Magnetic nanoparticles as biosensors

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There are an increasing number of studies that aim to use nanoparticles to improve the current healthcare standards. In our work we are focused in using magnetic nanoparticles to detect the presence of a biomarker in a solution via their modification of the alternating current (AC) magnetization cycles. In particular, changes in the AC magnetization can be observed when the MNP are functionalized with a ligand that specifically interacts with the biomarker, affecting the magnetic and hydrodynamic response: either via surface modification (detection based on single MNPs) or via the formation of MNPs aggregates.

Most of the applications based on magnetic nanoparticle (MNP) involve liquid suspensions where the Brownian displacements of MNPs are coupled by long-ranged magnetic and hydrodynamic couplings, however at present there is no efficient computational implementation of nanoscale magneto- hydrodynamics (NMH). To carry out our study we have developed a very efficient GPU computational algorithm that integrates the magnetization dynamics of the MNP taking into account both, the Brownian Relaxation (change of the magnetization due to the rotation of the particles) and the Nel relaxation (change of the magnetization because of the internal rotation/fluctuation of the magnetic moment). Our integrator of the magnetization has been written as a module of UAMMD [1], so it trivial to include hydrodynamic interactions in our simulations.

The Brownian relaxation of the particles is solved using Brownian Dynamics to integrate the rotation and the translation of the particles taking into account the torque exerted by the magnetic field on the particles,

$$\vec{\tau} = \vec{m} \times \vec{B} \tag{1}$$

The Neel relaxation is integrated using the Landau-Lifshitz-Gilbert (LLG) equation,

$$\frac{d\vec{m}}{dt} = \frac{-\gamma_0}{1+\alpha^2}\left(\vec{m} \times \vec{B}_{eff} + \alpha \cdot \vec{m} \times \vec{m} \times \vec{B}\right) \tag{2}$$

The detection of biomarkers using the surface modification is based on the change of the hydrodynamic size of the particles when a biomarker interacts with the ligands of the particle. The change in the hydrodynamic size increase the phase-lag between the magnetic field and the magnetization changing the shape of the magnetization cycles of the particles.

Using our algorithm we can reproduce the magnetization cycles of non-interacting magnetic nanoparticles under multiple conditions of field intensity and frequency. In addition from the changes in the shape of the magnetization cycles we can detect the presence of dextran molecules on the surface of the particles and measure the new hydrodynamic size of the particles when the dextran is attached to the surface of the MNP.

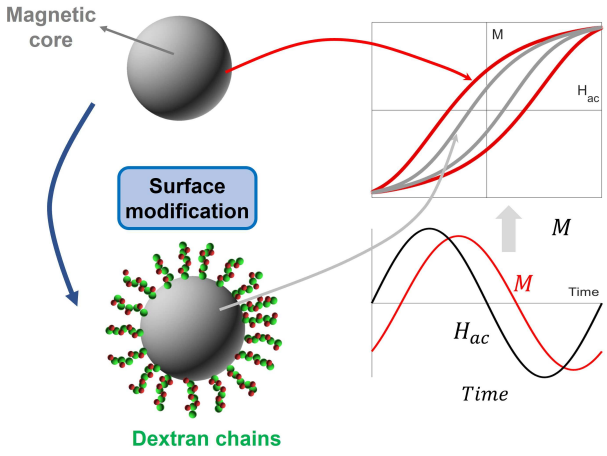

Fig. 1. The modification of the surface change the shape of the magnetization cycles.

On the other hand we have developed an algorithm to simulate the formation of MNP cross-linking structures when the biomarker can be linked to two different ligands, and we have studied multiple properties of the aggregates, in order to later simulate the response of the aggregates to an alternating current magnetic field.

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[1] https://github.com/RaulPPelaez/UAMMD/