COLLEGE OF ENGINEERING
THE UNIVERSITY OF ALABAMA IN HUNTSVILLE

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Brownian Dynamics of Interacting Anisotropic Magnetic Nanoparticles

Daniel Duke, and Isaac Torres-Díaz, Chemical & Materials Engineering

Motivation

Magnetized nanoparticles with shape anisotropy have potential applications in several fields, including optics (*e.g.*, windows with controlled transparency), biomedicine (*e.g.*, targeted drug delivery), and chemical catalysis (*e.g.*, catalyzing redox reactions)[1]. One particularly exciting area of interest is nanorobotics. Theoretically, two attached magnetized colloidal nanoparticles can swim by deforming and reforming under the influence of a time-varying magnetic field. However, simple nanorobots face an obstacle known as the Scallop Theorem, which states that a swimmer experiencing time-periodic motion in a Newtonian fluid cannot achieve net locomotion. Thus, to controllably maneuver the nanorobot, the return path from deformation must differ from the deformation path, breaking the symmetry of the periodic motion. Using various shapes of ellipsoidal particles offers one method of breaking the symmetry. But before the goal of fabricating nanorobots from anisotropic magnetic nanoparticles can be realized, the dipole-dipole interactions of these particles must be understood. This research aims to model the Brownian motion of two close anisotropic magnetic nanoparticles under the influence of an external magnetic field.

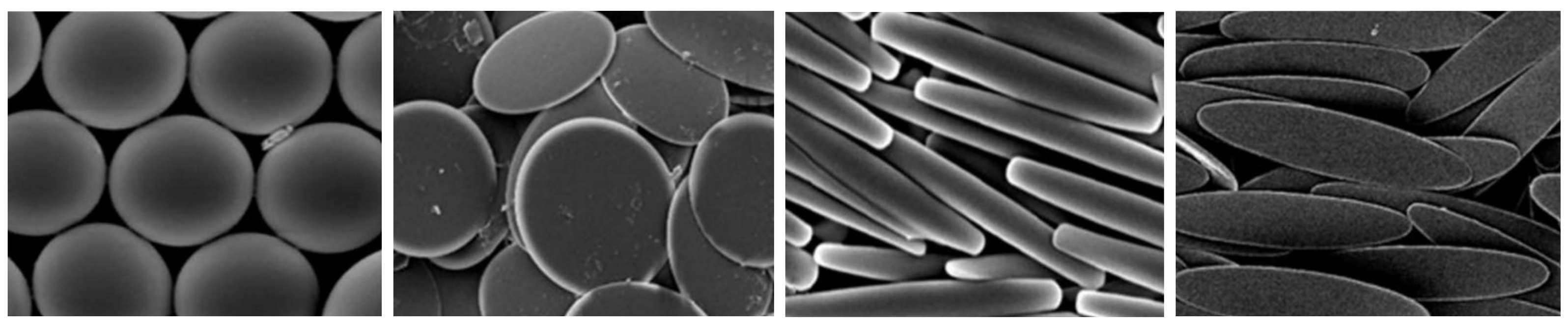

Figure 1. Left to right, ellipsoidal particles as spheres, circular disks, rectangular disks, and elliptical disks[2]

Methodology

Brownian dynamics of a particle *J* is described by

$$\begin{pmatrix}\boldsymbol{u}^J\\ \boldsymbol{\omega}^J\end{pmatrix} = \mathcal{M}^J \begin{pmatrix}\boldsymbol{F}^J_{dd}\\ \boldsymbol{\tau}^J_{dd}\end{pmatrix} + \mathcal{M}^J\begin{pmatrix}0\\ \boldsymbol{\tau}^J_{df}\end{pmatrix} + \mathcal{M}^J \begin{pmatrix}\boldsymbol{F}^J_{B}\\ \boldsymbol{\tau}^J_{B}\end{pmatrix} + \mathcal{M}^J\begin{pmatrix}\boldsymbol{F}^J_{rp}\\ \boldsymbol{\tau}^J_{rp}\end{pmatrix},$$

