Numerical Simulation of Optically Trapped Particles

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ABSTRACT

Some randomness is present in most phenomena, ranging from biomolecules and nanodevices to financial markets and human organizations. However, it is not easy to gain an intuitive understanding of such stochastic phenomena, because their modeling requires advanced mathematical tools, such as sigma algebras, the Itô formula and martingales. Here, we discuss a simple finite difference algorithm that can be used to gain understanding of such complex physical phenomena. In particular, we simulate the motion of an optically trapped particle that is typically used as a model system in statistical physics and has a wide range of applications in physics and biophysics, for example, to measure nanoscopic forces and torques.

Keywords: optical forces, Brownian motion, stochastic differential equations

1. INTRODUCTION

In this proceeding, we present a simple algorithm to simulate a Brownian particle in an optical trap [1]. We provide an implementation of this algorithm using MatLab[®], because this language is widely employed in the science and engineering. All algorithms can also be translated straightforwardly in the freeware programming language SciLab [2].

The interest of these simulations is dual. On the one hand, it is interesting to simulate an optically trapped particle to gain insight into how an optical trap works; since optical traps have found a widespread set of applications in fields as diverse as, e.g., cooling of single atoms, colloidal physics and biophysics, it can be useful for many students to understand how these optical traps work in simple and inexpensive simulations. On the other hand, an optically trapped particle constitutes a simple example of a stochastic phenomenon whose evolution is determined by both stochastic (the Brownian motion) and deterministic (the optical forces) forcing terms and can, therefore, be used as a model system for more general stochastic phenomena.

2. LANGEVIN EQUATION

An optically trapped particle can be described by the Langevin equation in one dimension [1,3]:

$$m\frac{d^2}{dt^2}x(t) = -\gamma\frac{d}{dt}x(t) - k\frac{d}{dt}x(t) + \sqrt{2k_BT\gamma}W(t) \tag{1}$$

where $x(t)$ is the trajectory of the particle with respect to the trap center, m is the particle mass, γ is the friction exerted by the surrounding medium on the particle, k is the optical trap stiffness, k_BT is the thermal energy unit, k_B is the Boltzmann constant, T is the absolute temperature and $W(t)$ is a Wiener process.

For microscopic particles immersed in a liquid, viscous forces are several orders of magnitude larger than inertial forces, i.e. the particle is in a *low-Reynolds-number regime* [4]. The Reynolds number is the ratio between inertial and viscous forces acting on an object moving in a fluid. If the object has a characteristic dimension L and is moving at velocity v through a fluid with viscosity η and density ρ, its Reynold number is Re = $Lv\rho/\eta$. In the low-Reynold-number regime, i.e for Re < 1, the viscosity dominates over inertia. Considering, for example, an *E. coli* bacterium in swimming in water [5], $L \approx 1\mu m$, $v \approx 30\mu m/s$, $\eta = 0.001$Pas and $\rho = 1000$kg/m3, so that Re = 3e-5 $\ll$ 1. One of the most striking aspect of low Reynolds number phenomena is that the speed of an object is solely determined by the forces acting on it at the

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moment; a good introduction to how is life at low Reynold numbers can be found in Ref. [4]. In general, most optical manipulation experiments take place at low Reynolds numbers, the exceptions being experiments in fluids with very low viscosity such as air [6]. Therefore, in Eq. (1) we can drop the inertial term obtaining:

$$\frac{d}{dt}x(t) = -\frac{k}{\gamma}\frac{d}{dt}x(t) + \sqrt{\frac{2k_B T}{D}}W(t) \tag{2}$$

where D is the Stokes-Einstein diffusion coefficient.

Eq. (2) is one of the simplest examples of a stochastic differential equation [7,8]. In general, stochastic differential equations are obtained from ordinary differential equations adding a noise term, i.e. the Wiener process $W(t)$. $W(t)$ is characterized by the following properties:

1. the mean $\langle W(t)\rangle = 0$ for all t;

2. $\langle W(t)^2\rangle = 1$ for each value t;

3. $W(t_1)$ and $W(t_2)$ are independent of each other for t_1 different from t_2. Because of these properties, a white noise is not a standard function. In particular, $W(t)$ is almost everywhere discontinuous and has infinite variation. In an intuitive picture, it can be seen as the continuous-time equivalent of a discrete sequence of independent random numbers.

