Kinetic Monte Carlo lecture

Initiation to the kMC methodology
Day 2

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Kinetic Monte Carlo lecture

Goal of lecture:

- **Understand the time evolution with probabilistic point of view**
- **Understand the structure the kMC algorithms**
- **Implementation of physical system**
- **Some optimization of algorithm**

Material:

- **kMC kernel code**

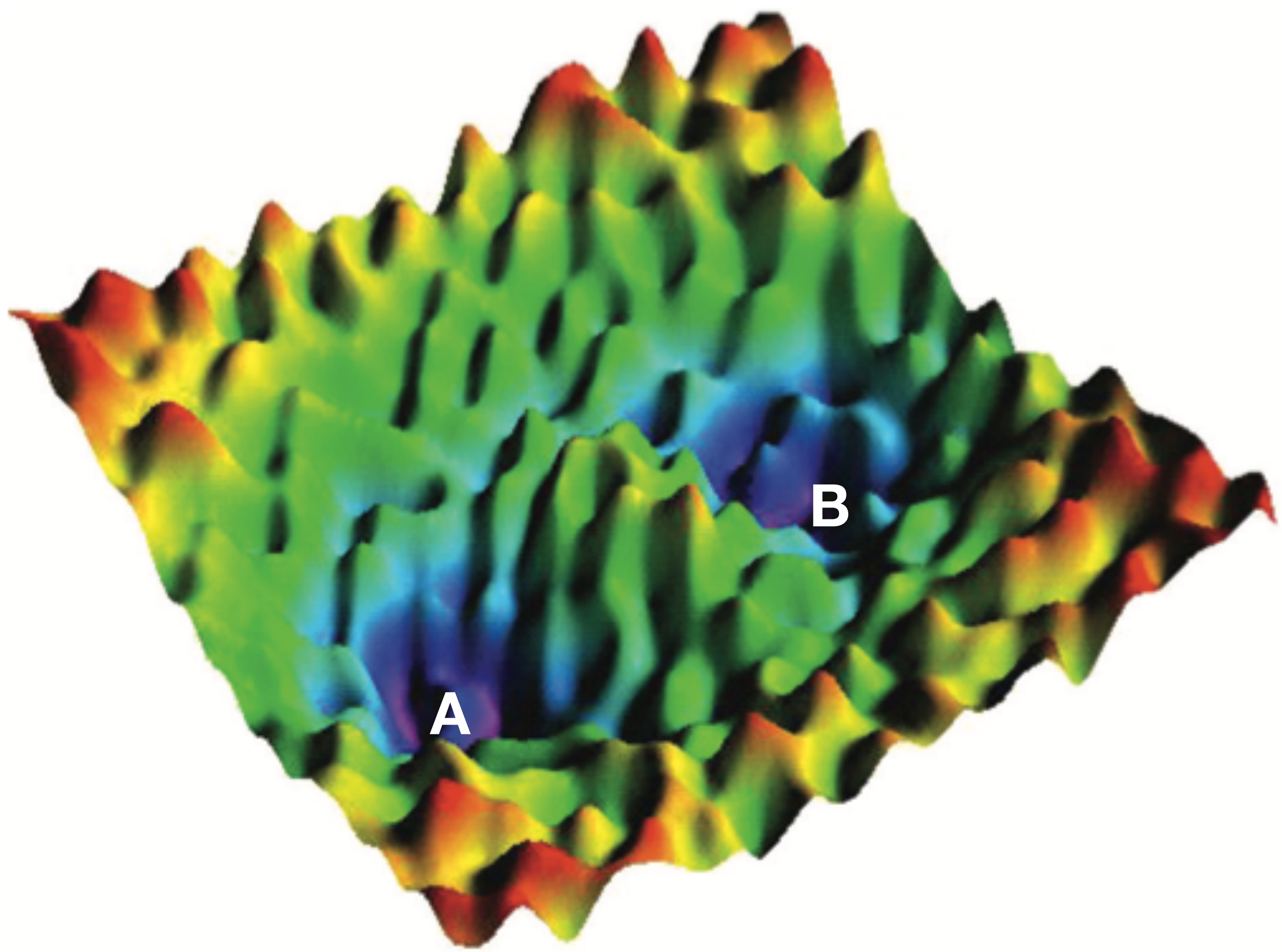
Step_3 : Some attention on complex system

