Simulation and modeling of natural processes

Week 1: Introduction and general concepts

The team

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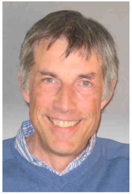


Prof B. Chopard

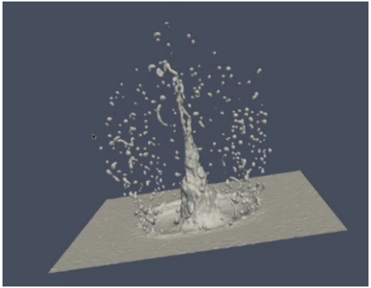
1. Objectives and Background

- Learn how to describe natural phenomena
- Give an introduction to several modeling techniques.
- Show how these models can be simulate on a computer (in-silico laboratory, numerical experiments)
- Learn more about science through modeling

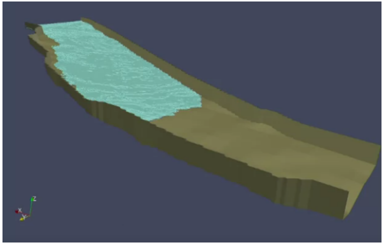
What natural processes are we interested in?

- Physics (Fluid mechanics), astrophysics, chemistry, climatology,...
- Environmental sciences (river modeling, Volcano plume)
- Biology: (Tissue growth), pattern on animal skins, cells, organs
- Ecosystems: competition between species, ant behavior, equilibrium between forest and savanna, propagation of epidemia,...
- Finance, social sciences, traffic, pedestrian motion,..
- ...

Movies

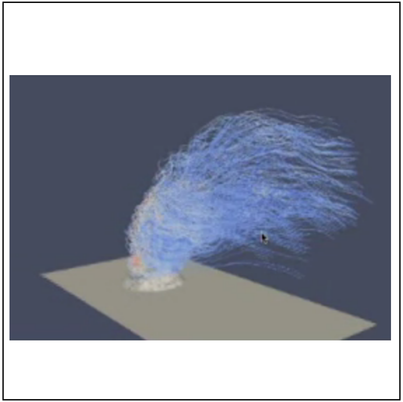


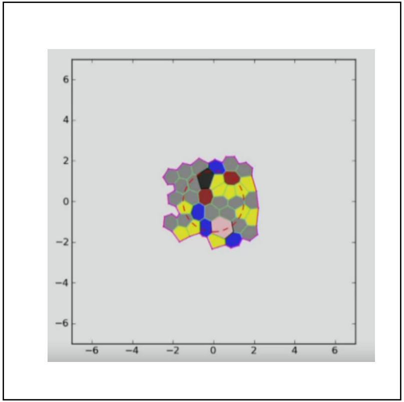
Droplet



River

Movies

Volcano: 

Tissue: 

What is a model?

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- This is not an apple just its graphical representation

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- Simplified abstraction of reality, allowing us to better describe and understand it
- An abstraction in which only the essential ingredients are retained, according to the question we ask about the system.
- It is the respresentation of a phenomena in a mathematical or computer-based language,

Computational Science

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- Computational Science is an emerging, multidisciplinary domain, based on the idea of "**computational thinking**".
- A computer-based description offers a new language, a new methodology to address scientific challenges, far beyond the scope of traditional numerical methods, and in fields where these classical approaches hardly apply.

Computational Science

- **Modeling and simulation** is a central part of computational sciences. It is a response to the new questions scientists want to solve, resulting from the avalanche of new experimental data, and the need to integrate many processes together rather than specializing in one single problem.

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- A computational scientists needs to be a physisict, a mathematician, a computer scientist, a biologist, an economists...

$\boxed{\textit{End of module}}$

Objectives and backgroud

$\boxed{\textit{Coming next}}$

Modeling and Simulation

2. Modeling and Simulation

Why a model?

- Describe, classify, but mostly
- Understand
- Predict
- Control a phenomena

What is a good model?

