The Fokker-Planck equation

From last lecture:

The Fokker-Planck equation describes the change of the probability distribution function with time:

$$\frac{\partial P(x,0)}{\partial t} \approx -\frac{\partial}{\partial x}\left[P(x,0)M_1\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[P(x,0)M_2\right],$$

where

$$M_n = \frac{1}{\Delta_t}\int d\tilde{x}\ \tilde{x}^n D(x+\tilde{x}, \Delta_t | x, 0).$$

Application of the Fokker-Planck equation

What is the stationary probability distribution for a particle in a one dimensional potential $U(x)$ at temperature T, with Brownian dynamics?

We then need to evaluate the integrals over $D(x+\tilde{x}, \Delta_t|x, 0)$, related to the dynamics,

$$x(\Delta_t) = x(0) + \frac{\Delta_t}{\alpha} F + \eta \Delta_t.$$

Write as a delta function!

$$D(x+\tilde{x}, \Delta_t|x, 0) = \delta\left(x + \frac{\Delta_t}{\alpha} F + \eta\Delta_t - (x+\tilde{x})\right) = \delta\left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t - \tilde{x}\right).$$

The relevant quantities are M_1 and M_2 *averaged over the random noise*:

$$M_n = \frac{1}{\Delta_t}\left\langle \int d\tilde{x}\, \tilde{x}^n\, \delta\left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t - \tilde{x}\right)\right\rangle = \frac{1}{\Delta_t}\left\langle \left(\frac{\Delta_t}{\alpha} F + \eta\Delta_t\right)^n \right\rangle.$$

Application of the Fokker-Planck equation. . . cont'd

$$\textit{With} \qquad M_n = \frac{1}{\Delta_t}\left\langle \left(\frac{\Delta_t}{\alpha} F + \eta \Delta_t \right)^n \right\rangle \qquad \textit{and}$$

$$F = -\partial U/\partial x, \qquad \langle \eta \rangle = 0, \qquad \langle \eta^2 \rangle = \frac{2T}{\alpha \Delta_t},$$

we get, to lowest order in Δ_t,

$$M_1 = -\frac{1}{\alpha}\frac{\partial U}{\partial x} + \frac{1}{\Delta_t}\langle \eta \rangle \Delta_t = -\frac{1}{\alpha}\frac{\partial U}{\partial x},$$

and

$$M_2 = \frac{1}{\Delta_t}\left[\left(-\frac{\Delta_t}{\alpha}\frac{\partial U}{\partial x} \right)^2 - \frac{\Delta_t}{\alpha}\frac{\partial U}{\partial x}\langle \eta \rangle \Delta_t + \langle \eta^2 \rangle \Delta_t^2 \right] = \frac{2T}{\alpha}.$$

Stationary solution

Our equation is

$$\frac{\partial P}{\partial t} \approx -\frac{\partial}{\partial x}\left[PM_1\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[PM_2\right].$$

With

$$M_1 = -\frac{1}{\alpha}\frac{\partial U}{\partial x}, \quad M_2 = \frac{2T}{\alpha},$$

this becomes

$$\frac{\partial P}{\partial t} \approx \frac{1}{\alpha}\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] + \frac{T}{\alpha}\frac{\partial^2 P}{\partial x^2},$$

Stationary solution. . . cont'd

We now want to demonstrate that $P \propto e^{-U/T}$ is the stationary solution to the F-P equation, i.e. that it gives $\partial P/\partial t = 0$. First note:

$$P \propto e^{-U/T}, \quad \frac{\partial P}{\partial x} = -\frac{1}{T}\frac{\partial U}{\partial x}P, \quad \frac{\partial^2 P}{\partial x^2} = \left[\frac{1}{T^2}\left(\frac{\partial U}{\partial x}\right)^2 - \frac{1}{T}\frac{\partial^2 U}{\partial x^2}\right]P.$$