Step_2 : Some optimization

Complex System

Complexity come from the quantity different element and event in the system and the dynamic competition between them

- **Create many local minium**
- **There are many different path possible from the same initial state of system**



Complex system

The first simulation occurs on « rigid network » (code exercice)

Useful for many simple system but totally relevant for the material and the diversity of configuration

Kinetic Monte Carlo « off-lattice » without predefined event library… « On the fly »

Identification of each different atomic environment (local minimum) -> Topology

Use an algorithm of research automatic of saddle point around local minimum

Use machin learning to predict the variation of rate with the environment

Complex System

- **Example of dissolution of Cr cluster in Fe-21Cr alloy**

10 simulations take different path → **Visit phase space**

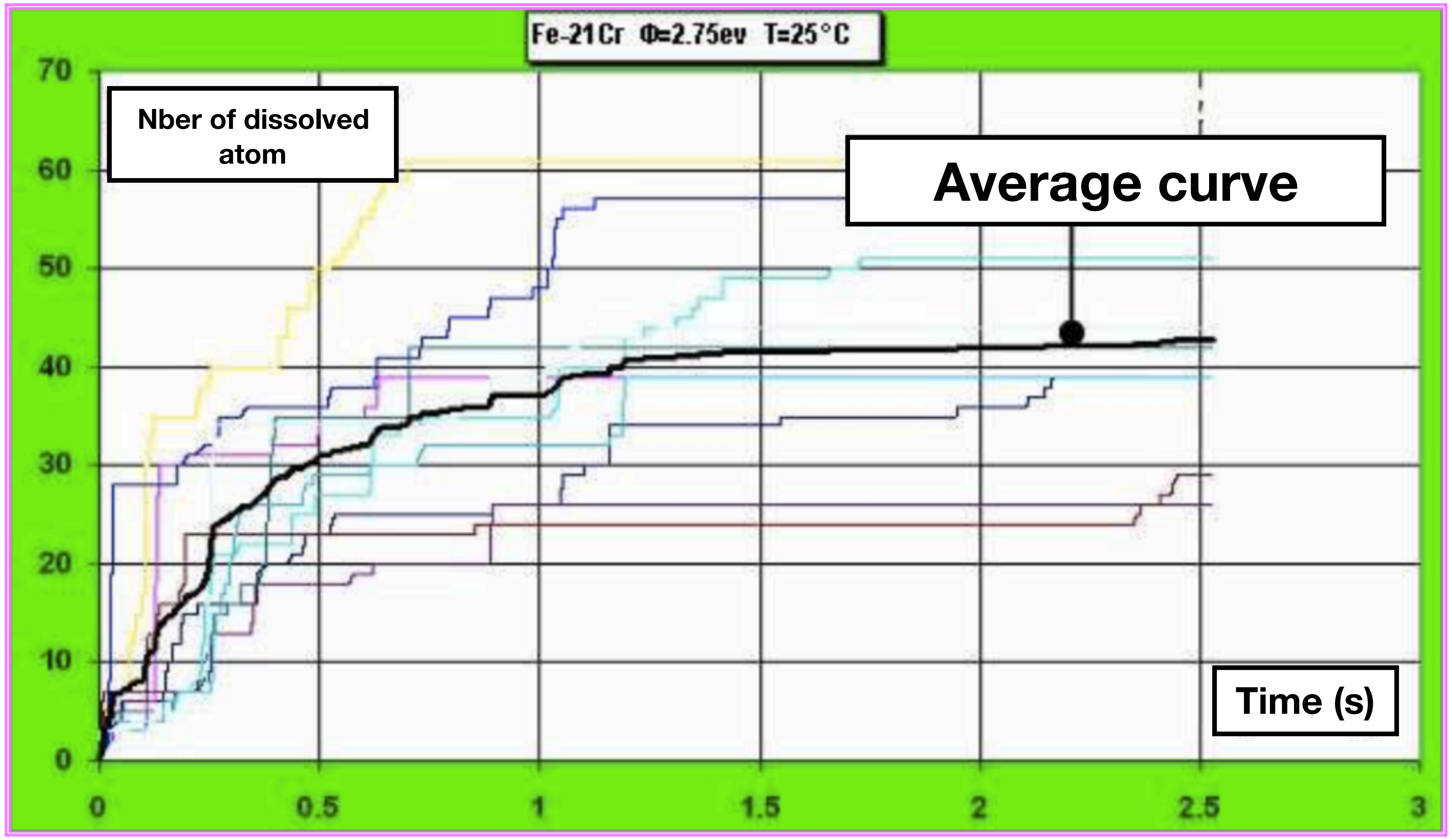
1 path is not revelent for complex system → **We build mean curve of all the path**

