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Simulation of Active Brownian Particles in Optical Potentials

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ABSTRACT

Optical forces can affect the motion of a Brownian particle. For example, optical tweezers use optical forces to trap a particle at a desirable position. Unlike passive Brownian particles, active Brownian particles, also known as microswimmers, propel themselves with directed motion and thus drive themselves out of equilibrium. Understanding their motion in a confined potential can provide insight into out-of-equilibrium phenomena associated with biological examples such as bacteria, as well as with artificial microswimmers. We discuss how to mathematically model their motion in an optical potential using a set of stochastic differential equations and how to numerically simulate it using the corresponding set of finite difference equations.

Keywords: optical forces, Brownian motion, stochastic differential equations, numerical simulations, active Brownian particles, microswimmers

1. INTRODUCTION

We present a simple algorithm to simulate an active Brownian particle, also known as microswimmer, in a two-dimensional field of optical forces [1], as discussed in more detail in Ref. [2-3]. We provide an implementation of this algorithm using MatLab®, because this language is widely employed in science and engineering. All algorithms can also be translated straightforwardly in the freeware programming languages SciLab [4] or Octave [5].

In first place, it is useful to simulate the motion of an active Brownian particle in a field of optical forces to gain insight into out of equilibrium physics and the interaction of active particles with physical potentials. Active Brownian motion, in fact, has attracted a lot of interest from the biology and physics communities [6-7]: several types of microscopic biological entities perform active Brownian motion and artificial active particles can be used to localize, pick up, and deliver nanoscopic objects, e.g., in bioremediation, drug delivery, and gene therapy [8-15]. While the motion of passive Brownian particles is driven by equilibrium thermal fluctuations, active Brownian particles are able to propel themselves, exhibiting an interplay between random fluctuations and active swimming that drives them into an out-of-equilibrium status [16-17]. Such artificial active Brownian particles propel themselves by several mechanisms, such as by a periodic deformation of their shape or by phoresis in, e.g., an electric field or a chemotactic or temperature gradient [18-28]. Studying the motion of these active particles in an optical potential can help understand basic principles of their interaction with surface and physical barriers to optimize delivery applications.

2. THEORETICAL MODEL

In a bidimensional homogeneous environment, the motion of an active particle can be modeled as the combined action of three different processes [29-30]: a random diffusion process, an internal self-propelling force and, in the case of chiral active particles, a torque. In particular, the position [x(t), y(t)] of a spherical particle with radius R undergoes Brownian diffusion with translational diffusion coefficient:

$$D_T = \frac{k_B T}{6\pi\eta R}$$

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where k_B is the Boltzmann constant, T the temperature and η the fluid viscosity. The particle self-propulsion results in a directed component of the motion, whose speed v we will assume to be constant and whose direction depends on the particle orientation φ(t), as illustrated in Figure 1(a). Finally, φ(t) undergoes rotational diffusion with rotational diffusion coefficient:

$$D_R = \frac{k_B T}{8\pi\eta R^3}$$

For chiral active particles, φ(t) also rotates with angular velocity Ω as a consequence of the torque acting on the particle [29-30], as shown in Figure 1(b). The sign of Ω determines the chirality of the particles. In the most general case, the motion of an active Brownian particle in a generic force field can be described by the following set of Langevin equations in two dimensions [2-3]:

$$\begin{cases} \dot{\varphi}(t) = \Omega + \sqrt{2D_R}W_\varphi \\ \dot{x}(t) = v\sin(\varphi(t)) + \sqrt{2D_T}W_x + F_x(t) \\ \dot{y}(t) = v\cos(\varphi(t)) + \sqrt{2D_T}W_y + F_y(t) \end{cases} \quad (1)$$

where W_φ, W_x and W_y are independent white noise terms. Inertial effects are neglected because of the low Reynolds number regime [31] and $[F_x(x(t),t), F_y(y(t),t)]$ is an optical force acting on the particle that can vary both in space and time.

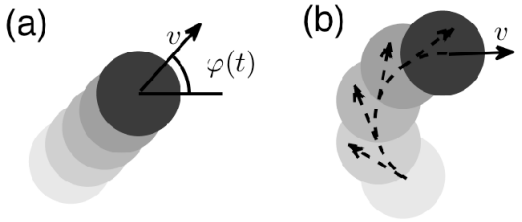

Figure 1. Active Brownian particles in two dimensions. (a) An active Brownian particle placed at [x(t), y(t)] is characterized by an orientation φ(t) along which it propels itself with speed v while it undergoes Brownian motion in both its position and orientation. (b) A chiral active Brownian particle also has a deterministic angular velocity Ω that, if the par- ticle's speed v > 0, translates into a rotation around an effective external axis.

The continuous-time solution [φ(t), x(t), y(t)] to the previous set of equations is approximated by the discrete-time sequence $[\varphi_i, x_i, y_i]$, which is the solution of the corresponding set of finite difference equations evaluated at regular time steps $t_i = i\Delta t$. If Δt is sufficiently small, $[\varphi_i, x_i, y_i] = [\varphi(t_i), x(t_i), y(t_i)]$ following the procedure explained in Ref. [2-3].

3. SIMULATION CODE

In this section we present the MatLab® code that implements Eq. (1) following the codes provided with Ref. [2-3]. This function implements Eq. (1) for the case of a monostable optical trap. Inputs: number of samples `N`, timestep `Dt`, initial position `x1`, particle radius `R`, temperature `T`, fluid viscosity `eta`, particle speed `V`, particle's angular velocity `W` and trap stiffness `k`. Outputs: particle position `x` in meters and time `t` in seconds.

```
function [x,t] = 1dtrapped_monostable(N,Dt,x1,R,T,eta,V,W,k)

% Parameters
```

```
kB = 1.38e-23;      % Boltzmann constant [J/K]
gamma = 6*pi*R*eta; % friction coefficient [Ns/m]
DT = kB*T/gamma;     % translational diffusion coefficient [m^2/s]
DR = 6*DT/(8*R^2); % rotational diffusion coefficient [rad^2/s


% Initialization
x = zeros(N,2);
x(1,:) = x1; % initial conditions (position)
theta = 0; % initial conditions (angle


% Finite Difference Simulation
for i = 1:1:N-1
    % Deterministic step
    x(i+1,:) = x(i,:) - k*Dt/gamma*x(i,:);
    % Translational diffusion step
    x(i+1,:) = x(i+1,:) + sqrt(2*DT*Dt)*randn(1,2);
    % Rotational diffusion step
    theta = theta + sqrt(2*DR*Dt)*randn();
    % Torque step
    theta = theta + Dt*W;
    % Drit step
    x(i+1,:) = x(i+1,:) + Dt*V*[cos(theta) sin(theta)];
end
t = [0:Dt:(N-1)*Dt];
```

4. COMPLEX FORCE FIELDS

The presence of more complex force fields, such as non-conservative force fields [32-38] or random optical potential [39-49], can be taken into account by modeling a generic force in Eq. (1) as explained in Ref. [2].

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