It depends on the question. Several models may be necessary for studying different aspects of the same phenomena

> *Everything should be made as simple as possible but not simpler*

A Einstein

Level of reality

The same system can be described at different scales, and different methods apply depending on the scale one is interested in:

- atoms, molecules, fluid elements, pressure field, climat
- cells, tissues, organs, living beings
- mechanical parts, cars, traffic

Level of reality

- One has to identify the important ingredients and their mutual interactions.
- Often, one defined a model at finer scale than the scale at which we ask a question.

Several models / different language of description

Partial differential equation for a fluid;

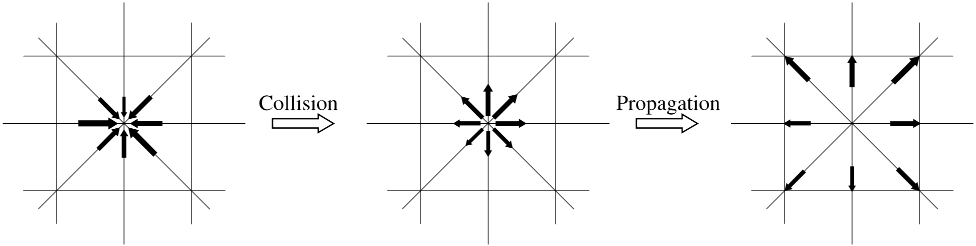
$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u}$$

$$\boxed{\textbf{phenomena} \rightarrow \textbf{PDE} \rightarrow \textbf{discretisation} \rightarrow \textbf{numerical solution}}$$

...to a virtual model of reality

One considers a discrete universe as an abstraction of the real word

$\boxed{\textbf{phenomena} \rightarrow \textbf{computer model}}$



- Mesoscopic *Rule* describing the phenomena

Example of modeling method

- N-body systems, molecular dynamics
- Mathematical equations, ODE, PDE
- Monte-Carlo methods (equilibrium, dynamic, kinetic)
- Cellular Automata and Lattice Boltzmann methods
- Multi-agents systems
- Discrete Events simulation
- Complex networks

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- It is a numerical experiment in **computer based virtual universe**
- One need to understand computer programs, software engineering, algorithms, data-structures, hardware (parallel machines, GPUs), code optimization, data-analysis.

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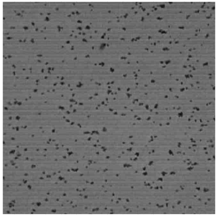
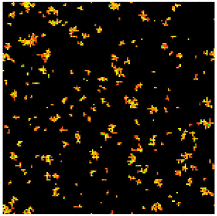
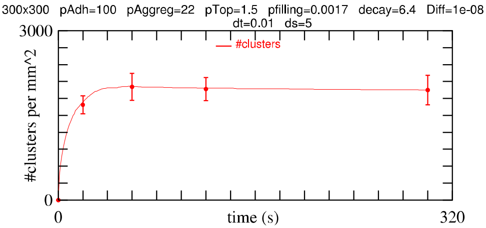
- One need enough knowledge of the phenomena to judge if its predictions are acceptable in new situations.

From a model to a simulation: illustration







$\boxed{\textit{End of module}}$

Modeling and Simulation

$\boxed{\textit{Coming next}}$

Modeling Space and Time

3. Modeling Space and Time

Space and time

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- Sometime one is only interested in the time evolution of a quantity, regardless of the spatial location (e.g the number of individuals) in a population
- Sometime, a process is stationary (no time evolution). Then only the spatial variations are of interest (e.g temperature in a room, in the middle or near the windows).

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- The time is discretized, but the process is followed **continuously** over its duration.

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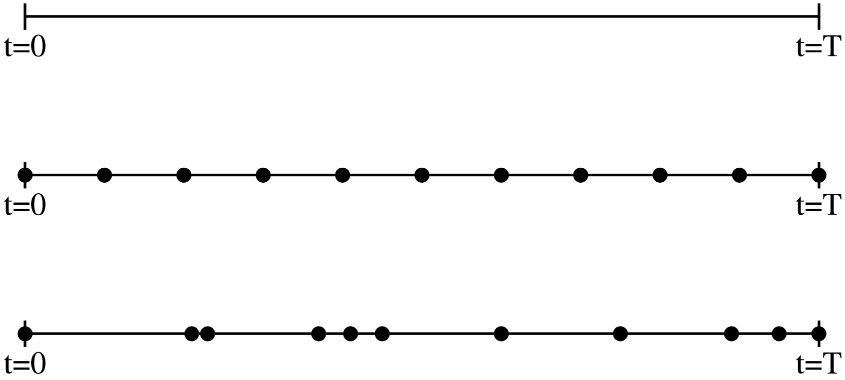
- This is the so-called Discrete-Event-Simulation (DES) approach

Time evolution



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- Space can be continuous (mathematical models) or discretized in cells, forming a mesh covering the region of interest.