3. FINITE-DIFFERENCE SOLUTION

In order to simulate Eq. (2) it is possible to employ a finite difference algorithm, where the continuous-time solution $x(t)$ is approximated by a discrete time sequence x_i evaluated at times $t_i = i\,\Delta t$. This is in practice done by doing the following substitutions in Eq. (2) [1,7]:

1. $x(t)$ $\rightarrow$ x_i

2. $\dfrac{d}{dt}x(t)$ $\rightarrow$ $\dfrac{x_i - x_{i-1}}{\Delta t}$

3. $W(t)$ $\rightarrow$ $\dfrac{w_i}{\sqrt{\Delta t}}$

where w_i is a sequence of Gaussian random numbers with the following properties:

1. the mean $\langle w_i\rangle = 0$;

2. $\langle w_i^2\rangle = 1$;

3. $\langle w_i w_j\rangle = 0$ for i different from j.

Notice how these properties mimic the ones of the Wiener process given above.

By making the aforementioned substitutions in Eq. (2) one obtains the following finite difference equation:

$$x_i = x_{i-1} - \frac{k}{\gamma}x_{i-1}\Delta t + \sqrt{2D\Delta t}\; w_i \tag{3}$$

which can now be solved numerically.

4. SIMULATION CODE

In this section we present the MatLab® code that implements Eq. (3) in one and 3 dimensions following the codes provided with Ref. [1].

4.1 1D Simulation Code

This function implements Eq. (3) in one dimension. Inputs: number of samples `N`, timestep `Dt`, initial position `x1`, particle radius `R`, temperature `T`, fluid viscosity `eta`, and trap stiffness `k`. Outputs: particle position `x` in meters and time `t` in seconds. Figure 1 shows the result of this simulation.

```
function [x,y,z,t] = trapped1d(N,Dt,x1,R,T,eta,k)

% Parameters
kB = 1.38e-23;       % Boltzmann constant [J/K]
gamma = 6*pi*R*eta;  % friction coefficient
D = kB*T/gamma;      % diffusion coefficient

% Initialization
x = zeros(1,N);
x(1)=x1;

% Finite Difference Simulation
for i = 2:1:N
    % Deterministic step
    x(i) = x(i-1) - k*Dt/gamma*x(i-1);
    % Diffusive step
    x(i) = x(i) + sqrt(2*D*Dt)*randn();
end
t = [0:Dt:(N-1)*Dt];

% Plot
figure
plot(t,x)
xlabel('x [m]')
ylabel('t [s]')
```
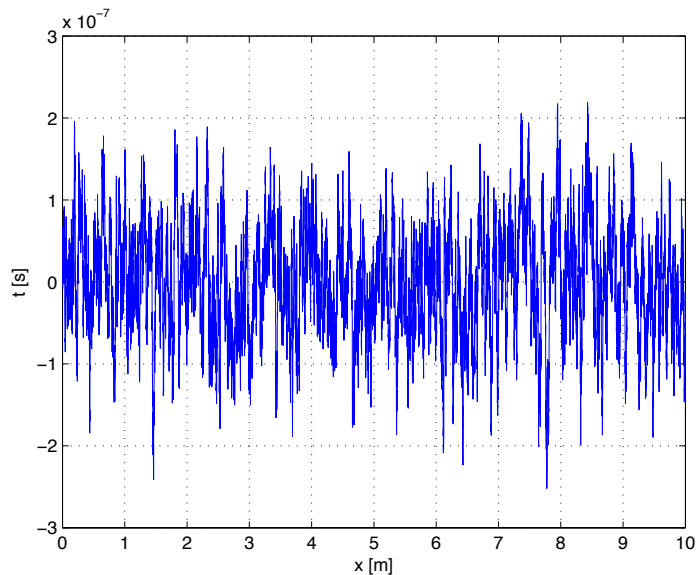

Figure 1. Simulation of an optically trapped particle in three dimensions with the following parameters: `N = 1e+4; Dt = 1e-3 [s]; x1 = 0 [m]; R = 1e-6 [m]; T = 300 [K]; eta = 0.001 [Pa s − water]; kx = 1e-6 [N/m] [N/m]`.

