

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

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

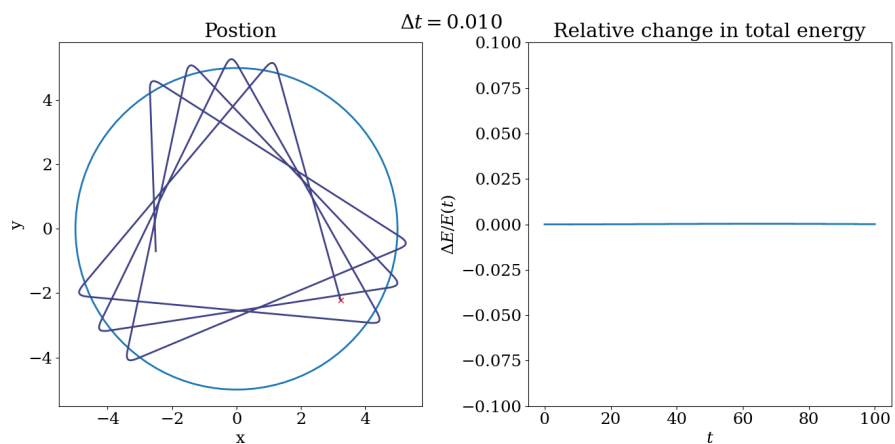
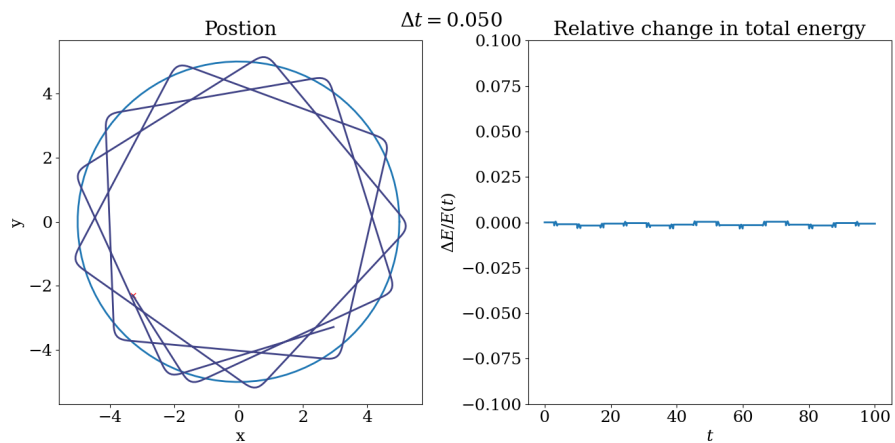
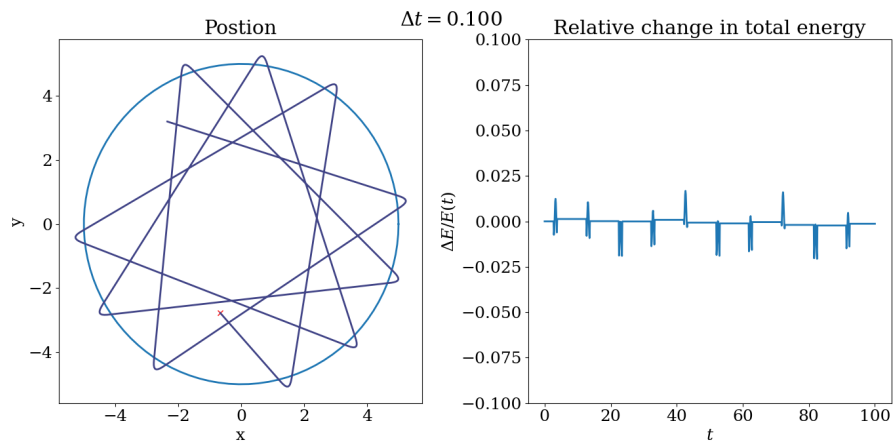
where $r = |\vec{x}|$. This leads to a force

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

This equation can be numerically integrated to simulate the trajectory of the particle. This project is done using verlet integration,

$$\begin{aligned} \vec{x}(t + \Delta t) &= \vec{x}(t) + \dot{\vec{x}}(t)\Delta t + \frac{1}{2}\vec{F}(\vec{x}(t))\Delta t^2 \\ \dot{\vec{x}}(t + \Delta t) &= \dot{\vec{x}}(t) + \frac{1}{2}\left[\vec{F}(\vec{x}(t)) + \vec{F}(\vec{x}(t + \Delta t))\right]\Delta t \end{aligned}$$

Everything is done in units defined by the parameters K, R and ϵ , so that mass of the particle disappears from the equations.



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