Simulating Magnetic Nanoparticles At UPRM... Plot Twist: They Have Shifted Dipoles [1]

Submitted by Angel Christian González Martell [2] on 31 July 2015 - 5:32pm

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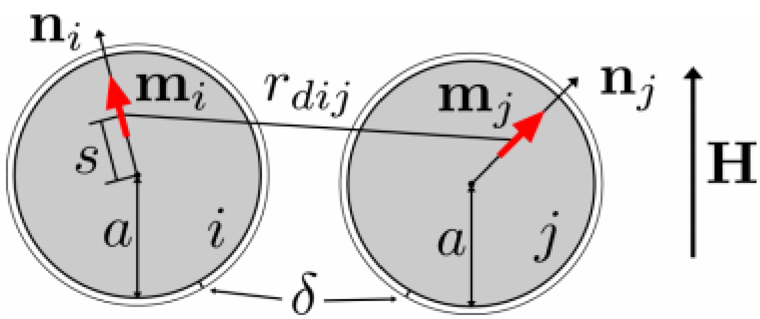
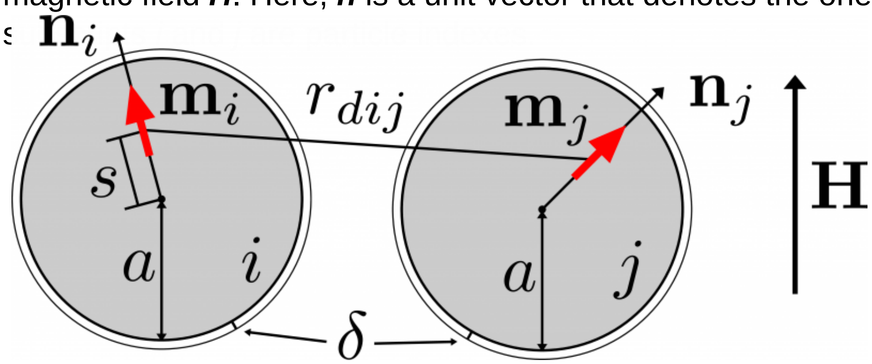


During this summer I had the opportunity to participate in a life-changing program at my own Campus, UPRM. The RMSM REU program provided me with the tools to conduct meaningful research and gave me the chance to meet a small group of people that I will call forever my friends. And as I wrote this, I just remembered something that a friend told me some time ago: "less is better". And it is that, even though this program didn't hosted a lot of students like others universities may do, being a small group of 11 strangers from different cultures, 10 weeks gave us enough time to make bonds that will most likely endure a lifetime. Moreover, during the program I came to the conclusion that I was looking for when I got enrolled on it... Go, or not to go to grad school? And, I'm glad to say today that, even though I don't picture myself as a grad student researcher in the near future, I will be continue working with my advisor, Dr. Ubaldo Córdova, during this upcoming semester and focus my future goals to the realization of a personal project in which I would love to establish my own company here in Puerto Rico. Said this, I will give you now an overview of the project that I have worked on for this summer and will continue developing.

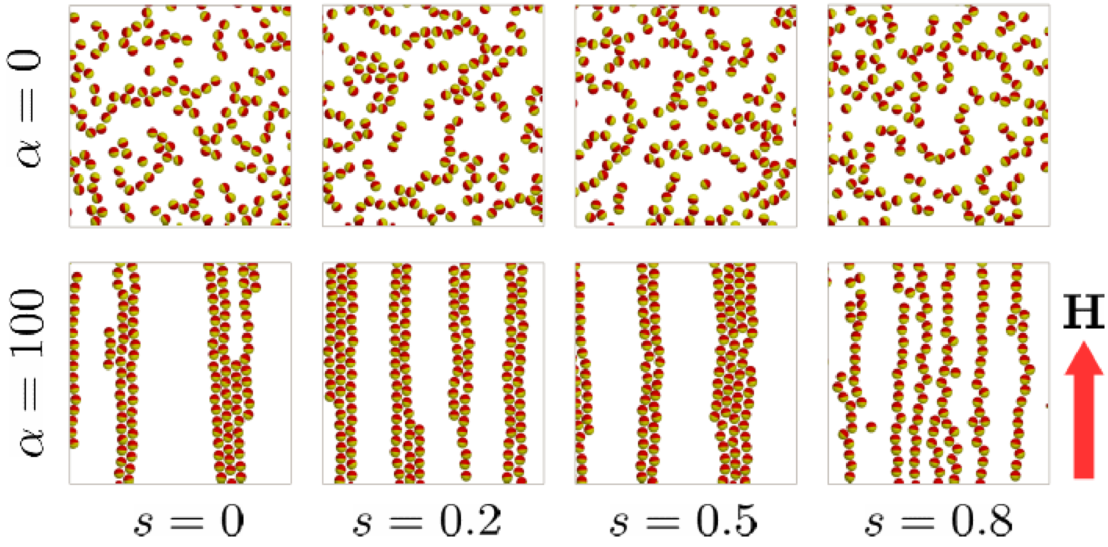
Magnetic nanoparticles with a centred-dipole have been well studied and, as I mentioned in my last post, their behavior in a colloidal scale has been already described in a numerical and experimental way. In summary, at this scale, these particles are suspended due to the governing Brownian motion on them. This motion is completely random and apply forces on the particles that prevents them from precipitating. To these forces is added a drag force opposed to the particle movement that depends on the viscosity of the suspension fluid. Then, as the particles that we consider are ferromagnetic, another interaction force works on the system, specifically from dipole to dipole. These particles have shown chain-like aggregation structures in presence of uniform external magnetic fields, and fractal-like aggregation in absence of one.

Variations of these particles have been recently studied having dipoles displaced from the center in two different ways: (1) collinear with the axis that crosses the center of mass of the particle and shifted toward the surface, and (2) parallel to the axis that goes through the particles center of mass. The first case have shown chain-like aggregation when they are exposed to an external magnetic field up to certain ratios in previous works, and the other one, have shown staggered chains (zigzags chains) aggregation. However, this field is yet to be studied and works regarding the dynamics of these systems are required to have further understanding of them.

In our study, we implemented the first case mentioned of shifted-dipole particles into quasi-two-dimensional Brownian dynamics simulations to measure their aggregation dynamics in time as can be seen in Figure 1. The particles were modeled as spheres of radius *a* and a steric layer *?* with a magnetic dipole moment ***m***, shifted at a radius ratio ***s***, and exposed to an external magnetic field ***H***. Here, ***n*** is a unit vector that denotes the orientation of the particle, while the s



Our work during the summer was mainly focused on the implementation of the actual physics of the system into the simulations, but in the last weeks we managed to get some preliminary results to see if the implementation had been well worked out. For this, we ran simulations at different shift ratios *s*, dipole-dipole strengths *?,* and external magnetic field strengths *?*. Snapshots of the simulations are shown ahead.



In these snapshots it can be seen how the particles aggregation is enhanced by the application of an external magnetic field and how the shift ratios affect this process as it increases. This happens because the particles have now (at high shift ratios) more unstable bonds with each other and the proximity of other particles to an already formed chain will just increment the energy of the bond and therefore, be repelled as it doesn't lead to a lower and stable energy state.

Future work on this matter will consider three-dimensional simulations and particles with shifted dipole moments parallel to the axis that goes through the particles center of mass.

Tags:

- UPR-Mayagüez REU RMSM Blog [3]

Links
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