4.2 3D Simulation Code

This function implements Eq. (3) in three dimensions. Inputs: number of samples `N`, timestep `Dt`, initial position `x1 y1 z1`, particle radius `R`, temperature `T`, fluid viscosity `eta`, and trap stiffness `kx ky kz`. Outputs: particle position `x y z` in meters and time `t` in seconds. Figure 2 shows the result of this simulation.

```
function [x,y,z,t] = trapped3d(N,Dt,x1,y1,z1,R,T,eta,kx,ky,kz)

% Parameters
kB = 1.38e-23;     % Boltzmann constant [J/K]
gamma = 6*pi*R*eta; % friction coefficient
D = kB*T/gamma;    % diffusion coefficient

% Initialization
x = zeros(1,N);y = zeros(1,N);z = zeros(1,N);
x(1)=x1;y(1)=y1;z(1)=z1;

% Simulation
for i = 2:1:N
    % Deterministic step
    x(i) = x(i-1) - kx*Dt/gamma*x(i-1);
    y(i) = y(i-1) - ky*Dt/gamma*y(i-1);
    z(i) = z(i-1) - kz*Dt/gamma*z(i-1);
    % Diffusive step
    x(i) = x(i) + sqrt(2*D*Dt)*randn();
    y(i) = y(i) + sqrt(2*D*Dt)*randn();
    z(i) = z(i) + sqrt(2*D*Dt)*randn();
end
t = [0:Dt:(N-1)*Dt];

% Plot
figure
plot3(x,y,z)
xlabel('x [m]')
ylabel('y [m]')
zlabel('z [m]')
axis equal
```
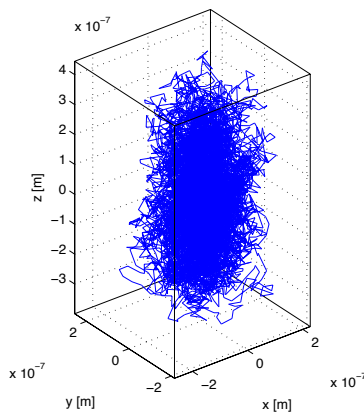

Figure 2. Simulation of an optically trapped particle in three dimensions with the following parameters: `N = 1e+4; Dt = 1e-3 [s]; x1 = 0 [m], y1 = 0 [m], z1 = 0 [m]; R = 1e-6 [m]; T = 300 [K]; eta = 0.001 [Pa s — water]; kx = 1e-6 [N/m], ky = 1e-6 [N/m], kz = 0.2e-6 [N/m]`.

5. DIFFUSION GRADIENTS

In the presence of diffusion gradients, which arise naturally, e.g., when a Brownian particle is trapped near another particle or near a surface, some additional correction are needed in order to account for a spurious drift [9,10,11,12]. This spurious drift results from the fact that the Wiener process is multiplied by a function of the particle position and is needed to correct an indetermination inherently occurring in stochastic differential equations with multiplicative noise. How to deal with these cases is explained in Refs. [13,14]. Similar considerations hold also in the case of diffusion gradients induced by, e.g., chemical gradients or temperature gradients [15,16,17].

6. FURTHER NUMERICAL EXPERIMENTS

Using the code provided in Section 4, it is possible to simulate an optically trapped particle under various conditions and verify, e.g., that the particle variance in the optical trap is inversely proportional to the trap stiffness [18]. Furthermore, it can be interesting to apply these simulation techniques to simulate and study the behavior of a Brownian particle in more complex force fields: for example, a Brownian particle in the presence of external forces or torques [19,20,21,22,23,24,25,26,27,28]. Also time-varying force fields can be considered, which leads to more complex phenomena, such as Kramers transitions [29], stochastic resonant damping [30] and stochastic resonance [31].

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