1 Optimizing the parallel tempering method

One considers a system of N identical point particles of mass m. The Hamiltonian is given by

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m} + V(\vec{x}^N) \tag{1}$$

where $V(\vec{x}^N)$ is the interaction potential, $\vec{p}_i$, the momentum of particle i, and $\vec{x}^N = (\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N)$ is a short-hand notation for the particle positions. In order to study the phase diagram, one performs a Monte Carlo simulation using the tempering method. It consists in performing simulation with M different boxes. Each box is in contact with a thermostat at the inverse temperature β_i. The inverse temperatures β_i are given by a increasing sequence $\beta_{i-1} < \beta_i < \beta_{i+1}$. The stochastic evolution of the system is given by two kinds of Markovian processes : single moves in each box using a Metropolis rule and particle swaps between two nearest neighbor boxes following also a Metropolis rule.

Let us denote the configurational integral of the canonical partition function as

$$Q(\beta) = \int d\vec{x}^N \exp\left(-\beta V(\vec{x}_N)\right) \tag{2}$$

where $d\vec{x}^N = \prod_{i=1}^N d\vec{x}_i$.

1. Express the joint probability distribution density of the particles $P(\beta, \beta', \vec{x}^N, \vec{x}'^N)$ of two boxes at the inverse temperature β and β' as a function of $Q(\beta)$ $Q(\beta')$, β, β' $V(\vec{x}_i)$ and $V(\vec{x}'_i)$.
2. Defining $P_a(\beta, \beta')$ the acceptance probability for particle swaps between neighboring boxes at the inverse temperatures β and β', justify that

$$P_a(\beta, \beta') = \iint d\vec{x}^N d\vec{x'}^N P(\beta, \beta', \vec{x}^N, \vec{x'}^N) \mathrm{Min}\left(1, \exp\left((\beta' - \beta)(V(\vec{x'}_N) - V(\vec{x}_N))\right)\right) \tag{3}$$

3. Justify that $P_a(\beta, \beta') = P_a(\beta', \beta)$
4. For the sake of simplicity, one now assumes that $\beta' > \beta$, show that

$$\mathrm{Min}\left(1, \exp\left([\beta' - \beta][\mathrm{V}(\tilde{\mathrm{x}}'_\mathrm{N}) - \mathrm{V}(\tilde{\mathrm{x}}_\mathrm{N})]\right)\right) = \exp\left(\frac{(\beta' - \beta)}{2}(\mathrm{V}(\tilde{\mathrm{x}}'_\mathrm{N}) - \mathrm{V}(\tilde{\mathrm{x}}_\mathrm{N}))\right)$$
$$\exp\left(-\frac{(\beta' - \beta)}{2}|V(\vec{x'}_N) - V(\vec{x}_N)|\right) \tag{4}$$

5. Introducing the variables $R = \frac{\beta'}{\beta}$ and $\overline{\beta} = \frac{\beta + \beta'}{2}$, show that

$$P_a(\beta, \beta') = \frac{Q^2(\overline{\beta})}{Q(\beta)Q(\beta')} \iint d\vec{x}^N d\vec{x'}^N P(\overline{\beta}, \overline{\beta}, \vec{x}^N, \vec{x'}^N) \exp\left(-\frac{R-1}{R+1}\overline{\beta}|V(\vec{x'}_N) - V(\vec{x}_N)|\right) \tag{5}$$

One aims to obtain an asymptotic estimate of P_a when $\beta' - \beta \ll 1$,namely $R - 1 \ll 1$.

6. Using the thermodynamic relation $C_v(\beta) = -\beta^2 \frac{\partial^2 \beta F(\beta)}{\partial \beta^2}$ (where $F(\beta)$ is the excess free energy of the system), show that

$$\frac{Q^2(\overline{\beta})}{Q(\beta)Q(\beta')} = 1 - \left(\frac{R-1}{R+1}\right)^2 Cv(\overline{\beta}) + O(|R-1|^3) \tag{6}$$

where C_v is the specific heat of the system.

