Temperature Measurements in Optical Tweezer Experiments

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1 Introduction

2 Motivation

3 Simulation

To study the problem on the computer, one needs certain techniques. These techniques and their application will be described in this section.

3.1 Molecular Dynamics

3.2 The Glass Nanoparticle

The glass particle from the experiment will be represented by a system of 864 particles, aligned regularly on a FCC (face centered cubic) lattice. This alignment is achieved by defining a minimum cell, containing points:

$$\begin{aligned} p_1 &= \{0, 0, 0\} \\ p_2 &= \{0.5, 0.5, 0\} \\ p_3 &= \{0.5, 0, 0.5\} \\ p_4 &= \{0, 0.5, 0.5\} \end{aligned}$$

The whole system is then created by copying this unit cell.
The interaction between the atoms is modeled by the Lennard-Jones potential. It has the form

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]. \tag{1}$$

To simplify the equation and computation of the potential and other quantities, like the forces or pressure, it is useful to introduce reduced units. In general, reduced units BLABLABLA THINK OF GOOD TEXT HEREJKA
The basic units in a system with Lennard-Jones interaction are length (σ), energy (ε or ε/k_B) and mass (m). Every quantity can now be written in terms of this units, so they become reduced quantities, denotet by an asterisk. The most important ones are:

$$\begin{aligned} r^* &= r/\sigma \\ T^* &= k_B/\varepsilon\, T \\ U^* &= U/\varepsilon \\ P^* &= P\sigma^3/\varepsilon \end{aligned}$$

With the above introduced reduced units, the Lennard-Jones potential can be written as

$$U(r^*) = 4\left[r^{*-12} - r^{*-6}\right]. \tag{2}$$

Since this is the most practical form, it will be used without the asterisk from here on.

The Lennard-Jones potential is an additive pair-potential, so the total energy of the system can be calculated by summing over all pairs of atoms:

$$U_{\text{tot}} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} 4 \left[{r_{ij}}^{-12} - {r_{ij}}^{-6} \right] \tag{3}$$

where r_{ij} denotes the distance between atom i and j.
The Velocity-Verlet algorithm uses the forces to calculate the positions and velocities for the next timestep, we need to calculate the derivative of the potential energy:

$$\begin{aligned} F_x &= -\frac{\partial}{\partial x} U(r) \\ &= -\frac{\partial}{\partial x} 4 \left[r^{-12} - r^{-6} \right] \\ &= -4 \left[(-12) r^{-13} - (-6) r^{-7} \right] \frac{\partial r}{\partial x} \\ &= 48 \left[r^{-13} - 0.5\ r^{-7} \right] \frac{x}{r} \\ &= 48 \left[r^{-14} - 0.5\ r^{-8} \right] x \end{aligned} \tag{4}$$

This is the component of the force in x-direction – the other components are calculated analogously.

4 Results

5 Conclusion

References