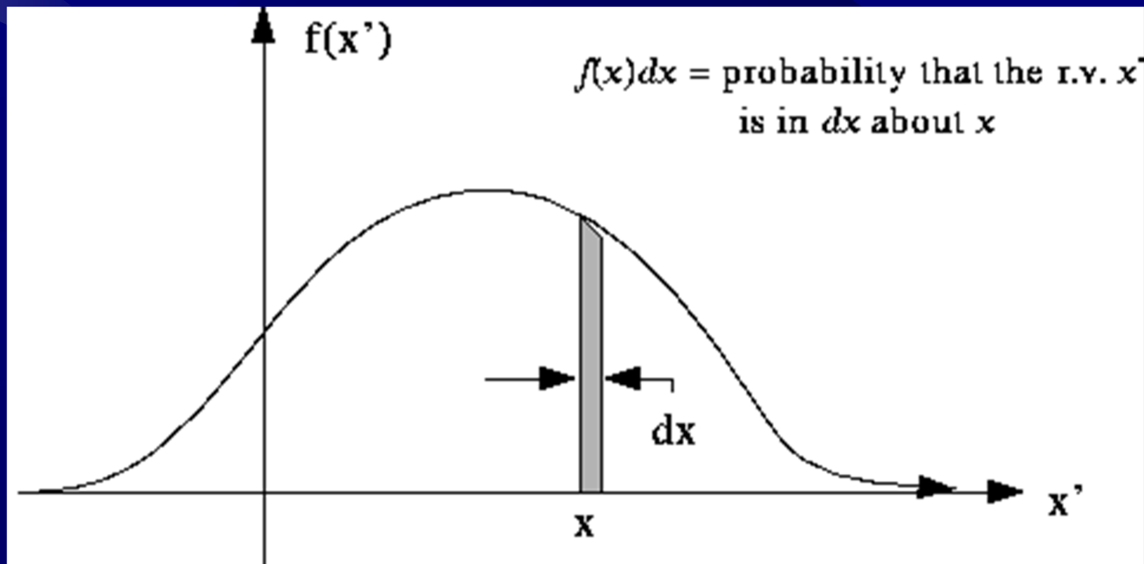
  E2 : top face is larger than 4

Probability Density Function

- PDF

  Probability that the random variable is in the interval $(x, x+dx)$

  $\text{Prob}(x \leq x' \leq x+dx) = P(x \leq x' \leq x+dx) = f(x)dx$

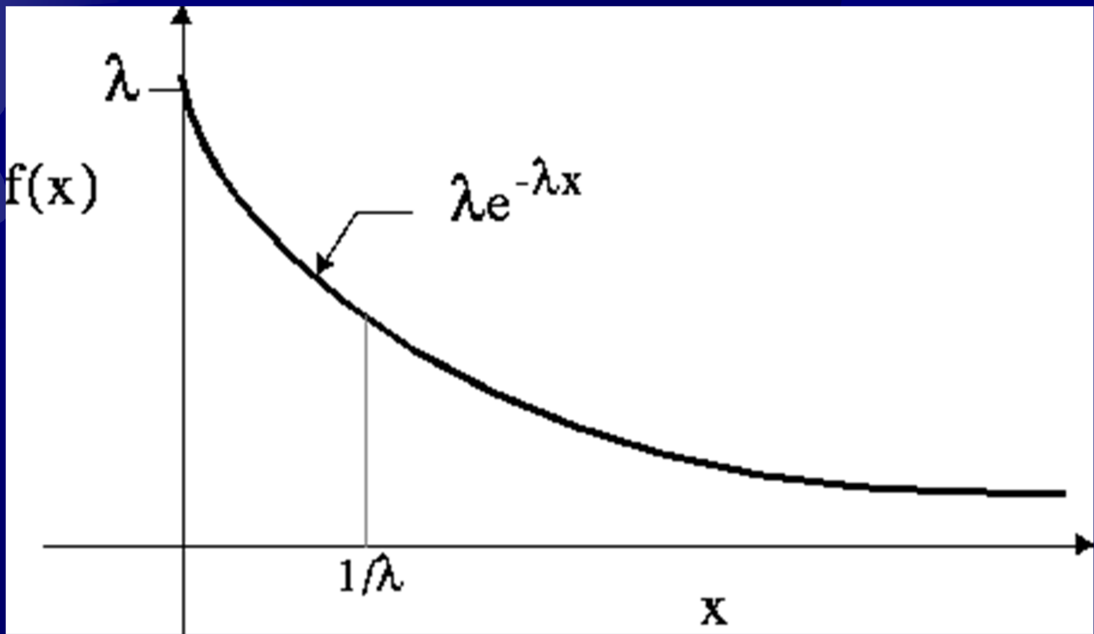


Types of PDF : Exponential

- Exponential Distribution

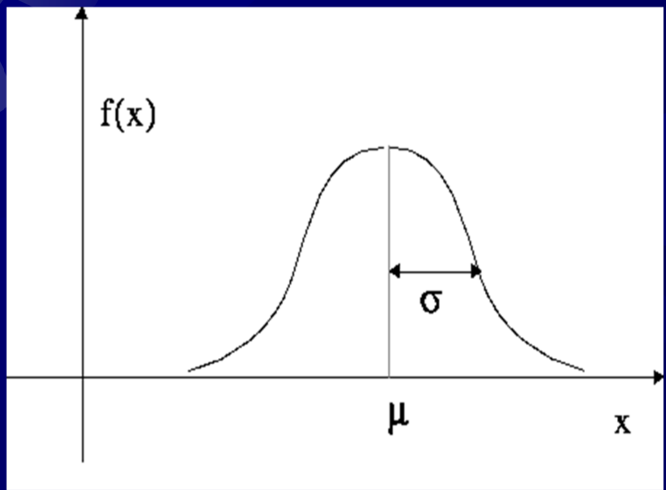
  $f(x)=\lambda e^{-\lambda x}$, $x \geq 0$, $\lambda > 0$

  applicable to radioactive nucleus to decay



Types of PDF : Gaussian

- Gaussian(Normal) Distribution
  - Two parameter distribution (σ, μ)
