SIMULATION OF PARTICLE DYNAMICS ON THE SURFACE OF A DEFORMABLE SPHERE

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August 20, 2024

Overview

Problem Statement

- Consider n particles scattered on the surface of a deformable sphere.
- The radius $R(t)$ of the sphere is a function of time.
- The particles interact through a general potential $V(r_{ij})$, where r_{ij} is the distance between particles i and j.
- Initially, the particles are placed randomly on the sphere and are at rest.
- Due to the potential, the particles will start to move.
- **Goal:** Determine the positions and velocities of all n particles at any given time, ensuring they remain constrained to the sphere's surface.

Example: n particles on the surface of a sphere interacting via the Lennard-Jones potential.

Total Kinetic Energy Of n Particles

The total kinetic energy T for n particles on the surface of a sphere is given by:

$$T = \sum_{i=1}^{n} \frac{1}{2} m \left(\dot{r}_i^2 + r^2 \dot{\theta}_i^2 + r^2 \sin^2(\theta_i) \dot{\phi}_i^2 \right)$$

where

- m is the mass of every particle,
- r is the radius of the sphere, which is a function of time,
- $\dot{r}_i$: This is the time derivative of the radius r,

TOTAL KINETIC ENERGY OF n PARTICLES

- θ_i : This is the polar angle, measured from the positive z-axis. It ranges from 0 to π (0 to 180 degrees). It describes the angle between the radius vector of the point and the z-axis,
- $\dot{\theta}_i$ This is the time derivative of θ, representing the rate of change of the polar angle with respect to time. It is the polar angular velocity,
- ϕ_i : This is the azimuthal angle, measured in the xy-plane from the positive x-axis. It ranges from 0 to 2π (0 to 360 degrees). It describes the angle between the projection of the radius vector onto the xy-plane and the positive x-axis,
- $\dot{\phi}_i$: This is the time derivative of ϕ, representing the rate of change of the azimuthal angle with respect to time. It is the azimuthal angular velocity.

Total Potential Energy Of n Particles

The potential energy V for n particles on the surface of a sphere is given by:

$$V = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(C_1 P - C_2 Q \right)$$

where

- $P = \frac{1}{r_{ij}^{m_1}}$, where r_{ij} is the distance between particles i and j,
- $Q = \frac{1}{r_{ij}^{m_2}}$, where r_{ij} is the distance between particles i and j,
- C_1 and C_2 are constants.

$$r_{ij} = \sqrt{2r^2 \left(1 - \sin(\theta_i) \sin(\theta_j) \cos(\phi_i - \phi_j) - \cos(\theta_i) \cos(\theta_j) \right)}$$

Total Potential Energy Of n Particles

- r is the radius of the sphere, which is a function of time,
- θ_i : This is the polar angle, measured from the positive z-axis. It ranges from 0 to π (0 to 180 degrees). It describes the angle between the radius vector of the point and the z-axis,
- ϕ_i : This is the azimuthal angle, measured in the xy-plane from the positive x-axis. It ranges from 0 to 2π (0 to 360 degrees). It describes the angle between the projection of the radius vector onto the xy-plane and the positive x-axis,

Governing Equations

The governing equations are given by:

$$\ddot{\theta}_i = \sin(\theta_i) \cdot (\dot{\phi}_i)^2 \cdot \cos(\theta_i) - \frac{2 \cdot \dot{r} \cdot \dot{\theta}_i}{r} + \frac{1}{4mr^2} \sum_{\substack{j=1 \\ j \neq i}}^{n} (C_1 m_1 A - C_2 m_2 B)$$

$$\ddot{\phi}_i = -\frac{2 \cdot \dot{\theta}_i \cdot \dot{\phi}_i}{\tan(\theta_i)} - \frac{2 \cdot \dot{\phi}_i \cdot \dot{r}}{r} + \frac{1}{4m(\sin(\theta_i))^2 r^2} \sum_{\substack{j=1 \\ j \neq i}}^{n} (C_1 m_1 C - C_2 m_2 D)$$