We then have

$$\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] = \frac{\partial P}{\partial x}\frac{\partial U}{\partial x} + P\frac{\partial^2 U}{\partial x^2} = -\frac{1}{T}\left(\frac{\partial U}{\partial x}\right)^2 P + \frac{\partial^2 U}{\partial x^2}P.$$

and we arrive at

$$\frac{\partial P}{\partial t} \approx \frac{1}{\alpha}\frac{\partial}{\partial x}\left[P\frac{\partial U}{\partial x}\right] + \frac{T}{\alpha}\frac{\partial^2 P}{\partial x^2} = 0.$$

Monte Carlo simulations

The theoretical treatment of Monte Carlo simulations starts from the concept of a Markov chain but since this is rather abstract we will...

1. introduce Monte Carlo by considering how the method is used for simulating a gas,
2. turn to the formulation in terms of Markov chains as a second step.

Monte Carlo for an interacting gas

In the standard implementation one loops over the particles, $i = 1, \ldots N$:

1. Suggest a *random* change of the position of particle i:

$$\mathbf{r}_i' = \mathbf{r}_i + \boldsymbol{\delta}_i,$$

   where the $\delta_i^{(x)}$, $\delta_i^{(y)}$, and $\delta_i^{(z)}$, are usually from a rectangular distribution centered around zero, $\in [-b, b)$.

2. Let ν denote the initial configuration and μ the new configuration where particle i is at $\mathbf{r}_i'$. Calculate the energy difference $\Delta U = U_\mu - U_\nu$.

3. Accept this new position with probability

$$\alpha_{\nu\to\mu} = \min\left(e^{-\Delta U/T}, 1\right).$$

   i.e. generate a random number $\xi \in [0, 1)$ and accept the change if $\xi < \alpha_{\nu\to\mu}$.

Monte Carlo simulations. . . a few remarks

- Monte Carlo is exact! (Other methods are correct only as $\Delta_t \to 0$.)
- To get a reasonably efficient simulation the range of the suggested changes $\boldsymbol{\delta}_i$ should be chosen such that the acceptance ratio is not too far from 50%, say between 30 and 70%.
- To compute the *change* in energy we use

$$\Delta U \equiv U_\mu - U_\nu = \sum_j [u(\mathbf{r}_i' - \mathbf{r}_j) - u(\mathbf{r}_i - \mathbf{r}_j)],$$

which is a computation of order N.
No need to calculate the $\sim N^2/2$ terms in

$$\sum_{i<j} u(\mathbf{r}_{ij}).$$

Markov chains

Note: matrices are here used as a means to describe the dynamics. They are never put into the computer.

Suppose that there is a finite number of possible configurations or multidimensional variables $x^{(\nu)}$.
A Markov chain is a random chain of these variables, x_1, x_2,... produced by means of a transition matrix $p_{\nu\mu}$ with the following properties:

1. $p_{\nu\mu} \geq 0$,
2. $p_{\nu\nu} \neq 1$,
3. $\sum_\mu p_{\nu\mu} = 1$ for all ν.

1. necessary since probabilities have to be non-negative,
2. the chain may never come to a halt,
3. the total probability to go to some state must always be equal to unity.

Markov chains. . . cont'd

If the chain is ergodic—i.e. if we are not stuck in a limited region of the phase space—then. . .

> *A random walk according to these transition probabilities will lead to a certain probability distibution* $\pi_\nu \equiv \pi(x^{(\nu)})$.

This is a profound result which makes Markov chains very useful.

(One can also relax the condition of a discrete set of possible configurations; Markov chains may also be defined for a continuous configuration space.)

To construct the transition matrix

How should we go about to choose the transition matrix such that a certain probability distribution π_ν is obtained?

A sufficient (but not necessary) condition is to require *detailed balance*, i.e.

$$\pi_\nu p_{\nu\mu} = \pi_\mu p_{\mu\nu}.$$

Consider the probability to be in state μ after a given step, which is

$$\sum_\nu \pi_\nu p_{\nu\mu} = \pi_\mu \sum_\nu p_{\mu\nu} = \pi_\mu.$$

(What is shown here: If we start in the desired probability distribution we will remain in that probability distribution.)