where the dipolar interaction force results

$$\tilde{\boldsymbol{F}}^J_{dd} = -\delta\tilde{U}_{dd}/\delta\tilde{\boldsymbol{X}}^J, \qquad \tilde{\boldsymbol{F}}^I_{dd} = -\delta\tilde{U}_{dd}/\delta\tilde{\boldsymbol{X}}^I = -\boldsymbol{A}^{IJ}\tilde{\boldsymbol{F}}^J_{dd},$$

and the dipolar interaction torque is

$$\tilde{\boldsymbol{\tau}}^J_{dd} = -\delta\tilde{U}_{dd}/\delta\tilde{\boldsymbol{\Phi}}^J, \qquad \tilde{\boldsymbol{\tau}}^I_{dd} = -\delta\tilde{U}_{dd}/\delta\tilde{\boldsymbol{\Phi}}^I = -\boldsymbol{A}^{IJ}\tilde{\boldsymbol{\tau}}^J_{dd}.$$

The pair dipolar interaction energy equals the sum of the interactions of particles *I* and J:

$$\tilde{U}^{IJ} = -\beta\cdot\tilde{\boldsymbol{M}}^J\cdot\boldsymbol{A}^{JI}\cdot\tilde{\boldsymbol{G}}^I\cdot\tilde{\boldsymbol{M}}^I, \qquad \tilde{U}_{dd} = \tilde{U}^{IJ} + \tilde{U}^{JI}.$$

Dipole-field interaction torque results

$$\tilde{\boldsymbol{\tau}}^J_{df} = -\delta\tilde{U}_{df}/\delta\tilde{\boldsymbol{\Phi}}^J, \qquad \tilde{U}^J_{df} = -\alpha\cdot\tilde{\boldsymbol{M}}^J\cdot\boldsymbol{A}^J\cdot\tilde{\boldsymbol{H}}_{ext}.$$

A repulsive potential is considered to avoid particle overlapping:

$$\tilde{U}_{rp} = Ze^{-\kappa D}, \qquad \tilde{\boldsymbol{F}}^J_{rp} = -\delta\tilde{U}_{rp}/\delta\tilde{\boldsymbol{X}}^J, \qquad \tilde{\boldsymbol{\tau}}^J_{rp} = \tilde{\boldsymbol{r}}^J\times\tilde{\boldsymbol{F}}^J_{rp}.$$

Brownian force and torque is generated using a Box-Muller transform with a Normal distribution of vectors:

$$\boldsymbol{r} = \sqrt{s^2}\cdot\sqrt{-2\ln(\boldsymbol{a})}\cdot\cos(2\pi\boldsymbol{c}).$$

Quaternion parameters are used to track particle orientation, and the transformation matrix **A** relates the fields in laboratory and particle coordinate systems:

$$\boldsymbol{A} = \begin{bmatrix}\chi^2+\eta^2-\xi^2-\zeta^2 & 2(\eta\xi-\chi\zeta) & 2(\eta\zeta+\chi\xi)\\ 2(\xi\eta+\chi\zeta) & \chi^2-\eta^2+\xi^2-\zeta^2 & 2(\xi\zeta-\chi\eta)\\ 2(\zeta\eta-\chi\xi) & 2(\zeta\xi+\chi\eta) & \chi^2-\eta^2-\xi^2+\zeta^2\end{bmatrix}.$$