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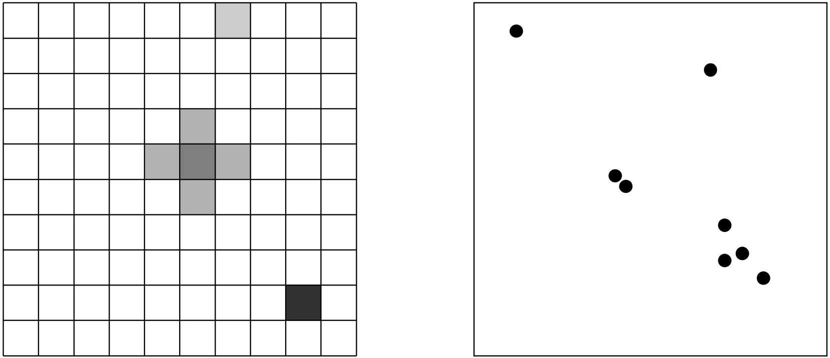
- This is the so-called **Lagrangian** approach: the observer take the point of view of the moving objects.

Modeling space



Eulerian point of view   Lagrangian point of view

Beyond the physical space: complex networks

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- It is rather whether these components see each others, or can interact.
- This is typically the case in social systems. Two persons can be very far away but still interact a lot by phone or other means

Beyond the physical space: complex networks

- For instance, the agent in an economical model can be represented as a **graph** (or a complex network): an edge connects pairs of agents that exchange information, money, goods,..

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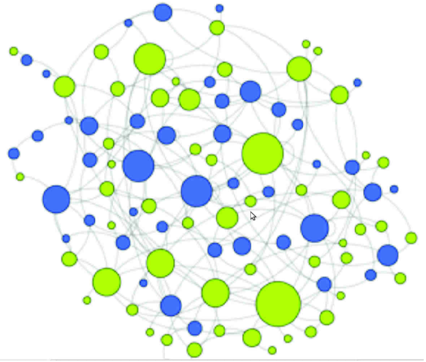
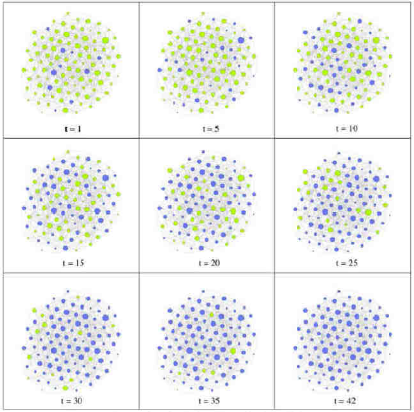
- Obviously, such a graph can be dynamical: creation of new links or destruction of old ones.

Exemple

A model of opinion propagation in a social network



(Lino Velasquez, UNIGE)



Réseau aléatoire, N = 100, p = 0.05, $\varepsilon = 0.3$

Complex networks

- Dynamical systems on complex networks is a fast developing field
- Graph topology imposes a rich "spatial" structure which constrains the dynamics
- Many quantities characterize the graph topology and can be related to some global properties of the system: degree distribution, clustering coefficient, centrality measures, assortativity, etc.