7. Show that

$$\iint d\vec{x}^N d\vec{x'}^N P(\overline{\beta}, \overline{\beta}, \vec{x}^N, \vec{x'}^N) \exp\left(-\frac{R-1}{R+1}\overline{\beta}|V(\vec{x'}_N) - V(\vec{x}_N)|\right) = 1 - \frac{R-1}{R+1}M(\overline{\beta}) + \left(\frac{R-1}{R+1}\right)^2 Cv(\overline{\beta}) + ... \tag{7}$$

where $M(\overline{\beta})$ is expressed as a mean average of $|V(\vec{x'}_N) - V(\vec{x}_N)|$.

8. Finally, by combining the above results, show that

$$P_a(\beta, \beta') = 1 - \frac{R-1}{R+1}M(\overline{\beta}) + O(|R-1|^3) \tag{8}$$

9. Using the Cauchy-Schwarz inequality $\langle|V(\vec{x'}_N) - V(\vec{x}_N)|\rangle^2 \leq \langle|V(\vec{x'}_N) - V(\vec{x}_N)|^2\rangle$, show that $M^2(\overline{\beta}) \leq 2C_V\overline{\beta})$

10. An optimal tempering Monte-Carlo method consists in having an equal acceptance between successive boxes. If the specific heat C_v (or M)is also constant in the range of $[\beta_{Max}, \beta_{Min}]$ show for N boxes that the inverse temperatures must be chosen as

$$R = \left(\frac{\beta_{max}}{\beta_{min}}\right)^{\frac{1}{N-1}} \tag{9}$$

and

$$\beta_i = R^{i-1}\beta_{min} \tag{10}$$

11. For the study of a first-order phase transition, can one assume a constant C_v ?

2 Clogging phenomenon in a channel : the Bridge model

One considers an one-dimensional stochastic model where particles enter a channel randomly according an exponential probability $P(\lambda) = \lambda e^{-\lambda t}$, where λ is the mean incoming flux. The time spent in the channel is the same for all particles and is denoted by $\tau = L/v$ where L is the length of the channel. When two particles are simultaneously present, the channel becomes blocked and no particle can enter the channel. After a finite duration τ_b, the blocked channel is released because one assumes that two particles exit the channel at the same time. Let us denote $P_0(t)$, $P_1(t)$ and $P_2(t)$, the probabilities of having a channel at time t with 0, 1 or 2 particles respectively.

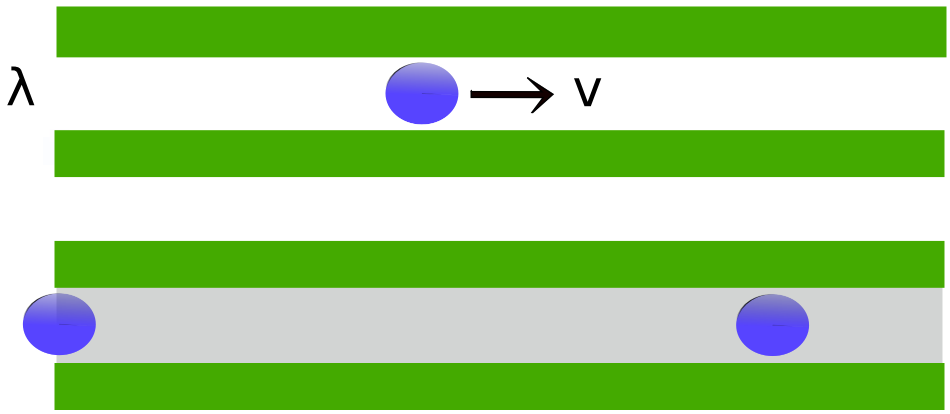

FIGURE 1 – Sketch of the model : (i) the passage is open when either zero or one particle is present. (ii) If a particle enters when another is already present, the passage is blocked preventing the entry of new particles. After time τ_b both trapped particles exit the passage.