References

1. D. Lisjak et al. Prog. Mater. Sci. 95, 286(2018)
2. J. Champion et al. PNAS 104(29), 11901(2007)

Results

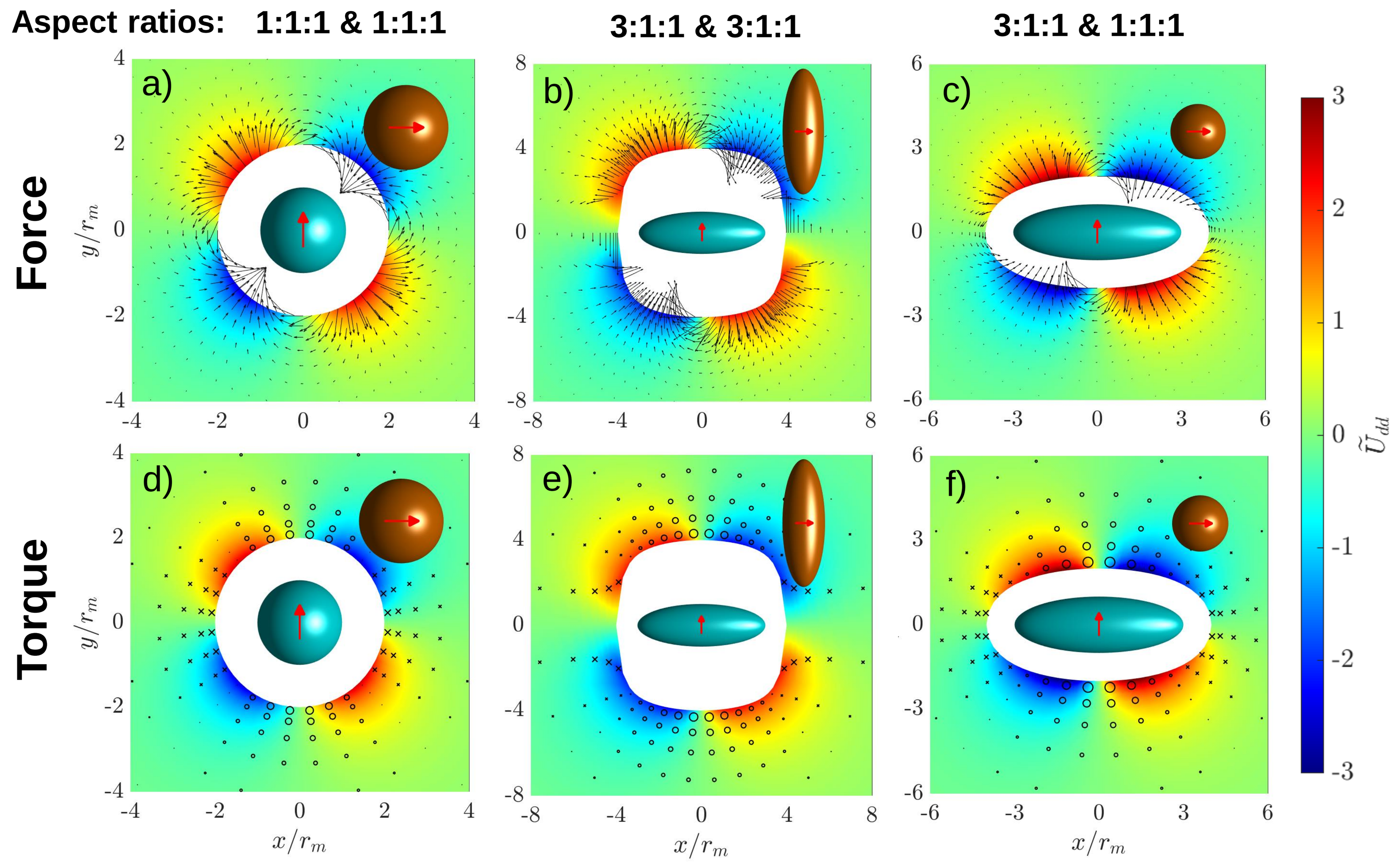

Figure 2. Dipole-dipole dynamics with $\beta_S = 10$. The force (top) and torque (bottom) fields are represented over the dipolar interaction energy.

Brownian dynamics of anisotropic particles

By integrating the linear and angular velocity of the particles over many infinitesimal time steps, the motion of the two particles was simulated in various scenarios and for various particle shapes. β_S characterizes the strength of dipole-dipole interactions, and α_S describes the strength of dipole-field interactions, both relative to Brownian energy.