Curve Average

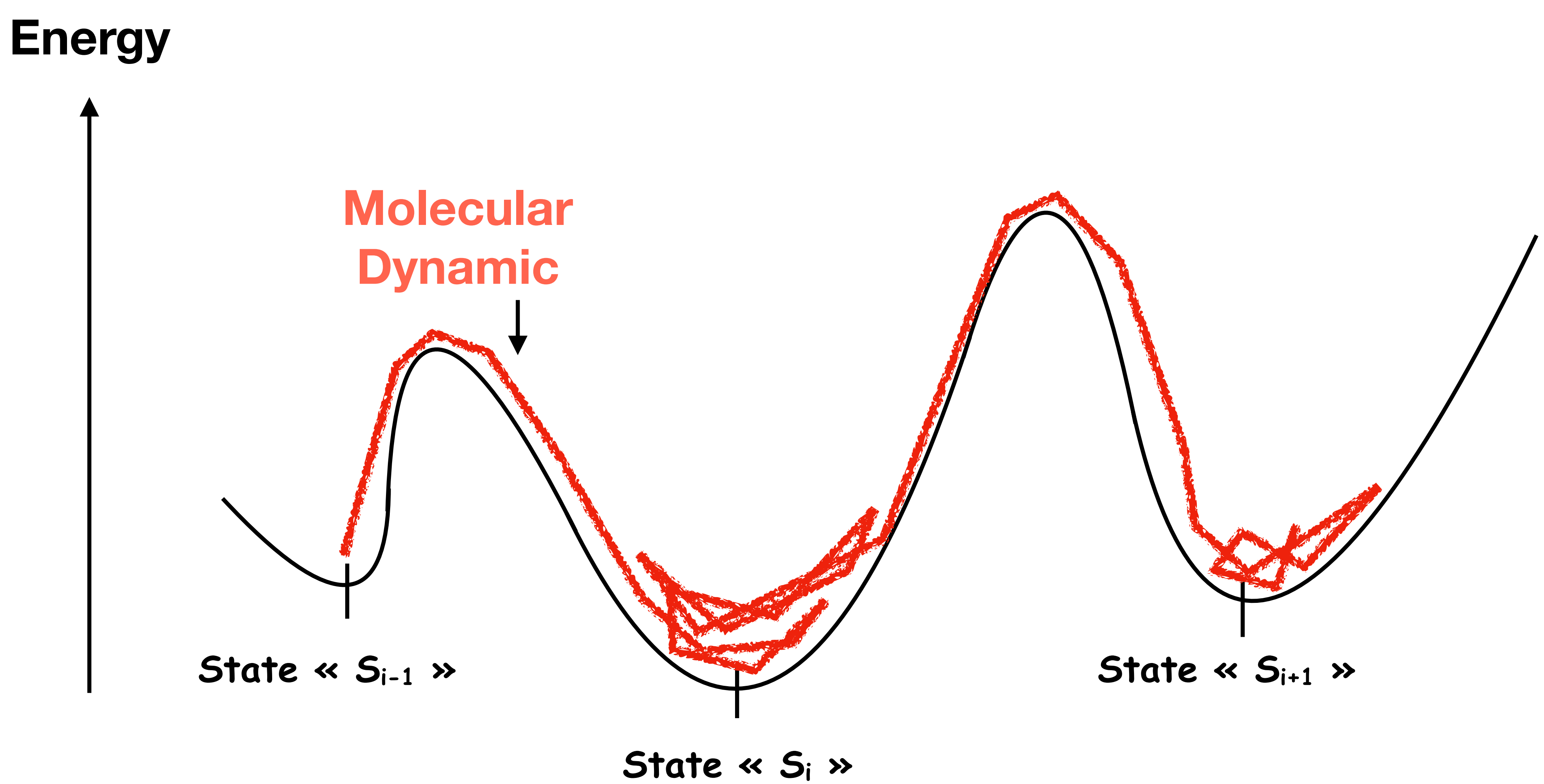
1) **Determine the kMC Time:**
   $T_{max} = \sup\{T_{max\_1}, T_{max\_2}, \ldots T_{max\_N}\}$