1. Show that the kinetic evolution of the system is given by the differential equations. (Each term must be clearly explained).

$$\frac{dP_0(t)}{dt} = -\lambda P_0(t) + \lambda e^{-\lambda\tau} P_0(t-\tau) + \lambda P_1(t-\tau_b) \quad (11)$$

$$\frac{dP_1(t)}{dt} = -\lambda P_1(t) + \lambda P_0(t) - \lambda e^{-\lambda\tau} P(0, t-\tau) \quad (12)$$

$$\frac{dP_2(t)}{dt} = \lambda P_1(t) - \lambda P_1(t-\tau_b) \quad (13)$$

2. Show the total probability $P(t) = P_0(t) + P(1,t) + P(2,t)$ is conserved by the process.
3. Starting with the initial condition with an empty channel, show that

$$\tilde{P}_0(u) = \frac{\lambda + u}{\Delta} \quad (14)$$

$$\tilde{P}_1(u) = \frac{\lambda(1 - e^{-(\lambda+u)\tau})}{\Delta} \quad (15)$$

where

$$\Delta = (\lambda + u)^2 - \lambda(\lambda + u)e^{-(\lambda+u)\tau} - \lambda^2 e^{-u\tau_b}(1 - e^{-(\lambda+u)\tau})$$

4. One defines the active probability of the channel as the sum of $P_0(t) + P_1(t)$. Using the above equations, obtain the active probability of the stationary state, $P_A(\infty)$.
5. One considers the stationary flux of particles exiting the channel denoted $J(\lambda)$. Find the relation between J and $P_A(\infty)$, and show that $J(\lambda)$ is given by

$$J(\lambda) = \lambda \frac{2 - e^{-\lambda\tau}}{2 - e^{-\lambda\tau}(1 + \lambda\tau_b) + \lambda\tau_b} \quad (16)$$

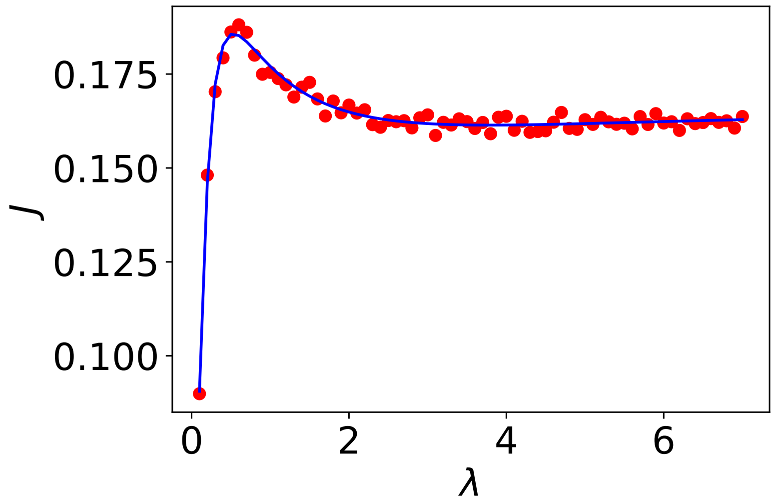

FIGURE 2 – Stationary flux as a function of λ : dots correspond to simulation results and full curve to exact result.

6. Give the leading term of the stationary flux when $\lambda \to 0$ and when $\lambda \to +\infty$. Give a physical interpretation of these results
7. Write a python code for this model. Fig.2 shows the stationary flux J versus λ at the value $\tau_b = 12$. τ is set to 1. Simulation results (dots) are obtained by the python code and compared with the exact result (full curve).

Glossary

— The Laplace transform of a function $f(t)$ is defined as

$$L(f(t)) = \tilde{f}(u) = \int_0^\infty f(t)e^{-ut}dt \tag{17}$$

— Basic properties :

$$\begin{aligned} \tilde{f}'(u) &= -f(0) + u\tilde{f}(u) \\ L(f(t-\tau)) &= e^{-u\tau}\tilde{f}(u) \\ f(\infty) &= \lim_{u\to 0} u\tilde{f}(u) \end{aligned}$$