

# Computational physics - Statistical Physics

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## Introduction

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

## Single particle

A single particle 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 modeling  $N$  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 particle  $k$  by this potential is

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

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