Brownian dynamics simulation method for the study of anisotropic active Brownian particles

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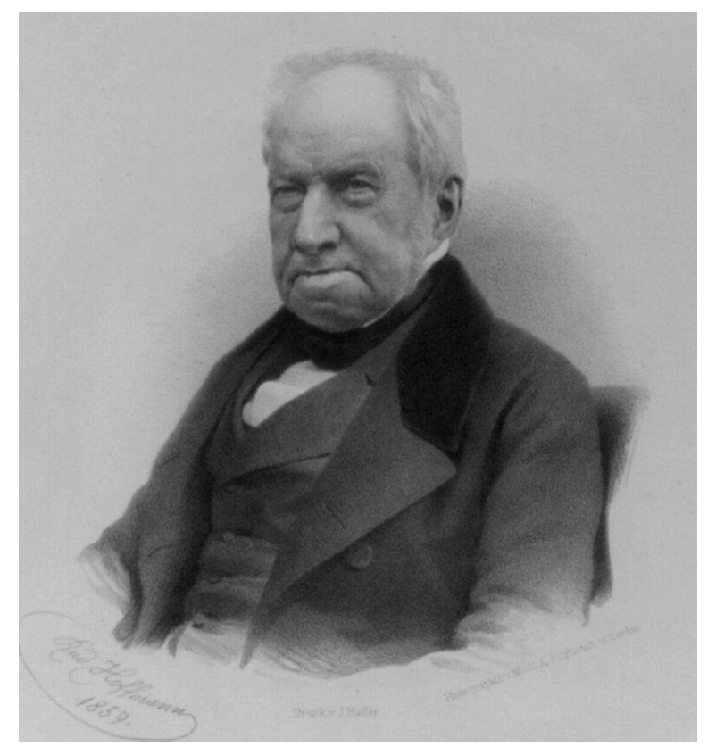
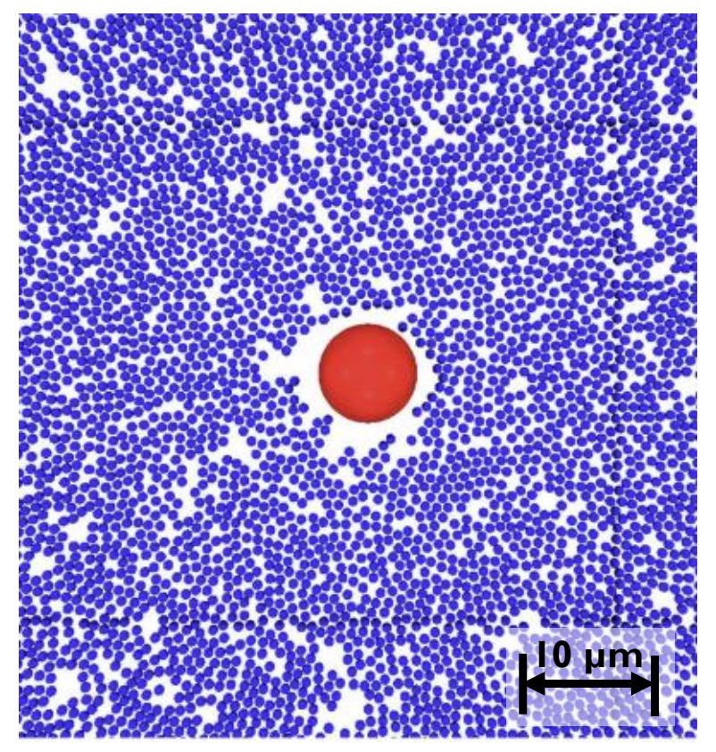
1 Abstract

