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Brownian dynamics simulations to explore experimental microsphere diffusion with optical tweezers.

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Abstract

We develop two-dimensional Brownian dynamics simulations to examine the motion of disks under thermal fluctuations and Hookean forces. Our simulations are designed to be experimental-like, since the experimental conditions define the available time-scales which characterize the solution of Langevin equations. To define the fluid model and methodology, we explain the basics of the theory of Brownian motion applicable to quasi-twodimensional diffusion of optically-trapped microspheres. Using the data produced by the simulations, we propose an alternative methodology to calculate diffusion coefficients. We obtain that, using typical input parameters in video-microscopy experiments, the averaged values of the diffusion coefficient differ from the theoretical one less than a 1%.

Keywords: Brownian dynamics simulations, colloids, Brownian motion, harmonic potentials, optical tweezers

1 Introduction

Brownian motion, i.e., the random movement of objects immersed in a fluid, was theoretically described by Einstein more than a century ago [32] from a microscopic perspective, demonstrating the molecular structure of the fluid [11]. The Einstein's classical approach neglected hydrodynamics memory and inertia effects, since they appear at very short-time scales, something experimentally available only very recently [24]. This assumption theoretically implies that the particle velocity cannot be defined and the trajectories of Brownian particles are fractal [27]. Therefore, the study of Brownian motion is determined by the available experimental set-up, which defines the detected time-resolution of the stochastic jumps.

The standard experimental methodology to study Brownian motion is to mix a small concentration of micro-nanospheres with a certain fluid. The suspension sample is deposited into a glass cell which is inserted in an optical instrument, such as a video-microscopy or an interferometry set-up, where the trajectories of the beads can be recorded for ulterior analysis. A

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common practice to facilitate the study of particles' motion is using optical tweezers [1]. This technique exerts a restoring force under the object, allowing the experimentalist to move the particle inside the fluid in a quasi-twodimensional plane. Many optical tweezers set-ups allow to trap several objects, but single-particle tracking is usually employed to improve spatial and temporal resolution.

During the last decades, optical traps have permitted to develop a wide variety of experiments in colloidal motion. To cite some examples: about the effects caused by confinement [21], the hydrodynamic interaction between particles [10], discovering resonances from hydrodynamic memory at short-time scales [15], regarding micro-rheology [31], or even to produce Brownian Carnot engines [26], along with many other applications [16].

In spite of the evident benefits of optical tweezers in the research of colloidal physics, this experimental methodology generates an external force under the bead which can modify the dynamics of the particle [25]. This force can be also itself modified by the thermo-physical properties of the surrounding complex fluid [7]. Therefore, a good dynamical characterization of the external harmonic potential detected by stochastic particle motion is needed to correctly measure the values of the diffusion coefficient.

Here, we study by experimental-like computer simulations the diffusion of a single sphere observed in a two-dimensional plane under optical tweezers, *i.e.*, we investigate the Brownian motion of a disk under harmonic potentials. In this work, we show how the solution of the Fokker-Planck equation [29] allows us to propose an iterative approach as an alternative methodology to calculate the diffusion coefficient of the disk. Our objective in this work is to emulate the dynamics of a trapped single-bead in a video-microscopy experiment by means of Brownian dynamics simulations. These simulations are designed to be experimental-like using typical input parameters but without the limitations which appear in an experimental set-up, like image analysis miscalculations or confinement effects in the bead's diffusion.

2 Brownian dynamics simulations

We develop Brownian dynamics simulations, which are a simplification of Stokestian dynamics, but neglecting hydrodynamic interactions (HI) between particles [18]. Our model of colloidal fluid is designed to be compared with video-microscopy (VM) experiments, where we can observe real-time motion of the colloids in two dimensions and where we can storage the particles' position for defined temporal steps, according to the frame-rate of the camera. The software simulates a suspension of micro-spheres in a Newtonian fluid in a 2D or pseudo-2D configuration of sedimented micro-particles [8]. In analogy with a image-based VM lab, we are able to change external parameters, expressed in physical units, such as the concentration of particles in the suspension, the viscosity of the fluid, the focal distance, the size of the spheres or the temperature of the bath.

Our simulation model has been implemented using an open-source Java-based software named "Easy Java/JavaScript Simulations" (EjsS) [13], allowing to create visual simulations of physical systems based on ordinary differential equations. The equations described in this section have been resolved numerically by EjsS using a Euler-Richardson algorithm —alternative algorithms are available but they provided the same results. This simulation methodology has been successfully developed and tested in more complex systems composed of many Brownian particles under different internal and external forces [9, 8].

Theoretically, the movement of particles under thermal fluctuations is studied by means of the Langevin equation [22], which is the Newton's second law equation including a stochastic