Magnetic nanoparticles for medical applications – Theory and simulations

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The fast and reliable control of the magnetization dynamics in magnetic materials has been a topical area of research for the last two decades. A promising medical application concerns the use of magnetic nanoparticles as diagnostic and/or therapeutic use, for instance in cancer treatment (hyperthermia). Cancer cells are very sensitive to alterations of their near environment such as the presence of radiation or heat. Hyperthermia tries to exploit this sensitivity by subjecting cancerous cells to a strong localized heat source.

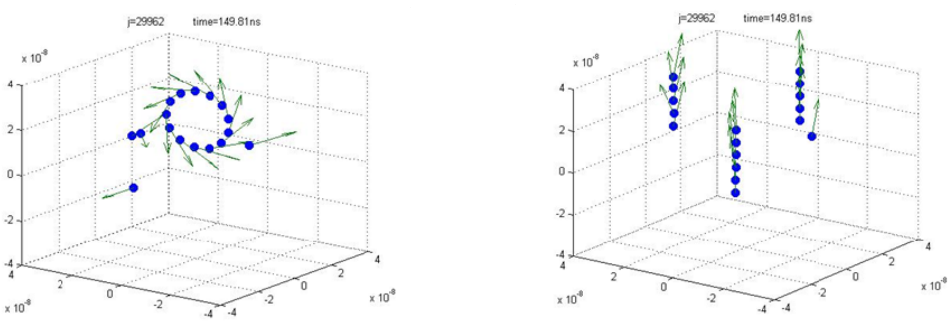
A possible way to achieve this goal is to use magnetic nanoparticles (NPs), particularly single-domain superparamagnetic NPs, which carry a magnetic moment (macrospin) resulting from the internal interactions that align all its atomic spins along the same direction. The basic idea is to excite such NPs with oscillating magnetic fields. The NPs can be very effective in absorbing the electromagnetic energy, and subsequently release it to their environment as heat, leading to a temperature increase.

Many factors can influence the heating efficiency of an ensemble of magnetic NPs, such as the structural and magnetic properties of the NPs and the magnitude and frequency of the magnetic field. A crucial factor for magnetic hyperthermia is the effect of the magnetic dipolar interaction between individual NPs, whose role has not yet been completely elucidated.

The goal of this project is to develop – through theoretical and computational modeling – a better understanding of these phenomena and thus, in the long run, to improve the efficiency of magnetic hyperthermia for cancer treatment. The main objective will be to find the most effective configuration that maximizes the energy exchanges between the NPs and their environment, for given (and possibly low) amplitude and frequency of the magnetic field.

The simulations will be based on a molecular-dynamics approach, generalized to include the macrospin evolution and the magnetic dipolar interactions. The interaction of the particles with their environment will also be simulated in order to describe the thermal exchanges between the NPs and the fluid substrate. Preliminary results show the formation of straight chains or circular structures, depending on the number of NPs (see figure).

The challenge will be to fully understand how these structures react under magnetic excitation, how they absorb energy and finally release it to their environment as heat. It will also be possible to investigate the formation and evolution of temperature gradients in the fluid substrate, induced by the magnetic heating of the NPs.



Self-consistent assembly of magnetic NPs under the action of viscosity and dipolar interactions, without (left frame) and with (right frame) an external magnetic field