Colloidal or Brownian particles are tiny particles (1 µm to 10 nm) immersed in a Newtonian viscous fluid and subjected to Brownian motion. This motion is due to thermal fluctuations of the fluid molecules that induce irregular (or stochastic) movement in the particle dynamics. The particles become active Brownian particles (ABPs) if they can move autonomously or self-propel by transforming energy into mechanical motion. This self-propulsion ability of ABPs ("smart ABPs") offers immense potential in applications such as biomedicine (e.g. drug delivery mechanisms) and nanotechnology (e.g. nanorobots). It is therefore crucial to understand the dynamics of these particles under external influence. The present work aims to develop the governing equations that mathematically model the dynamic behavior of isotropic (spherical) and anisotropic (e.g., ellipsoidal) ABPs in a uniform magnetic field. This work also implements the equations using a well-established computational method called Brownian dynamics (BD) simulation. Upon completion of this computational approach, a complete characterization of the interaction between isotropic and anisotropic ABPs can be performed.

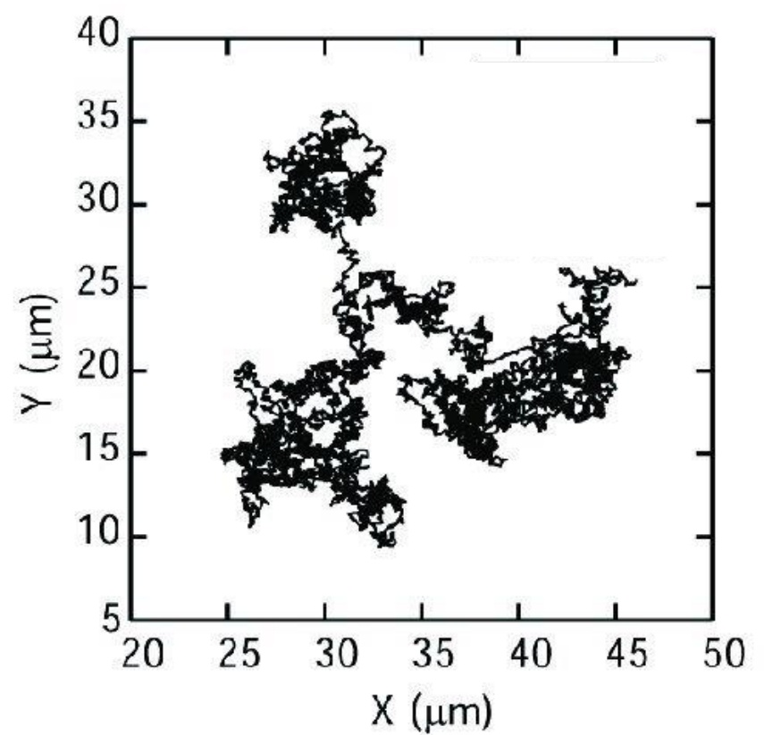
2 Introduction

In 1827, Scottish botanist Robert Brown discovered randomized, incessant, and irregular motion inherent to mesoscopic particles suspended in a fluid. This kind of motion is now named Brownian motion, after its discoverer. This phenomenon is characteristic of all particles in the mesoscopic size range (1 µm to 10 nm) [1]. Thanks to their small size and their ability to move in complex environments, they are desirable for applications in biomedicine (e.g., drug delivery, nanosurgery). However, a limitation of Brownian particles is that their "passive" motion is uncontrolled and randomized. For use in these applications, it is necessary for the particles to be "active" (self-propelled) and controllable.


Robert Brown (1773-1858)

