Computatonal physics - Statistical Physics

Martin Johnsrud

March 10, 2020

Introduction

By numerically integrating Newtons equation of motion og many particles, confined to a box and interacting via the Leonard-Jones potential, it is possible to see the emergence of statistical behvior like the Maxwell-Boltzmann distribution. In this exercice, we explor this behavior, and ... (more to come)

Single particel

A single particel with position $\vec{x} = (x_1, x_2)$ in a box is modeled in a potential

$$V_w(\vec{x}) = \begin{cases} \frac{1}{2}K(r-R)^2, & r > R \\ 0, & r < R, \end{cases}$$

where $r = |\vec{x}|$. This leads to a force

$$\vec{F}_w(\vec{x}) = -\nabla V_w(\vec{x}) = \begin{cases} -K(r-R)\hat{x}, & r > R \\ 0, & r < R. \end{cases}$$

N particles

When moddeling N particles $\{\vec{x}_k\} = \{(x_1^{(k)}, x_2^{(k)})\}$, each one of them is subject to the force from the potential $V_w(\vec{x}_k)$, as well as a modified Leonard-Jones potential the interaction potential. The potential felt by particle k is then

$$V_k(\vec{x}_j) = \sum_{r_{kj} < a} \epsilon \left[\left(\frac{a}{r_{kj}} \right)^{12} - 2 \left(\frac{a}{r_{kj}} \right)^{6} + 1 \right]$$

Here, $r_{kj} = |\vec{x}_k - \vec{x}_j|$. The force on particel k by this potential is

$$F_k(\vec{x}_j) = -\nabla_k V(\vec{x}_j) = \sum_{r_{kj} < a} 24\epsilon \left[\left(\frac{a}{r_{kj}} \right)^{12} - \left(\frac{a}{r_{kj}} \right)^{6} \right] \frac{\hat{x}_{kj}}{r_{kj}},$$

where $\hat{x}_{kj} = (\vec{x}_k - \vec{x}_j)/r_{kj}$