$\boxed{\textit{End of module}}$

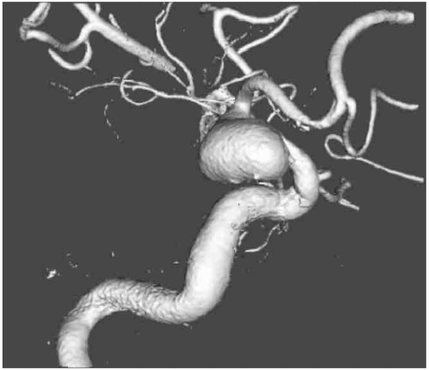
Modeling Space and Time

$\boxed{\textit{Coming next}}$

Example of bio-medical Modeling

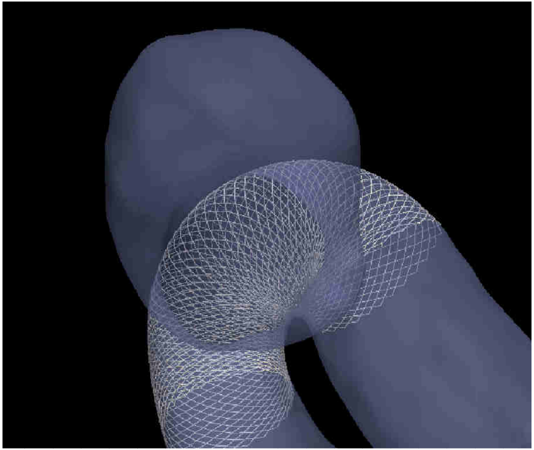
4. Example of bio-medical Modeling

Thrombosis in cerebral aneurysms



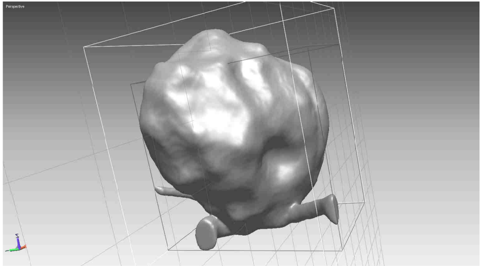
The evolution of aneurysms is driven by bloodflow, biomechanics and biology

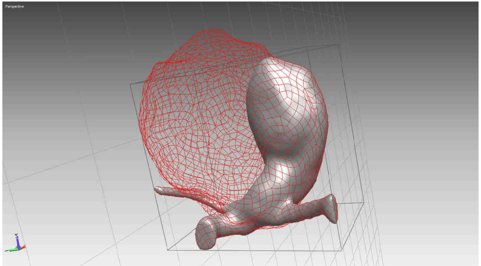
How to treat them: Stents/flow diverter



- The flow-diverter **reduces bloodflow** in the aneurysm
- **Clotting is induced in the aneurysm**

Example of a thrombus in a segmented aneurysms



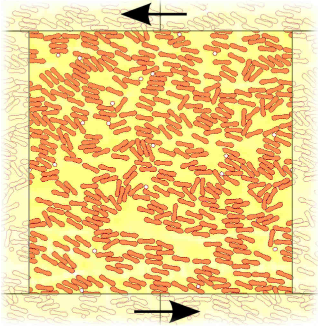


movie

(Image processing: Guy Courbebaisse, INSA-Lyon)

Micro-model (University of Amsterdam)

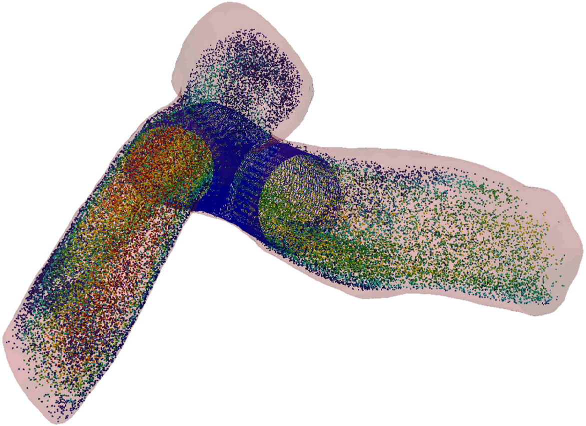
- Red Blood Cells and platelets are modeled as
- deformable objects
- in suspension in the plasma fluid



- Platelets and RBC in a 2D shear
- 3D suspension model

(L. Mountrakis, E. Lorenz and A.G. Hoekstra)

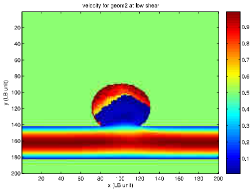
Macroscopic flow simulation in an aneurysm

