22.106 Neutron Interactions and Applications

Special Project

Monte Carlo simulation of Solid State Diffusion

Based on:

G.E. Murch,
Monte Carlo calculation as an aid in teaching solid-state diffusion,
Am. J. Phys. **47**, 78 (1979)

And also:

G.E. Murch,
Monte Carlo demonstration of solid-state diffusion in an electric field,
Am. J. Phys. **47**, 958 (1979)

C.A. Whitney,
Casino physics in the classroom,
Am. J. Phys. **54**, 1079 (1986)

Motivation

- Acquire a broader perspective on Monte Carlo **simulations**

Monte Carlo methods in science = using randomness to solve problems

- (Metropolis) Calculation of thermodynamical properties of a system of many interacting particles
- Importance sampling – numerical evaluation of integrals / weighted sums

Mathematically similar:

$$\langle A \rangle = \sum_i p(\chi_i) A(\chi_i) \text{ or } \int p(\chi) A(\chi) d\chi$$

where χ belongs to a space of possible configurations/values

$$\rightarrow \langle A \rangle = \sum_{i \text{ SAMPLED}} A(\chi_i)$$

- Optimization – search for global minima

  → *"to go downhill, and uphill once in a while…"*

- **Simulations of physical phenomena**

  ☺ Creativity to interpret different phenomena probabilistically or to identify stochastic behavior

- other…

Simulations of physical phenomena

- Radiation transport - MCNP

  Neutrons (or photons) travel across a given material where they can be scattered, absorbed, leak ... go through fission (neutrons), pair production (photons), etc.

- Absorption in space / Nuclear decay in time

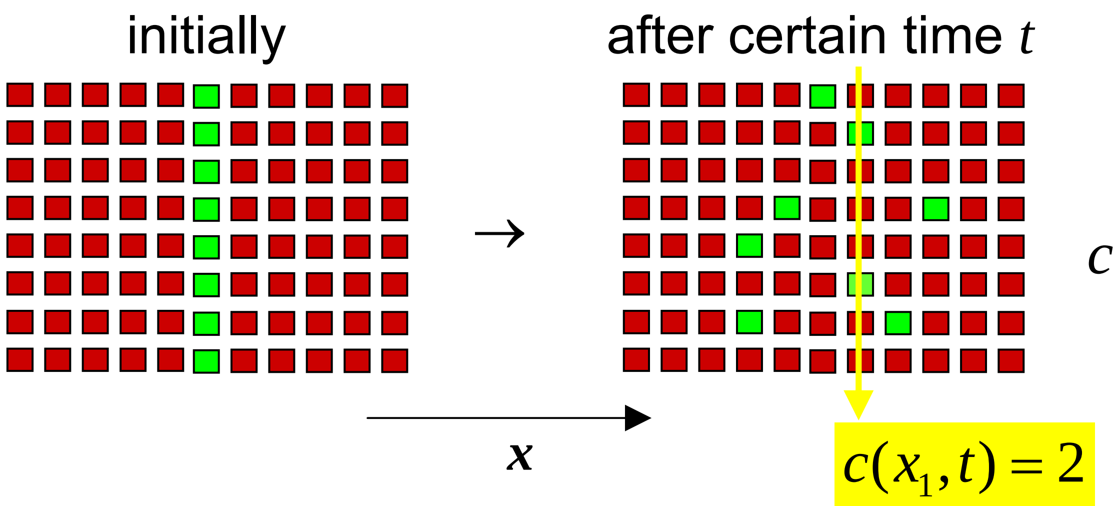
  Particles that survive with probability p or don't with probability $1\text{-}p \rightarrow$ laws of the type e^{-px}, e^{-pt} where p is related to c.x., life-times, etc.

- Random walks

- Solid-state diffusion

- other…

Statement of the problem



■ ■ Same type of atoms: self-diffusion

$c(x,t) =$ concentration of ■ along the $\hat{x}$ direction

$$J = -D\frac{\partial c}{\partial x}$$ Fick's law

$$\frac{\partial J}{\partial x} = -\frac{\partial c}{\partial t}$$ eq. of continuity

$$D\frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial t}$$ (time dependent) diffusion eq.