To construct the transition matrix. . . cont'd

The transition probability may be thought of to consist of two parts.

$$\text{We write} \qquad p_{\nu\mu} = q_{\nu\mu}\alpha_{\nu\mu}, \qquad \text{where}$$

$$\begin{aligned} q_{\nu\mu} &= \text{probability for the transition to be suggested} \\ \alpha_{\nu\mu} &= \text{probability for the transition to be accepted} \end{aligned}$$

Note that $q_{\nu\mu}$ in our gas is non-zero only for the small subset of all possible configurations μ with $\mathbf{r}_i^{(\mu)} = \mathbf{r}_i^{(\nu)}$ for $N-1$ particles and $\mathbf{r}_i^{(\mu)} = \mathbf{r}_i^{(\nu)} + \boldsymbol{\delta}$ for the remaining particle.

Detailed balance may be fulfilled with the following choice for $\alpha_{\nu\mu}$:

$$\alpha_{\nu\mu} = \min\left(\frac{\pi_\mu q_{\mu\nu}}{\pi_\nu q_{\nu\mu}}, 1\right)$$

The Metropolis algorithm

This simplifies for symmetric targeting probabilities $q = q_{\nu\mu} = q_{\mu\nu}$.

$$\alpha_{\nu\mu} = \min\left(\frac{\pi_\mu}{\pi_\nu}, 1\right)$$

We now demonstrate that this expression leads to detailed balance,

$$\pi_\nu p_{\nu\mu} = \pi_\mu p_{\mu\nu}.$$

With $p_{\nu\mu} = q\alpha_{\nu\mu}$:

$$\pi_\nu p_{\nu\mu} = \pi_\nu q\ \alpha_{\nu\mu} = \pi_\nu q \min\left(\frac{\pi_\mu}{\pi_\nu}, 1\right) = q\ \min(\pi_\nu, \pi_\mu).$$

$$\pi_\mu p_{\mu\nu} = \pi_\mu q\ \alpha_{\mu\nu} = \pi_\mu q \min\left(\frac{\pi_\nu}{\pi_\mu}, 1\right) = q\ \min(\pi_\mu, \pi_\nu).$$

(The same derivation works for the more general $\alpha_{\nu\mu}$.)

Monte Carlo and expectation values

How do we calculate expectation values? Two cases:

- Experiments, MD and MC, with n measurements:

$$\langle A \rangle = \frac{1}{n} \sum_{\nu=1}^{n} A_\nu .$$

  Here the configurations appear with a probability $\propto e^{-E_\nu / T}$.

- Statistical physics:

$$\langle A \rangle = \sum_{\nu} A_\nu P_\nu = \frac{1}{Z} \sum_{\nu} A_\nu e^{-E_\nu / T} .$$

  The sum is here over all possible configurations.

Program structure

The program usually consists of a few different parts:

1. **Initialization** – Assign initial values to the positions in some way. (Positions from an earlier run. Just random values).
2. **Equilibration** – Some time is needed before the Markov chain starts to give configurations from to the correct probability distribution. ("Thermalization." This sometimes needs very long times.)
3. **Production** – The actual run when data are collected. Results could also be written to a data file for later analysis.
4. **Print out results** – The averages are obtained from `v1sum`. (See below!) With `v2sum` it also becomes possible to determine the standard error.

Production

The part of the run when data are collected. Also write to a data file and a config file for later use.

The below is a good structure for the simulation.

```
for iblock=... {
  for isamp= ... nsamp {
    mc_update(pos);
    measure(pos, vsum);
  }
  write_data(vsum);
  write_conf(pos);
  v1sum[ ] += vsum[ ];
  v2sum[ ] += vsum[ ] * vsum[ ];
}
```