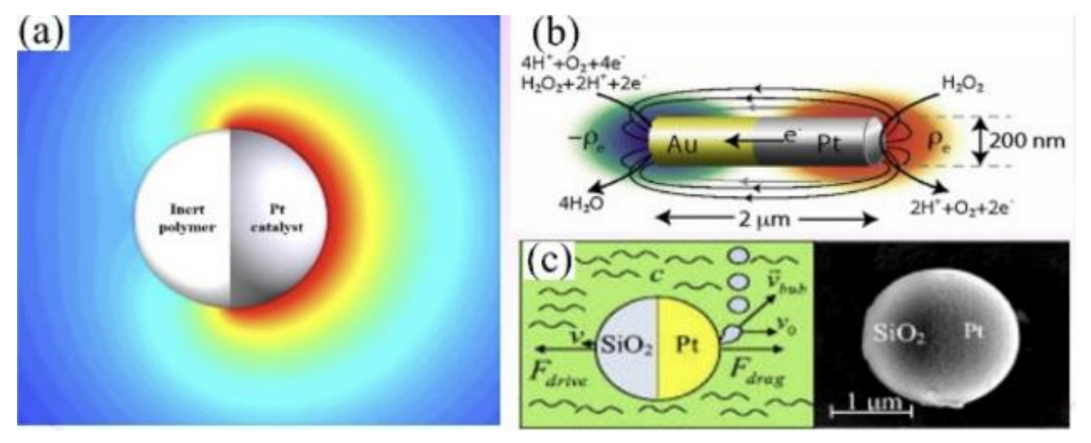


Brownian particle (red) surrounded by fluid molecules (blue) [2]

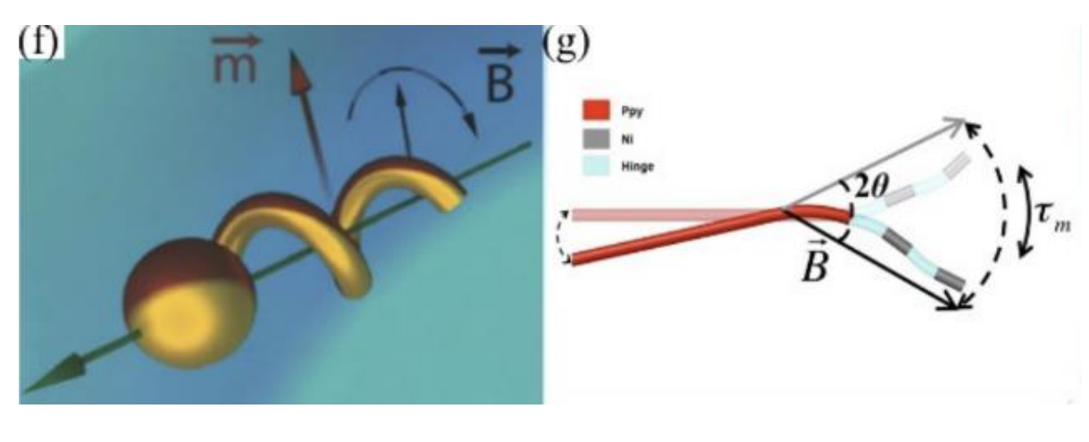


Trajectory of a Brownian Particle [3]

Magnetic active Brownian particles (ABPs) are able to overcome these limitations. They are autonomous and self-propelled by, for example, converting chemical energy into mechanical energy. Furthermore, external magnetic fields can limit their Brownian motion. The magnetic field is also able to guide the direction of motion of the ABP. An example of ABPs is catalytic nano- and micromotors.