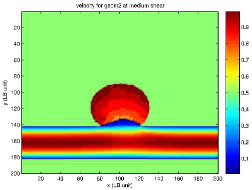


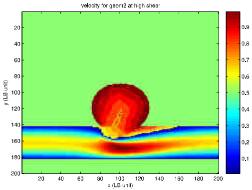
(see movie)

Numerical Model of Clotting

Under proper flow conditions and depending on the vessel wall biological response, a clot develops: a solidification of the blood from the wall







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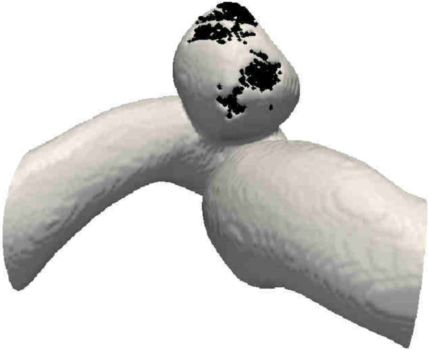
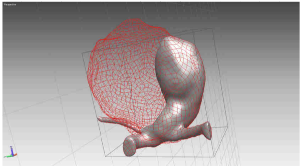


[Pulsatile](#) versus [steady](#) flow

Qualitative validation

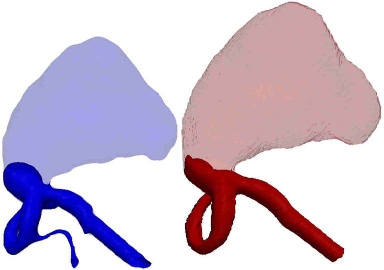
As observed in giant aneurysms, the simulation shows

- Partial or total aneurysm thrombosis,
- Spontaneous stop and start of the clot



Blue: patient   Red: simulation

[movie]



$\boxed{\textit{End of module}}$

Bio-medical Modeling

$\boxed{\textit{Coming next}}$

Monte-Carlo methods

5. Monte-Carlo methods I

Background

- The goal of Monte-Carlo methods is the sampling of a process in order to determine some statistical properties
- For instance, we toss a coin 4 times. What is the probability to obtain 3 tail and 1 head?
- Mathematics gives us the solution:

$$P(3\text{ head}) = \binom{4}{3}\left(\frac{1}{2}\right)^3\left(1-\frac{1}{2}\right)^1 = \frac{1}{4}$$

- But we could also do a simulation

A Monte-Carlo computer simulation

```
from random import randint

success=0

attempts=10000
for i in range(attempts):
    if randint(0,1)+randint(0,1)+randint(0,1)+randint(0,1)==3:
        success+=1

print "Number of attempts=", attempts
print "Number of success=", success
```

We get for instance:

```
Number of attempts= 10000
Number of success= 2559
```

More difficult problems

- For the coin tossing problem, no need for a simulation

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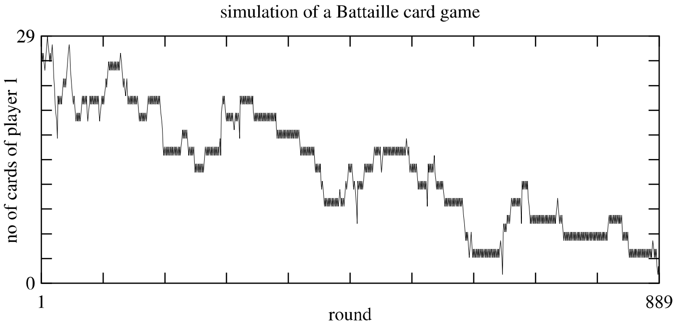
More difficult problems

- For the coin tossing problem, no need for a simulation
- But we can think of other problems for which probability theory could hardly be applied
- For instance: what is the average duration of the card game called “war” (or battle)?

The *war* card game with 52 cards



Historical note

- The method was name in the 1940s by **John von Neumann**, **Stanislaw Ulam** and **Nicholas Metropolis** after the name of the *Monte-Carlo casino*, where Ulam's uncle used to gamble ...and loose his money
- The motivation was to find out the probability that a Canfield solitaire will finish sucessfully.
- Ulam found it easier to play many Canfield solitaires and estimate the number of successes, rather than trying to apply combinatorics and probability theory.
- Then the Monte-Carlo methods was successfully applied to the *Manhattan project* (nuclear weapon) in the Los Alamos National Laboratory.