Analytical solution:
(for infinite medium
$\Rightarrow$ no boundaries)

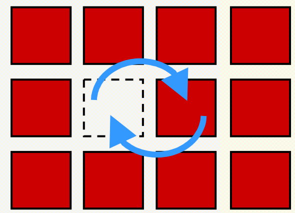
$$c(x,t) = \frac{c_0}{2\sqrt{\pi D t}} e^{-\frac{x^2}{4Dt}}$$

- Gaussian profile
- $\langle \Delta x^2 \rangle = 2\, t\, D$

Monte Carlo simulation

Atomistic approach: the vacancy mechanism

Causes for vacancies:
- Impurity doping
- Radiation damage
- Thermal activation



the vacancy moves
and interchanges
places with the atoms

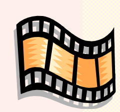
$\rightarrow$ the vacancy
follows a **random walk**

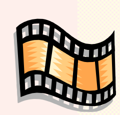
MC simulation

keep track of the wandering of the atoms:
final distance traveled = Δx

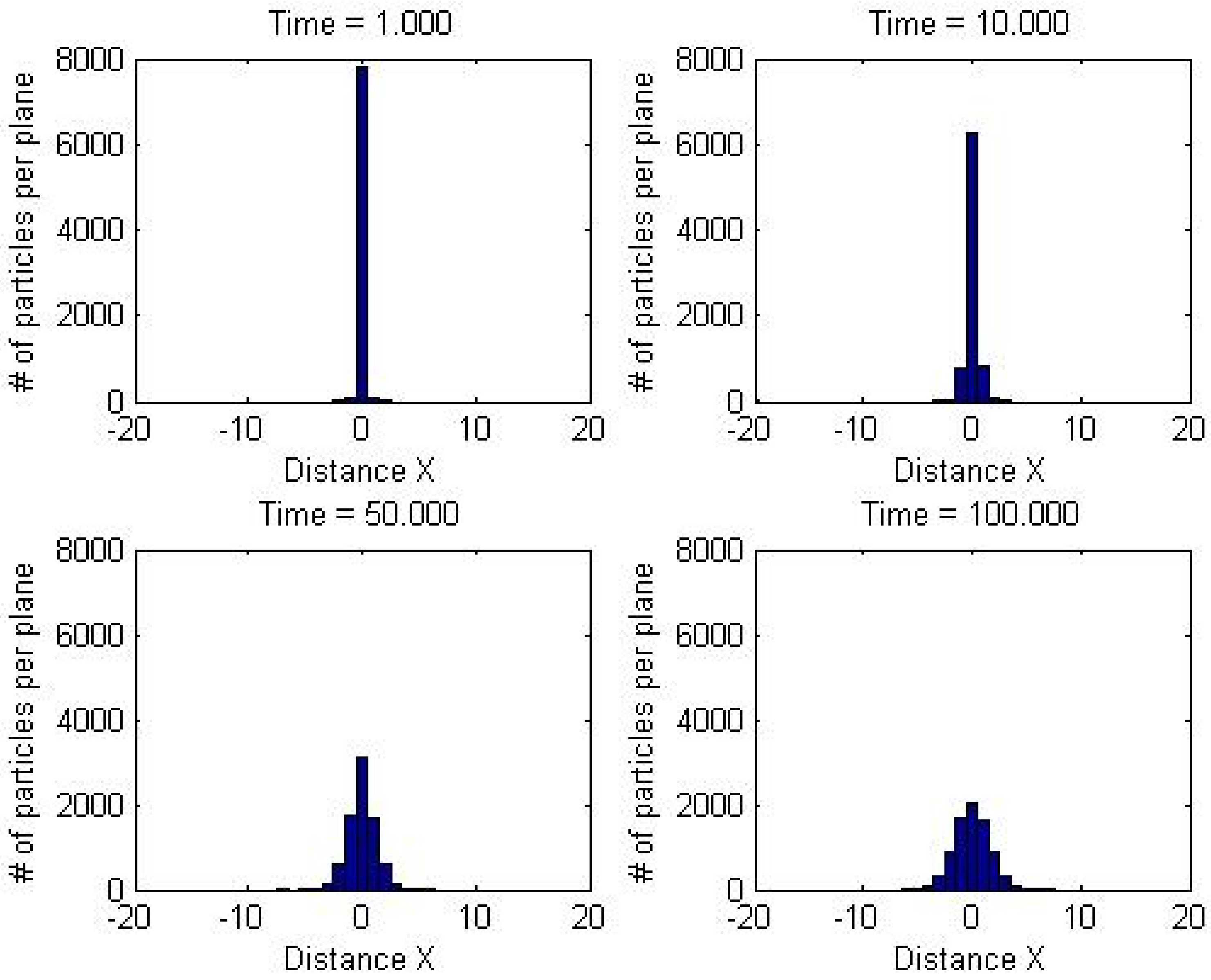
histogram

computer = finite medium
$\Downarrow$
Periodic Boundary Conditions
(for the vacancy)