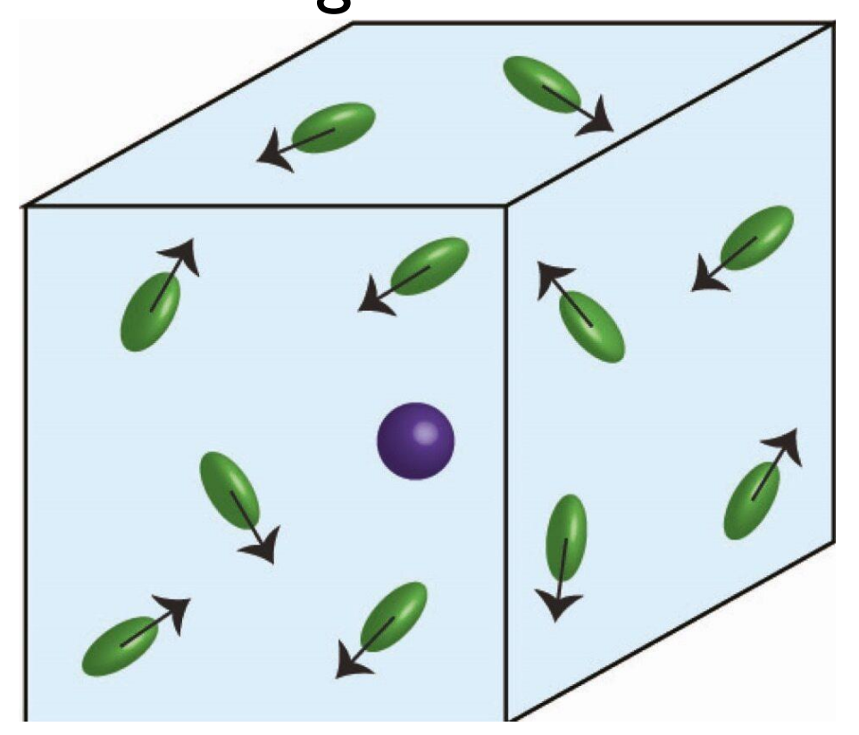


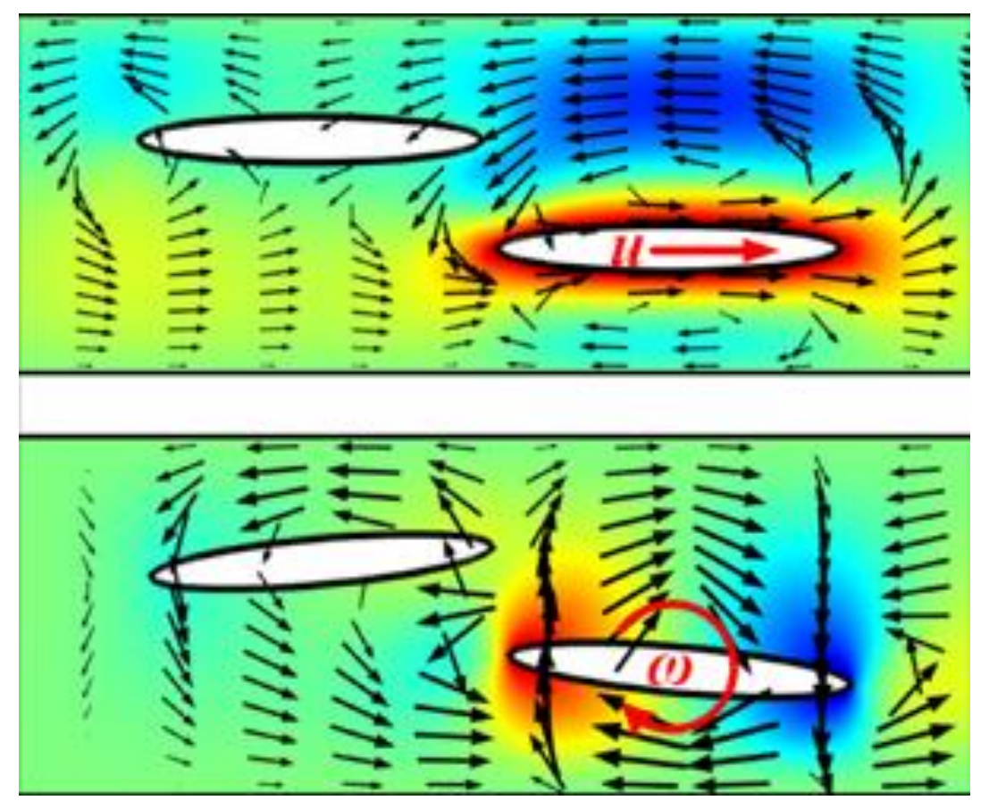
Chemically-powered ABPs [4]



ABPs controlled by magnetic field [4]

Due to their easy treatment, isotropic, spherical, magnetic ABPs have been extensively studied in active soft matter. However, studying anisotropic (e.g., rods, plates, ellipsoids) self-propelled Brownian particles continues to be challenging due to their complexity ranging from experimental fabrication to their theoretical/numerical treatment. An advantage of these particles is that their anisotropic hydrodynamic mobility allows them to reach geometrically-complex environments where spherical particles are not able to go.