$\boxed{\textit{End of module}}$

Monte-Carlo Methods I

$\boxed{\textit{Coming next}}$

Monte-Carlo Methods II

6. Monte-Carlo Methods II

Markov-Chain Monte-Carlo (MCMC)

- We consider a stochastic process whose goal is to explore the state space of a system of interest.

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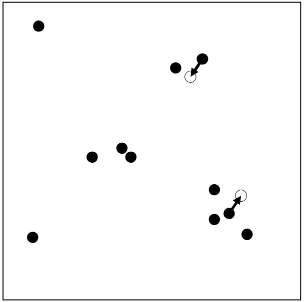
- Let x be a point in this state space. Let us asssume that this point moves across the space by jumping randomly to another point x'.
- The jump from location x to location x' takes place with probability $W_{x \to x'}$. This advanced the system time from t to $t + 1$ (Markov chain)

Markov-Chain Monte-Carlo (MCMC)



- We want this process to sample a prescribed probability $\rho(t,x)$. This stochastic process should be at point x at time t with a probability $\rho(t,x)$.
- How do we choose $W_{x\to x'}$?

$$\rho \propto \exp(-E(x)/k_B T)$$

Sampling the diffusion equation in 1D

The probability that our random exportation is at location x at time t is

$$p(t+1, x) = \sum_{x'} p(t, x') W_{x' \to x}$$

Sampling the diffusion equation in 1D

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- Let us consider a 1D discrete space: $x \in \mathbf{Z}$.

Sampling the diffusion equation in 1D

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Sampling the diffusion equation in 1D

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- The equation for $p(t, x)$ simplifies to

$$p(t+1, x) = p(t, x-1)W_+ + p(t, x)W_0 + p(t, x+1)W_-$$

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$$p(t+1,x) = p(t,x-1)W_+ + p(t,x)W_0 + p(t,x+1)W_-$$

- In order to have $p=\rho$, one need $W_+ = W_- = \Delta t D/(\Delta x)^2$ and $W_0 = 1 - 2\Delta t D/(\Delta x)^2 = 1 - W_+ - W_-$, and thus $\Delta t D/(\Delta x)^2 \leq 1/2$

Monte-Carlo simulation of Diffusion

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Monte-Carlo simulation of Diffusion

- Therefore a random walk is a way to sample a density ρ that obeys the diffusion equation.
- With a random walk, it is easy to add obstacles, or aggregation processes, hard to include in the differential equation.

More general case: Master equation

The probability to find the random exploration at location x at time t is $p(t, x)$ given by

$$
\begin{aligned}
p(t+1,x) &= \sum_{x'} p(t,x') W_{x' \to x} \\
&= \sum_{x' \neq x} p(t,x') W_{x' \to x} + p(t,x) W_{x \to x} \\
&= \sum_{x' \neq x} p(t,x') W_{x' \to x} + p(t,x)(1 - \sum_{x' \neq x} W_{x \to x'}) \\
&= p(t,x) + \sum_{x' \neq x} [p(t,x') W_{x' \to x} - p(t,x) W_{x \to x'}]
\end{aligned}
\tag{1}
$$

Detailed balance

In a steady state, the condition $p(x) = \rho(x)$ requires that

$$\sum_{x' \neq x} [\rho(x') W_{x' \to x} - \rho(x) W_{x \to x'}] = 0$$

We can then choose $W_{x \to x'}$ according to the **detailed balance** condition

$$\rho(x') W_{x' \to x} - \rho(x) W_{x \to x'} = 0$$

Metropolis Rule

Let us consider a physical system at equilibrium whose probability to be in state x is given by the Maxwell-Boltzmann distribution

$$\rho(x) = \Gamma \exp(-E(x)/kT)$$

We can sample this distribution with a stochastic process by choosing $W_{x \to x'}$ according to the **Metropolis rule**:

