Introduction to Computer Midterm II
Program Algorithm (Total 30 pts)

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Program Question Open: 12/6/2022 17:00 - 12/8/2022 17:00

Kinetic Monte Carlo

REF: https://en.wikipedia.org/wiki/Kinetic_Monte_Carlo

The kinetic Monte Carlo (kMC) method is a Monte Carlo method computer simulation intended to simulate the time evolution of some processes occurring in nature.

A simple kMC algorithm for simulating the time evolution of a reaction, where all possible processes can occur with known rates k_p, can be written as follows:

1. Set the time t = 0.
2. Set an initial state i.
3. Form the list of all possible N transition rates in the system , from state i into a generic state p.
4. Calculate the cumulative total rate $k_{tot} = \sum_{p}^{N} k_p$.
5. Get a uniform random number $u_1 \in (0,1]$.
6. Find the ***m*** event to carry out by finding the ***m*** for which $\sum_{p}^{m-1} k_p < u_1 \cdot k_{tot} \leq \sum_{p}^{m} k_p$ (this can be achieved efficiently using binary search).
7. Carry out event **m** (update the current state i —> m).
8. Get a second uniform random number $u_2 \in (0,1]$.
9. Update the time with $t_{new} = t_{old} + \Delta t$, where $\Delta t = \frac{\ln(1/u_2)}{k_{tot}}$.
10. Return to step 3.

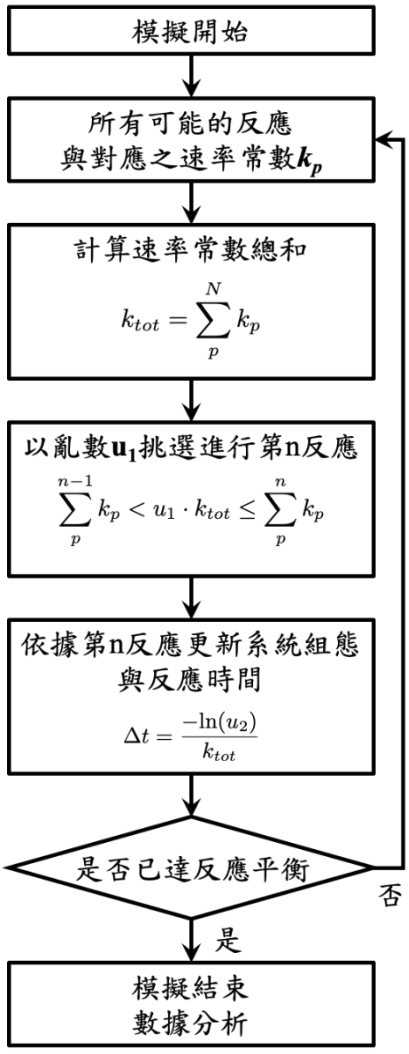

圖 動態蒙地卡羅計算流程

Example:
Consider a reversible reaction:

$$A \xrightarrow{k_1} B$$
$$A \xleftarrow{k_{-1}} B$$
$$k_1 = 10 \text{ and } k_2 = 1$$

For 10 molecules started in A, the time evolution of the system can be calculate by kMC:

MC Step 1

1. All 10 molecules in state A, and calculate cumulated rates:

Reaction	$A \xrightarrow{k_1} B$	$A \xleftarrow{k_{-1}} B$
Rate	k_1 x [A] = 10x10 = 100	k_{-1} x [B] = 1x1 = 0
Cumulated rate	100	100

2. calculate $k_{tot} = \sum_p k_p = 100$
3. Get a uniform random number $u_1 \in (0,1]$,
   In C, you can generate $u_1 = \text{rand}()/\text{RAND\_MAX}$
   assume you get $u_1 = 0.386$
4. Find the reaction event to carry out by finding ***m*** for which $\sum_p^{m-1} k_p < u_1 \cdot k_{tot} \leq \sum_p^{m} k_p$. For $u_1 = 0.386$, the 1st reaction is picked. That is one molecule is changed from A to B
5. Carry out event **m,** update the current state i —> m:

	A	B
Number	10 —> 9	0 —> 1

6. Get a second uniform random number $u_2 \in (0,1]$.
7. Update the time with $t_{new} = t_{old} + \Delta t$, where $\Delta t = \frac{\ln(1/u_2)}{k_{tot}}$.
8. Output current time and states.

MC Step 2

1. Current state:

Reaction	$A \xrightarrow{k_1} B$	$A \xleftarrow{k_{-1}} B$
Rate	k_1 x [A] = 10x9 = 90	k_{-1} x [B] = 1x1 = 1
Cumulated rate	90	91

2. calculate $k_{tot} = \sum_p k_p = 91$
3. Get a uniform random number $u_1 \in (0,1]$,
   In C, you can generate $u_1 = \text{rand}()/\text{RAND\_MAX}$
   assume you get $u_1 = 0.824$
4. Find the reaction event to carry out by finding ***m*** for which
   $\sum_p^{m-1} k_p < u_1 \cdot k_{tot} = 74.984 \le \sum_p^{m} k_p$. For $u_1 = 0.824$, the 1st reaction is picked.
   That is one molecule is changed from A to B
5. Carry out event **m,** update the current state i —> m:

	A	B
Number	9 —> 8	1 —> 2

6. Get a second uniform random number $u_2 \in (0,1]$.
7. Update the time with $t_{new} = t_{old} + \Delta t$, where $\Delta t = \dfrac{\ln(1/u_2)}{k_{tot}}$.
8. Output current time and states.

Continue the kMC procedure with more MC steps