Isotropic & anisotropic active particles



Hydrodynamic coupling of anisotropic particles [5]

Characterization of the dynamics of anisotropic, magnetic ABPs is important because understanding how particles at the colloidal size range move in a fluid will help the development of nanotechnology that can be used in medicine, such as nanosurgery robots and targeted medication delivery systems

Additionally, since viruses and bacteria exist at the colloidal size range, understanding their motion will allow disease specialists to better understand mechanisms of infection and eradication of pathogenic diseases.

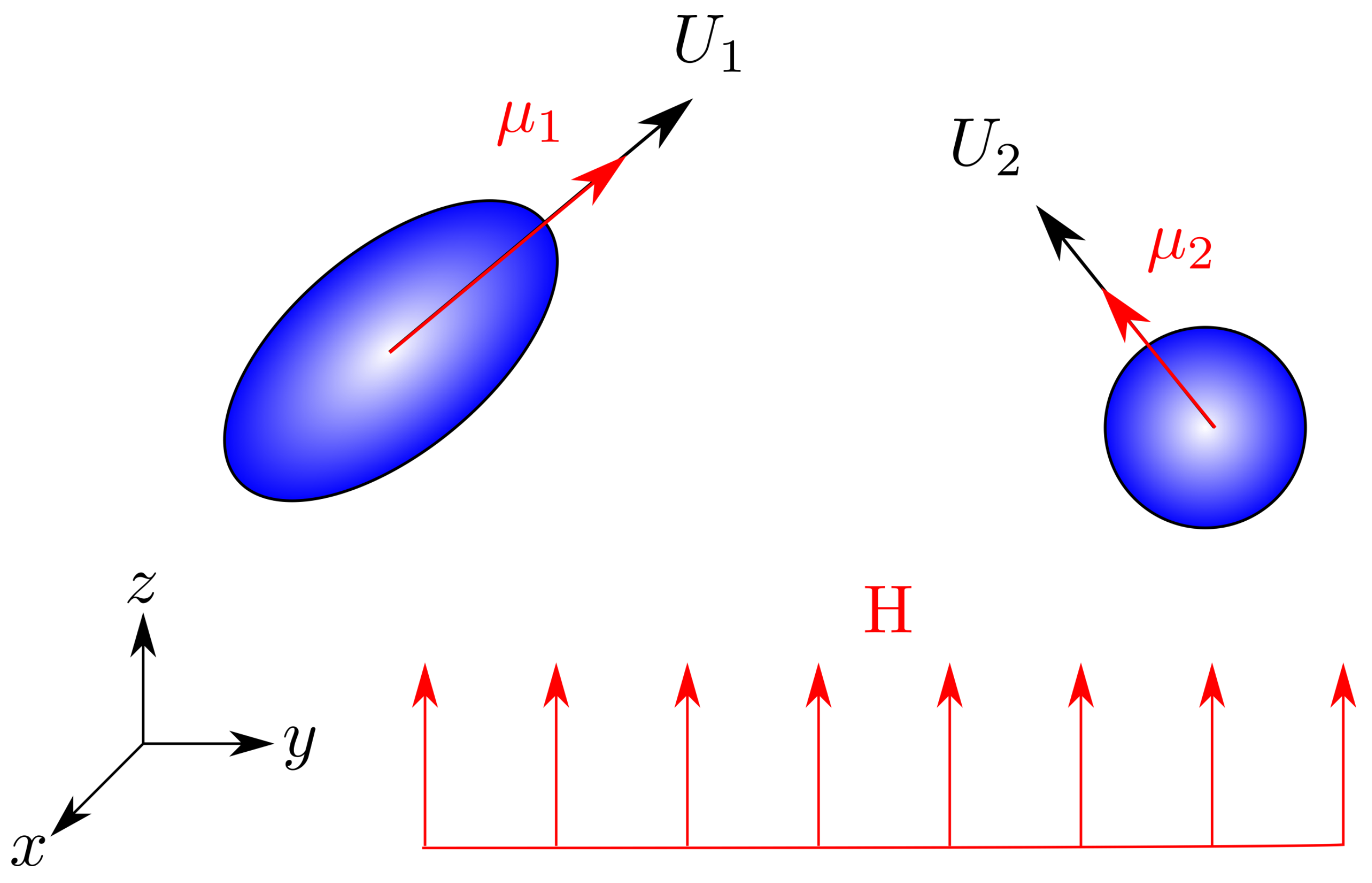
3 Objective

The objective is to collect Brownian dynamics equations from existing literature. These equations mathematically describe the motion of a spherical and ellipsoidal active Brownian particle. The equations will then be synthesized and non-dimensionalized for use with the BD simulation method.

The BD simulation method will be implemented in a Fortran program using a modular approach. The new code will be based on an existing Fortran program that accomplishes a similar simulation but for a single spherical particle [6]. The goal of creating the new program is to optimize and streamline the code, as well as to document it properly for use by future projects, since the previous code has "black box" segments.