Governing Equations

Where:

$$A = \frac{x}{z^{\left(\frac{m_1}{2}+1\right)}}$$

$$B = \frac{x}{z^{\left(\frac{m_2}{2}+1\right)}}$$

$$C = \frac{y}{z^{\left(\frac{m_1}{2}+1\right)}}$$

$$D = \frac{y}{z^{\left(\frac{m_2}{2}+1\right)}}$$

Governing Equations

$$z = 2r^2 - 2r^2 \sin(\theta_i)\sin(\theta_j)\cos(\phi_i - \phi_j) - 2r^2 \cos(\theta_i)\cos(\theta_j)$$

$$x = -\left(2r^2 \cos(\theta_i)\sin(\theta_j)\cos(\phi_i - \phi_j) + 2r^2 \sin(\theta_i)\cos(\theta_j)\right)$$

$$y = 2r^2 \sin(\theta_i)\sin(\theta_j)\sin(\phi_i - \phi_j)$$

Solving Problem Using Lennard-Jones Potential for Nitrogen Molecule

We consider a system with the following parameters:

$$
\begin{aligned}
\sigma &= 3.798\,\text{Å} \\
\epsilon &= 16.4\,\mathrm{u}\cdot\text{Å}^2\cdot\mathrm{ps}^{-2}\cdot\mathrm{particle}^{-1} \\
m_1 &= 12 \\
m_2 &= 6 \\
C_1 &= 4\epsilon\sigma^{m_1} \\
C_2 &= 4\epsilon\sigma^{m_2} \\
m &= 28.014\,\mathrm{u} \\
n &= 2 \\
\text{timespan} &= [0, 300]\,\mathrm{ps}
\end{aligned}
$$

Solving Problem Using Lennard-Jones Potential For Nitrogen Molecule

The initial conditions for the angles θ and ϕ are given by:

$$\theta_0 = \mathbf{1}_n \cdot \frac{\pi}{6}$$

where $\mathbf{1}_n$ is a column vector of ones with dimension n.

$$\phi_0 = \begin{bmatrix} 1 \\ 2 \\ \vdots \\ n \end{bmatrix} \cdot \frac{2\pi}{n+1}$$

Solving Problem Using Lennard-Jones Potential For Nitrogen Molecule

Consider the following functions where the radius of the Nitrogen molecule (N_2) varies with time:

$$\text{N2\_radius} = 0.54885\,\text{Å}$$

$$r(t) = 5 \times \text{N2\_radius}$$

$$\dot{r}(t) = 0$$

Solving Problem Using Lennard-Jones Potential For Nitrogen Molecule

Click here to watch the video.

Solving Problem Using Lennard-Jones Potential For Xenon

We consider a system with the following parameters:

$$
\begin{aligned}
\sigma &= 4.10\,\text{Å} \\
\epsilon &= 177.503\,\text{u} \cdot \text{Å}^2 \cdot \text{ps}^{-2} \cdot \text{particle}^{-1} \\
m_1 &= 12 \\
m_2 &= 6 \\
C_1 &= 4\epsilon\sigma^{m_1} \\
C_2 &= 4\epsilon\sigma^{m_2} \\
m &= 131.293\,\text{u} \\
n &= 10 \\
\text{timespan} &= [0, 300]\,\text{ps}
\end{aligned}
$$

Solving Problem Using Lennard-Jones Potential For Xenon

The initial conditions for the angles θ and ϕ are given by:

$$\theta_0 = \mathbf{1}_n \cdot \frac{\pi}{6}$$

where $\mathbf{1}_n$ is a column vector of ones with dimension n.

$$\phi_0 = \begin{bmatrix} 1 \\ 2 \\ \vdots \\ n \end{bmatrix} \cdot \frac{2\pi}{n+1}$$

Solving Problem Using Lennard-Jones Potential for Xenon

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Reference

https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Physical_Properties_of_Matter/Atomic_and_Molecular_Properties/Intermolecular_Forces/Specific_Interactions/Lennard-Jones_Potential

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