  - most important pdf in probability and statistics

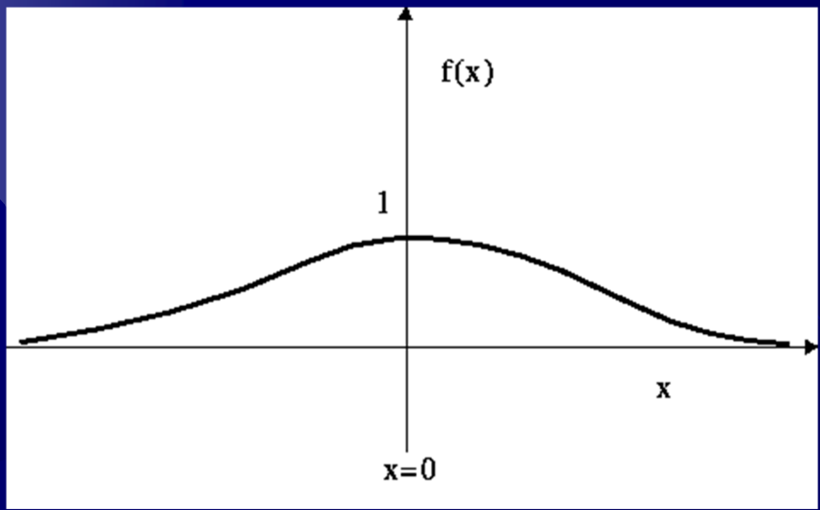


$$f(x) = \frac{1}{(2\pi\sigma)^{1/2}} e^{\frac{(x-\mu)^2}{2\sigma^2}}, -\infty < x < \infty$$

Types of PDF : Cauchy

- Cauchy Distribution

  non-exist mean value



$$f(x) = \frac{a}{a^2 + x^2}, -\infty < x < \infty$$

Sampling from PDF

- Simulation of physical system
  - = Random sampling from PDF + Supplementary computations needed to describe the system evolution

Physics and mathematics of system ← Random sampling of possible states from PDF

Transformation of PDF

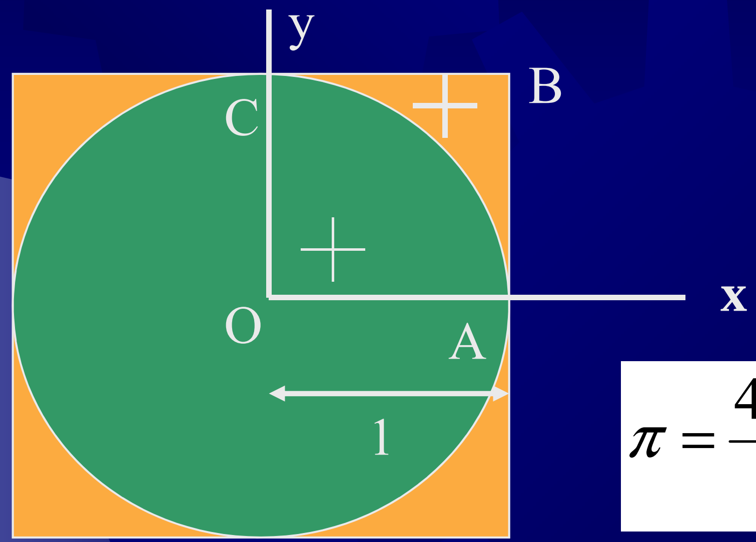
PDF f(x) → y=y(x) → PDF g(y)