4 Model system

Equations will be developed for application in a new model system. The new model system consists of two ABPs suspended in a viscous Newtonian fluid. One is spherical and the other one is ellipsoidal. Both particles are magnetic; therefore, they bear fixed magnetic dipoles μ_1 and μ_2 about their center of gravity. The Brownian motion of these particles is controlled by an external uniform magnetic field H applied along the z-axis of a coordinate system x-y-z. Since the particles are active, they self-propel with constant speeds U_1 and U_2 as illustrated in the figure.



5 Equations for use in BD simulation

Langevin equations for particle displacement:

$$\mathbf{F} = \mathbf{F}_{hyd} + \mathbf{F}_{Brow}$$

$$\mathbf{T} = \mathbf{T}_{hyd} + \mathbf{T}_{Brow}$$

Hydrodynamic force and torque for an isotropic particle:

$$\mathbf{F}_{hyd} = 6\pi \mathbf{U} R$$

$$\mathbf{T}_{hyd} = 8\pi\eta\omega R^3$$

Hydrodynamic force and torque for an anisotropic particle:

$$\mathbf{F}_{hyd} = \eta \hat{\mathbf{K}} \cdot \mathbf{U}$$

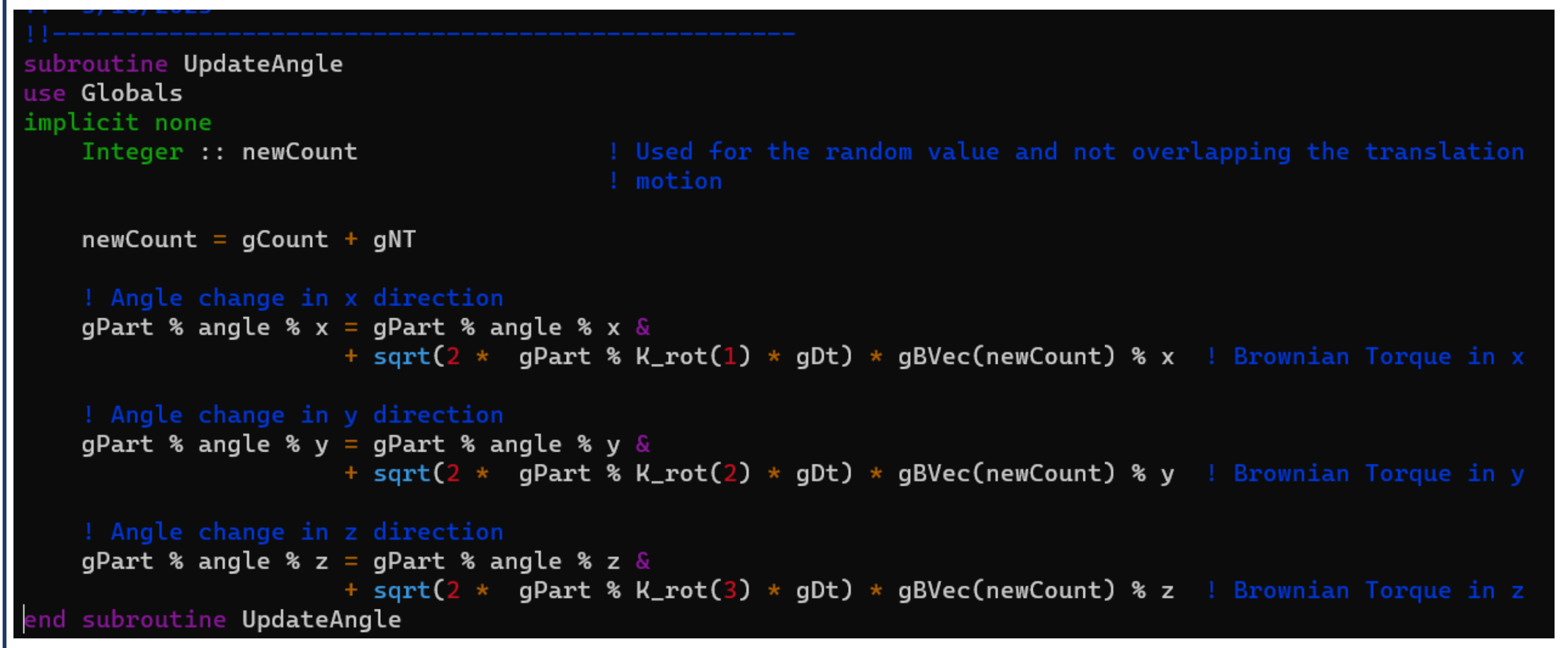
$$\mathbf{T}_{hyd} = \eta \hat{\mathbf{K}}'_r \cdot \omega'(t)$$