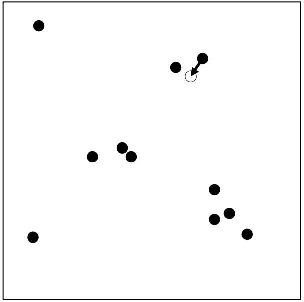
$$W_{x \to x'} = \begin{cases} 1 & \text{si } E' < E \\ \exp[-(E'-E)/kT] & \text{si } E' > E \end{cases}$$

The Metropolis Rule in practice

- In a gas, one selects one particle at random.
- One moves it by an amount Δx.
- One computes the energy E' of the gas with this new position.
- One accepts this change if

$$\text{rand}(0,1) < \min(1, \exp[-(E'-E)/kT])$$

- By sampling ρ with $W_{x \to x'}$, one can compute average physical properties, such as for instance the pressure in the gas.



The Metropolis obeys the detailed balance

Let us assume that $E' > E$. Detailed balance is obeyed because

$$\begin{aligned}\rho(x)W_{x\to x'} &= \Gamma\exp(-E/kT)\exp[-(E'-E)/kT] \\ &= \Gamma\exp(-E'/kT) \\ &= \rho(x')\times 1 \\ &= \rho(x')W_{x'\to x}\end{aligned}$$

And similarly if $E' \leq E$

Glauber Rule

This is an alternative to the Metropolis rule. $W_{x \to x'}$ is given by

$$W_{x \to x'} = \frac{\rho(x')}{\rho(x) + \rho(x')}$$

which also clearly obeys detailed balance
With $\rho = \Gamma \exp(-E(x)/kT)$, one obtains

$$W_{x \to x'} = \frac{\exp(-E'/kT))}{\exp(-E/kT) + \exp(-E'/kT)}$$

$\boxed{\textit{End of module}}$

Monte-Carlo Methods II

$\boxed{\textit{Coming next}}$

Monte-Carlo Methods III

7. Monte-Carlo Methods III

Kinetic / Dynamic Monte-Carlo

Let us consider the chemical equations

$$A \xrightarrow{k_1} B \qquad B \xrightarrow{k_2} A$$

They can be written as an ordinary equation

$$\frac{d}{dt}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$$

Analytical solution

$$A(t) = \frac{k_2}{k_1 + k_2}(A_0 + B_0) + \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t}$$

$$B(t) = \frac{k_1}{k_1 + k_2}(A_0 + B_0) - \frac{A_0 k_1 - B_0 k_2}{k_1 + k_2} e^{-(k_1+k_2)t}$$

where A_0 and B_0 are the initial concentration of A and B.
When $t \to \infty$,

$$A \to A_\infty = \frac{k_2}{k_1 + k_2}(A_0 + B_0) \qquad B \to B_\infty = \frac{k_1}{k_1 + k_2}(A_0 + B_0)$$

Monte-Carlo Simulation

1 One defines a time step Δt, small enough so that $k_1\Delta t$ et $k_2\Delta t$ are smaller than 1. They are the **probabilities** that, during Δt, one A particle get transformed into one B particle, or conversely.

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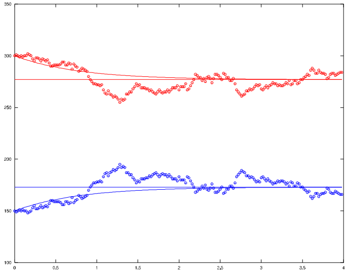
5 One repeats (2)-(4) until $t = t_{max}$

Results



$\Delta t = 0.02$ and $k_1 = 0.5$, $k_2 = 0.8$.
The Monte-Carlo simulation fluctuate around analytic solution.
We should average over several runs

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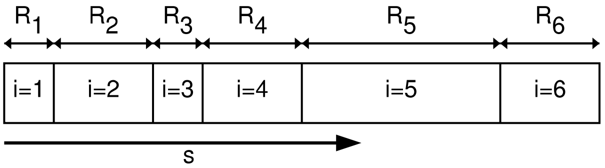

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- Only one event takes place during the time interval Δt.

$\boxed{\textit{End of module}}$

Monte-Carlo method III

$\boxed{\textit{End of Week 1}}$

Thank you for your attention!