- y(x) is one-to-one relation with x
- Probability of the random variable x' occurring in dx about x =
  Probability of the random variable y' occurring in dy about y

$$f(x)dx = \text{probability}(x \le x' \le x + dx)$$

$$g(y)dy = \text{probability}(y \le y' \le y + dy)$$

Example : MC Integration



$$\pi = \frac{4 * \text{Area under the curve } CA}{\text{Area of the } OABC} = \frac{4\tau_{hit}}{\tau_{shot}}$$

- A number of Shots
  - Two independent random number in [0,1]
  - Set number as coordinates of a point
  - Check Distance from origin
- Record hit and miss

Importance Sampling

$$I = \int_a^b dx f(x) = (b-a) < f(x) >$$

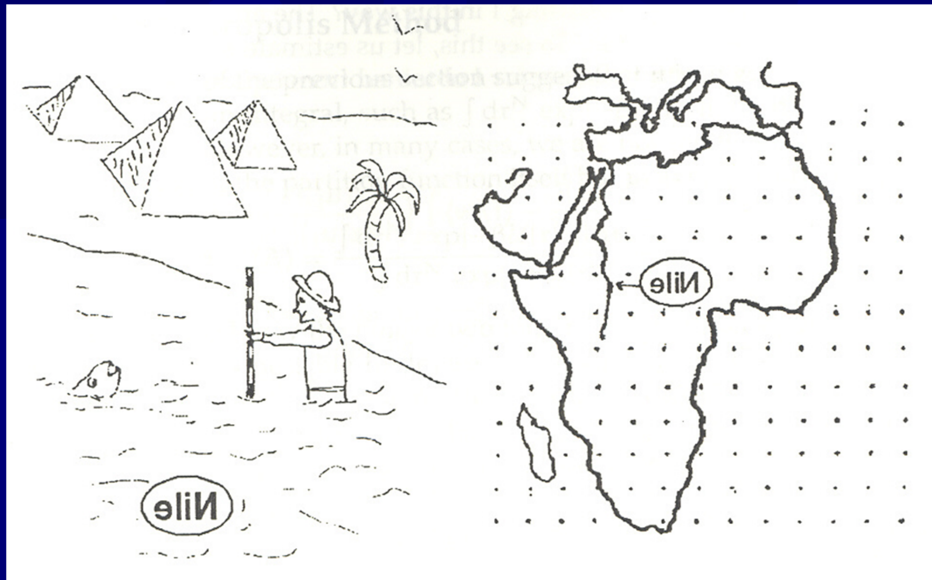
- Many points in the region where Boltzman factor is large and few elsewhere

$$I = \int_a^b dx f(x) = \int_0^1 dx\, w(x) \frac{f(x)}{w(x)} = \int_0^1 du \frac{f(x(u))}{w(x(u))}$$

- Generate L random values of u uniformally distributed in the interval [0,1]

$$I \cong \frac{1}{L} \sum_{i=1}^{L} \frac{f(x(u_i))}{w(x(u_i))}$$

Metropolis Method



- **Random walk** is constructed
- **Trial move** is rejected(if out of water) or accepted
- Depth of water is measured at every trial move
- **Average depth of Nile River**

Criteria of trial move acceptance

- Probability of accepting a trial move from **o** to **n**

  (U(o) < U(n))

  acc(o→n)=exp{-β[U(n)-U(o)]} < 1

  IF generated Random number from [0,1],

  Ranf < acc(o→n) : accept

  Ranf > acc(o→n) : reject

A Basic MC algorithm

- For equilibrium properties of classical many-body system,
  - Select a particle at random and
    Calculate its energy $U(r^N)$
  - Give the particle a random displacement :
    $r' = r + \triangle$ and calculate its new energy $U(r'^N)$
  - Accept the move from r^N to r'^N with probability

$$\mathbf{acc(o \rightarrow n)} = \min(1, \exp\{-\beta[U(n)-U(o)]\})$$