2) **Choose the number of step (importante for the smoothing of curve)**

3) **For each intervalle do the average of property**



kMC permit to visit a big part of phase space

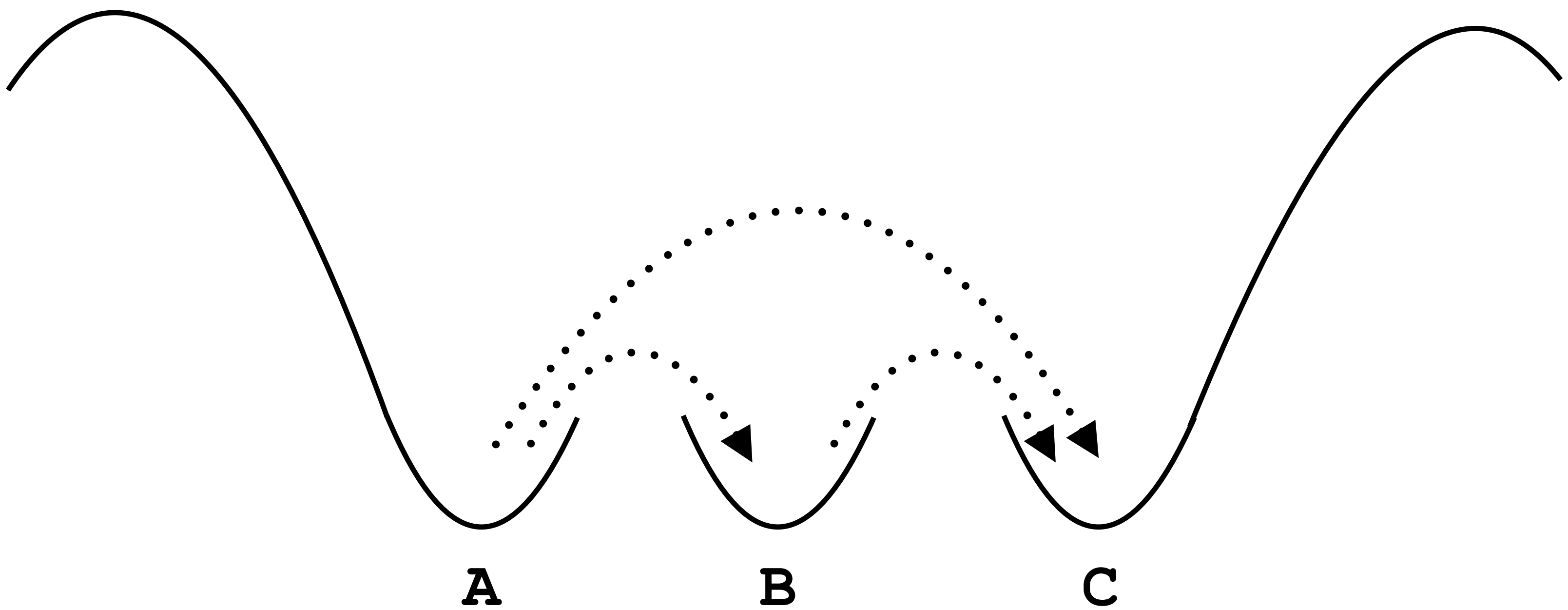


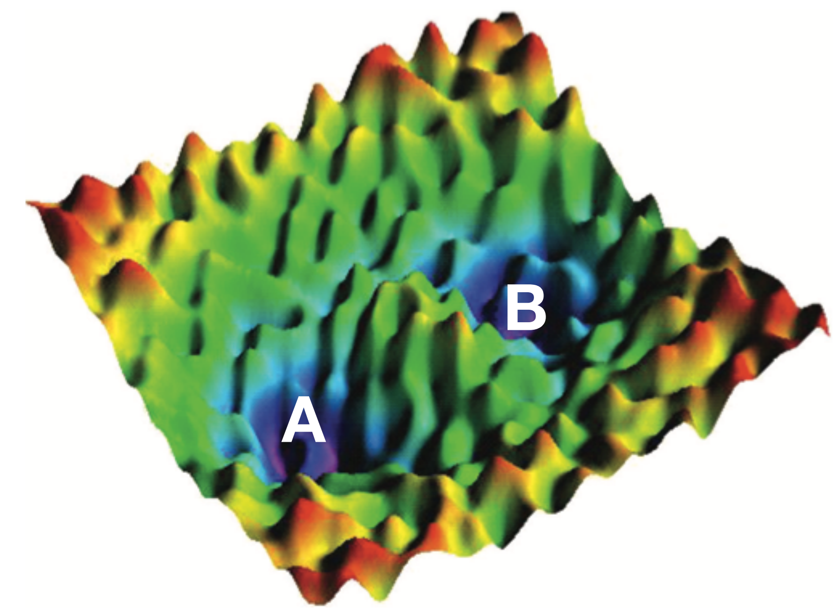
Kinetic Monte Carlo Markovian chain of state $\{S_{i-1}, S_i, S_{i+1}\}$

Complex System

Flinkering state:

Sometime the system can be trapped in loop of event between local minimum.
The system can be oscillate in this loop long time.





Use the Mean-rate Method to compute escape rate $\langle R_{A->j} \rangle$

1) Detect the flickering state => bassin A
2) Identification of escape event to bassin j={B, C, D,…}
3) Compute the escape rate $\langle R_{A->j} \rangle$ from the bassin A to bassin j.
4) We choose an escape event with $Q=\mathrm{Sum}_j \langle R_{A->j} \rangle$

kMC Optimization

1) Local update of event:

In certain case the carry out of an event modify just the rate of event close to it.