 trajectory of the vacancy in 3D

 dynamics in 2D

Recovering results…



Observations

we can calculate $D = \langle \Delta x^2 \rangle / 2t$ with

$$\langle \Delta x^2 \rangle = \frac{1}{M} \sum_{i=1}^{M} x_i^2 \qquad M = \#\ particles\ tracked$$

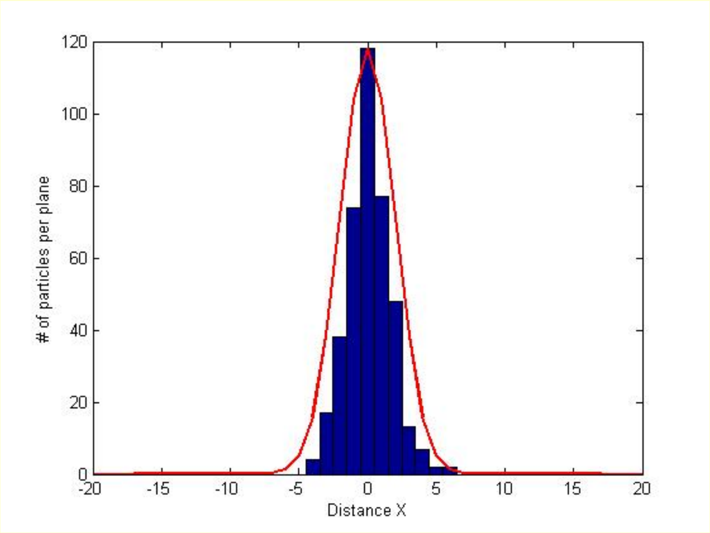
or by fitting: $Ln(c) = const - x^2/(4Dt)$

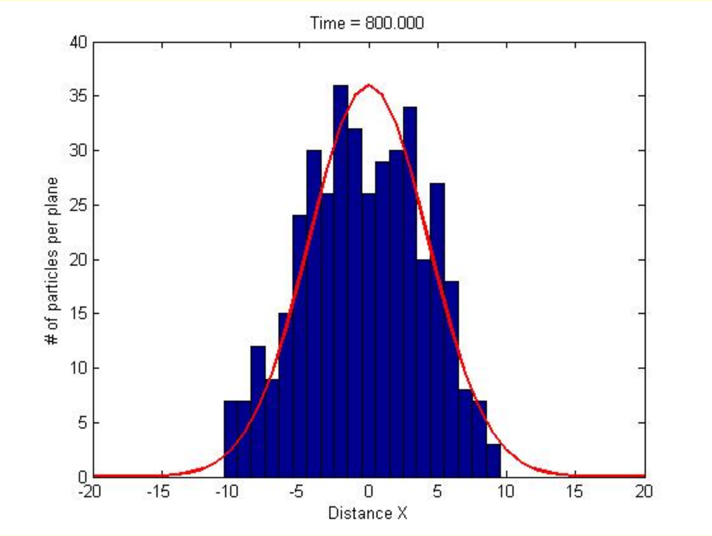
D = 2x10^{-5} - 1.4x10^{-5}

(1.36x10^{-5} in the paper)

(physical units)

PBC ≠ infinite medium, because there is a maximum distance!





To simulate an infinite medium at large t, we must take a larger lattice

Conclusions

- We simulated solid state self diffusion using a Monte Carlo algorithm

- MC can be used to simulate very different systems & dynamics

- Random numbers are very useful to solve a large variety of problems.