



Numerical simulation and characterization of systems for Magneto-thermal and Magneto-mechanical interaction with the living matter

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The aim of the present thesis is to investigate and understand the physical phenomena and parameters associated with magnetic particle hyperthermia and the magnetomechanical effect.

The main research question to be answered is whether the theoretical models of the interaction of magnetic field and magnetic nanoparticles with the living matter are reliable. Validation of the theoretical models was achieved by comparison with literature and experimental measurements and data. This main research question contains individual questions that were answered during the conduction of the present thesis. More specifically:

1. At which length scale does the optimum effect of magnetic particle hyperthermia take place? The three cases examined computationally are: (i) at nano-scale where we studied the heating distribution and temperature increase at the magnetic nanoparticles level, with their number less than 100, (ii) at micro-scale where we studied the heating distribution and temperature increase at the intracellular level ($\leq 100 \mu\text{m}$) and (iii) at macro-scale where we studied the heating distribution and temperature increase at the tissue level.
2. How much does anisotropy of magnetic nanoparticles affect their thermal and mechanical performance?
3. What role do the physical properties (thermal, electrical, mechanical) of biological materials play in their interaction with magnetic nanoparticles and the various externally applied magnetic fields (static, alternating, pulsatile)?

This thesis examines the numerical simulation and characterization of the interactions between magnetic fields and magnetic nanoparticles when they are both applied to living matter, focusing on the physics of magnetic particle hyperthermia and the Magneto-mechanical effects of magnetic nanoparticles. In this context, magnetic energy is converted to mechanical stress by forces (magneto-mechanical effect) in the frequency range below 100 Hz and to heat by magnetic particle hyperthermia at frequencies of 100-1000 kHz. In the first case, the effect of the field gradient on the movement of the nanoparticles and how it affects, through the generated mechanical forces, the activation of cellular mechanisms (in vitro) was investigated. In magnetic particle hyperthermia, the thermal performance of magnetic nanoparticles was evaluated (i) in a non-living environment, i.e. in materials that simulate the properties of living biological tissue (ex vivo), (ii) in a liquid solution (ferrofluid, in-vitro) and (iii) in a living biological tissue (in-vivo). In each case, both the magnetic response of the nanoparticles and the energy transfer (mechanical or thermal) to the biological material were simulated, and the factors that influence the whole process such as the characteristic properties of the nanoparticles (size, shape, magnetic anisotropy), the magnetic field (frequency, amplitude, gradient), the protocol (dosage, duration of application, magnetic nanoparticles concentration, type of magnetic field) were investigated for all three cases.