# METROPOLIS ALGORITHM FOR THE GRAND CANONICAL ENSEMBLE 

$$\Xi(\mu, V, T) = \sum_{N=0}^{\infty} e^{\beta\mu N} \frac{1}{\lambda^{3N} N!} \int d^{3N}q \; e^{-\beta U(r_1 \dots r_N)}$$

We should update both $N$ and $\{r_1 \dots r_N\}$

(a) At given iteration the system consists in $N$ particles located in $\{r_1, \dots r_N\}$
We update their positions using the usual canonical Metropolis update

b) We must change the number $N$, i.e. $N \to N \pm 1$
We use the Metropolis algorithm.

As usual we must discuss the proposal for the insertion move $(N \to N+1)$ and the deletion move $(N \to N-1)$. [We propose them with the same prob]

We have $N$ particles in $\{r_1, \dots r_N\}$

(a) INSERTION

We choose a random point in the box: (cubic $L^3$).

$\bar{r}$ = (L*RAN( ), L*RAN( ), L*RAN( ))

We choose a label in $\{1, \dots N+1\}$ (label $= i$)

The new configuration is

$$\bar{r}_1, \dots \bar{r}_{i-1}, \bar{r}, \bar{r}_{i+1}, \dots \bar{r}_N, \bar{r}_i$$

[$\bar{r}_i$ has been moved at the end, and $\bar{r}$ replaces $\bar{r}_i$]

Note that if $i = N+1$ the new configuration is simply

$$\bar{r}_1 \dots \bar{r}_N, \bar{r} \qquad [\bar{r} \text{ is appended at the end}]$$

(b) DELETION

We choose a random label $i$ in $\{\cancel{0}, \dots, N\}$ and delete particle in $\bar{r}_i$. The new conf. is

$$\bar{r}_1, \dots \bar{r}_{i-1}, r_N, r_{i+1}, \dots r_{N-1}$$

Note that we have moved, the last particle in the "hole".

The insertion / deletion move have been chosen so that it is possible to go back and forth with a non vanishing probability

$$N \text{ part.} \quad r_1 \dots \quad r_N \qquad \text{choose } i$$

$$\downarrow \text{insert}$$

$$(N+1) \text{ part} \quad r_1, \dots r_{i-1}, r, r_{i+1}, \dots r_N, r_i$$

$$\downarrow \text{delete} \qquad \text{choose the same } i$$

$$(N\text{-part}) \quad r_1 \dots r_{i-1}, r_i, r_{i+1} \dots r_N$$

SAME CONF AS THE ONE WE STARTED FROM

We wish now to compute $P^{(0)}$

$$P^{(0)}\Big[N,\{\bar r_1\ldots \bar r_N\} \to N+1,\{r_1,\ldots,\overset{\text{in position}(i)}{r},\ldots r_N, r_i\}\Big]$$

$$= \frac{1}{N+1}\cdot\frac{1}{V}\cdot\frac{1}{2}$$

$\frac{1}{2}$ ← probability of proposing a move ($N\to N+1$)

$\frac{1}{V}$ ← We choose a point in the box ($P^{(0)}$ is a prob. DENSITY)

$\frac{1}{N+1}$ ← we choose a label among $(N+1)$ possibilities

$$P^{(0)}\Big[N+1,\{r_1,\ldots,r,\ldots,r_N,r_i\}\to N,\{r_1\ldots r_N\}\Big]$$

$$= \frac{1}{N+1}\cdot\Big(\leftarrow \text{we choose a particle among } (N+1) \text{ available}\Big)\times\frac{1}{2}$$

$\frac{1}{2}$ ← [probability of proposing $N+1\to N$]

$$R(N\to N+1) = \frac{P^{(0)}(N+1\to N)\,\pi(N+1)}{P^{(0)}(N,N+1)\,\pi(N)}$$

[coordinates are not written explicitly]

$$= \frac{\dfrac{1}{2(N+1)}}{\dfrac{1}{2(N+1)V}}\;\frac{e^{\beta\mu(N+1)}\,\dfrac{1}{\lambda^{3N+3}(N+1)!}\,e^{-\beta U_{N+1}}}{e^{\beta\mu N}\,\dfrac{1}{\lambda^{3N}\,N!}\,e^{-\beta U_N}}$$

same notation as in the Widom algorithm

$$= \frac{e^{\beta\mu}V}{\lambda^3(N+1)}\,e^{-\beta(U_{N+1}-U_N)}$$

$$A(N,N+1) = \min\left(1,\ \frac{e^{\beta\mu}V}{\lambda^3(N+1)}\,e^{-\beta(U_{N+1}-U_N)}\right)$$

$$A(N+1, N) = \min\left(1, R(N+1,N)\right)$$
$$= \min\left(1, \frac{1}{R(N,N+1)}\right)$$
$$= \min\left(1, \frac{\lambda^3 (N+1)}{V e^{\beta\mu}} e^{\beta(U_{N+1} - U_N)}\right)$$
$$A(N, N-1) = \min\left(1, \frac{\lambda^3 N}{V e^{\beta\mu}} e^{\beta(U_N - U_{N-1})}\right)$$

<u>IN PRACTICE</u>: if we have $N$ particles in $\{r_1 \dots r_N\}$

(a) Choose which move to perform
[ $x = RAN()$. if $x < 0.5$ delete one particle
if $x \geq 0.5$ add one particle ]

(b1) delete choose one particle to be deleted
Compute $U_N - U_{N-1}$ and accept the move
with prob
$$\min\left(1, \frac{\lambda^3 N}{V e^{\beta\mu}} e^{\beta(U_N - U_{N-1})}\right)$$

(b2) alternatively add one particle
Compute $U_{N+1} - U_N$ and accept the move
with probability
$$\min\left(1, \frac{V e^{\beta\mu}}{\lambda^3 (N+1)} e^{-\beta(U_{N+1} - U_N)}\right)$$

COMMENT: The reorganization of the labels is only needed in the proof, but not in the practical implementation

The insertion is usually defined in the following way.

We choose a point $\bar{r} = (L\,RAN(\,),\, L\,RAN(\,),\, L\,RAN(\,))$ and the new configuration is

$\bar{r}_1, \ldots \bar{r}_N, \bar{r}$ ($\vec{r}$ is appended at the end)

Deletion is unchanged. If we use the same acceptances as before, the new algorithm is still correct: it does not satisfy detailed balance, but it satisfies stationarity