Tensors for anisotropic particle equations:

$$\hat{\mathbf{K}} = 16\pi a_1 a_2 a_3 \left(\frac{\mathbf{e}_1\mathbf{e}_1}{\chi_0 + a_1^2\alpha_0} + \frac{\mathbf{e}_2\mathbf{e}_2}{\chi_0 + a_2^2\beta_0} + \frac{\mathbf{e}_3\mathbf{e}_3}{\chi_0 + a_3^2\gamma_0} \right)$$

$$\hat{\mathbf{K}}'_r = \frac{16\pi}{3} \left(\frac{a_2^2 + a_3^2}{a_2^2\varepsilon_2 + a_3^2\varepsilon_3} \mathbf{i}_{x'}\mathbf{i}_{x'} + \frac{a_3^2 + a_1^2}{a_3^2\varepsilon_3 + a_1^2\varepsilon_1} a_2^2\varepsilon_2 + \frac{a_1^2 + a_2^2}{a_1^2\varepsilon_1 + a_2^2\varepsilon_2} \mathbf{i}_{z'}\mathbf{i}_{z'} \right)$$

6 Implementation of BD simulation



```
!!------------------------------------------------------
subroutine UpdateAngle
use Globals
implicit none
    Integer :: newCount                    ! Used for the random value and not overlapping the translation
                                           ! motion

    newCount = gCount + gNT

    ! Angle change in x direction
    gPart % angle % x = gPart % angle % x &
                      + sqrt(2 *  gPart % K_rot(1) * gDt) * gBVec(newCount) % x  ! Brownian Torque in x

    ! Angle change in y direction
    gPart % angle % y = gPart % angle % y &
                      + sqrt(2 *  gPart % K_rot(2) * gDt) * gBVec(newCount) % y  ! Brownian Torque in y

    ! Angle change in z direction
    gPart % angle % z = gPart % angle % z &
                      + sqrt(2 *  gPart % K_rot(3) * gDt) * gBVec(newCount) % z  ! Brownian Torque in z
end subroutine UpdateAngle
```

Sample Fortran code implementing a BDS equation for updating the position of an ellipsoidal Brownian particle

7 Future work

With the implementation of equations completed, the next step is to run tests using the computer simulation program. The tests will yield results of position and velocity, which can be analyzed to characterize the diffusivity of the particles and how they interact. This could later be expanded into work with other shapes than the ones covered in this investigation.

8 References

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