## Numerical simulations of interactions between magnetic nanoparticles and living matter through magnetothermal and magnetomechanical experimental setups

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In this work we quantify numerically the interactions between magnetic nanoparticles (MNPs) and the living matter which take place under varying external magnetic fields and frequencies through two different procedures: The MNPs magnetic energy density transformation (i) into mechanical forces and (ii) into heat. For the first case magnetic field gradients are induced by permanent magnets which are placed on a 3D polymer disk and in close proximity to seeded cells (above the magnets in Fig1a). With COMSOL 3.5a Multiphysics we estimate the mechanical forces exerted on different lines of cancer cells by cell-internalized MNPs. Those forces are generated by high-gradient magnetic fields (Fig.1d) and dictate MNPs movements within the cellular environment. Mechanical stress mediated by localized nanoparticles in HT.29 (human colorectal adenocarcinoma) and CT 26 cells leads to a significant decrease of cells viability. On the other hand in magnetic hyperthermia (Figs 1b, 1c) the combination of alternating magnetic fields and magnetic nanoparticles allows one to cause apoptosis via heat induction. We simulate the heating process of a single MNP inserted in a biological tissue under an external applied magnetic field. The thermal response of MNPs with different morphological features is analysed. The results demonstrate the impact of nanoparticle shape and surface coating in temperature dissipation in and around the nanoparticle. Finally we model the experimental setup of magnetic hyperthermia for in - vitro experiments. The simulations are repeated for both experimental setups of the laboratory, one consisting of two circular coils and one of eight squared coils surrounding the solution (Figs 1e, 1f). COMSOL can easily extend convectional models for one type of physics into multiphysics models that solve coupled physics phenomena simultaneously and so the electrical and the thermal problem were solved, calculating the magnetic field and the temperature of the coil and the solution respectively.



**Figure 1:** From theory to experiment and vice versa: Magnetic flux density mapping of a permanent NdFeB magnet placed in the centre of the 3D polymer magnetomechanical disk (1a,1d), Magnetic field distribution generated by two circular coils (1b,1e) and temperature distribution in the eight squared coils (1c,1f).