Simulation of Water Nuclear Magnetic Relaxation Induced by Superparamagnetic Nanoparticles Trapped in a Biological Tissue
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The high-field $T_1$ relaxation of water molecules trapped in a biological tissue loaded with superparamagnetic iron oxide nanoparticles (SPIONs) is simulated using a Monte Carlo algorithm. The tissue is modeled as a periodic arrangement of semi-permeable membranes, and the influence of the membrane permeability on the relaxation is studied.

I. Context

- Various models describe the $T_1$ relaxation induced by SPIONs in an homogeneous medium.
- The diffusion of water molecules in the magnetic field inhomogeneities caused by the magnetic particles induces the relaxation [1].
- In vivo diffusion is constrained by cell membranes, which drastically alters the water diffusion coefficient $D$ [2].
- This effect is too complex to be described analytically, but can be studied through Monte Carlo simulations.

II. Methodology: the algorithm

1. Generation of the simulation space, with its cubic cells and fixed nanoparticles.
2. Proton diffusion to a distance $\sqrt{6D\tau}$ where $\tau$ is the simulation time step. Upon meeting a membrane, the probability to cross it depends on the membrane permeability.
3. Dephasing of the proton magnetic moment depending on the magnetic field at its position.
4. Computation of the total magnetization at each time, and extraction of the system $T_1$ from an exponential fit.

III. Results, discussion and future prospects

![Graph showing the effect of the membrane permeability on the relaxation rate in different settings.](image)

Clearly, the impact of the permeability is not negligible and should be further studied. The model could be improved:
- by modelling the cells more realistically (in size and shape);
- by studying the effect of the aggregation of the nanoparticles in the cells which is experimentally observed [3];
- by adding the extracellular medium;
- ...