2) Selection of event with u1 r.n. following N(0;1):

$$\sum_{j}^{\mu-1} r_{i,j} < u_1 \,.\, r_i \leq \sum_{j}^{\mu} r_{i,j}$$

Binary tree research of event:

$$G_j^k = \sum_{i=1+2(j-1)}^{2j} G_i^{k-1}$$

r_0, r_1, r_2, r_3, …, r_i, …, r_M

k=1 $G^1{}_0$, $G^1{}_1$, $G^1{}_2$, …, $G^1{}_i$, …, $G^1{}_{M/2}$

k=2 $G^2{}_0$, $G^2{}_1$, …, $G^2{}_i$, …, $G^2{}_{M/(2*2)}$

.
.
.

k=K $G^K{}_0$

Mean-rate Method

We are in bassin I connected with other bassins J. The rate to escape from bassin I depend only on the escape event and not on the event inside the bassin.

We define the transition matrix **T** between the bassin: $$T_{IJ} = \frac{R_{I\to J}}{\sum_K R_{I\to K}} = \tau_I^1 R_{I\to J}$$

We calculate the in-bassin occupation probability vector as:

$$\Theta^{tot} = (\mathbb{I} - T)^{-1} . \Theta(0)$$

Then we obtain the mean residence time in bassin I: $$\tau_I = \tau_I^1 \Theta^{tot}$$

Finally the escape rate write: $$< R_{I\to J} > = \frac{\tau_I}{\sum_K \tau_K} R_{I\to J}$$