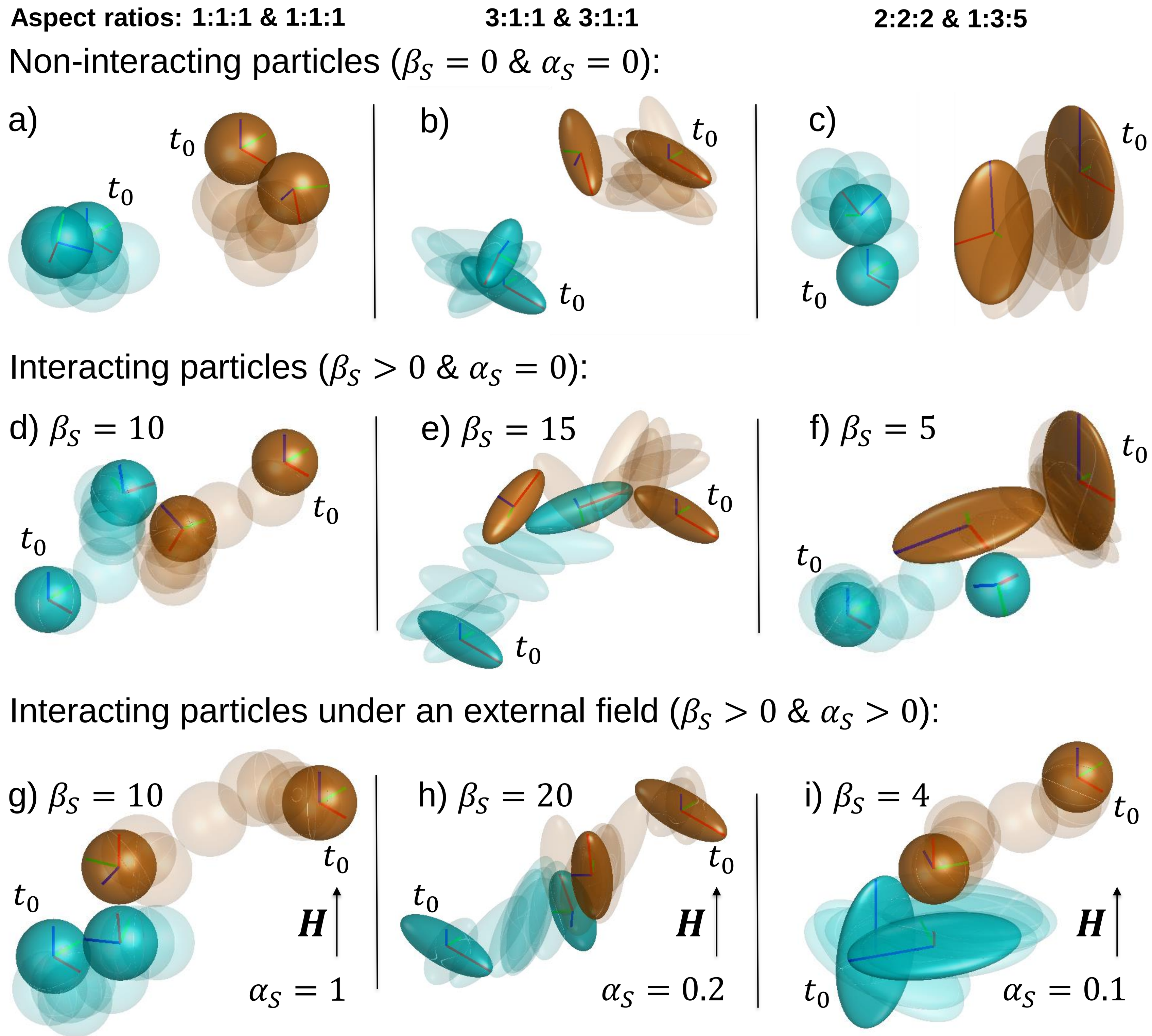

Figure 3. Simulation snapshots with various particle shapes and in various conditions. All using 2000 time steps and $dt = 0.12$. The magnetic moment of each particle points in the positive x-direction (red axis). t_0 represents the initial configuration.

Conclusions and Future Work

We developed a reliable model to quantify the dynamics of the dipolar interaction between multi-shaped ellipsoids. In the future, the dynamics of longer and larger system will be considered. We aim to use the dipole interaction model to simulate the motions of nano-robots.

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