# NMR transverse relaxation induced by cubic nanoparticles: a Monte Carlo simulation study

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## 1. Introduction

- Iron oxide superparamagnetic nanoparticles (IONP) are used as contrast agents in MRI and mainly shorten proton transverse relaxation time $T_2$ [1].
- In the theoretical relaxation models describing the $T_2$ relaxation induced by IONP, the nanoparticles are always supposed to be spherical.
- Several experimental studies show that the nanoparticle shape seems to have a crucial influence on the relaxation times (see figure 1 and reference [2]).
- **Aim of this study : theoretically predicting $T_2$ for the case of cubic nanoparticles using simulations**

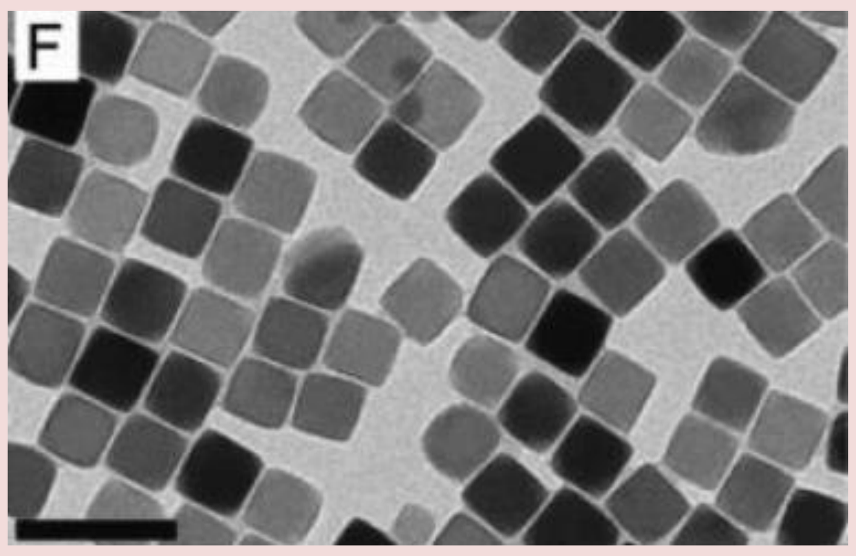


Figure 1: TEM samples of iron oxide nanocubes from reference [3]

## 2. Methods

To simulate the relaxation, three main steps are achieved [4]:

(1) Computation of the exact magnetic field produced by the cubic or spherical IONP using a finite element solver software (COMSOL).

(2) Simulation of the diffusion of the protons around the nanoparticles (random walk) and computation of their spin interaction with the IONP magnetic field. Nanoparticles are considered as impenetrable.

(3) Computation of the average spin evolution and fitting the resulted curve to extract the relaxation time value.

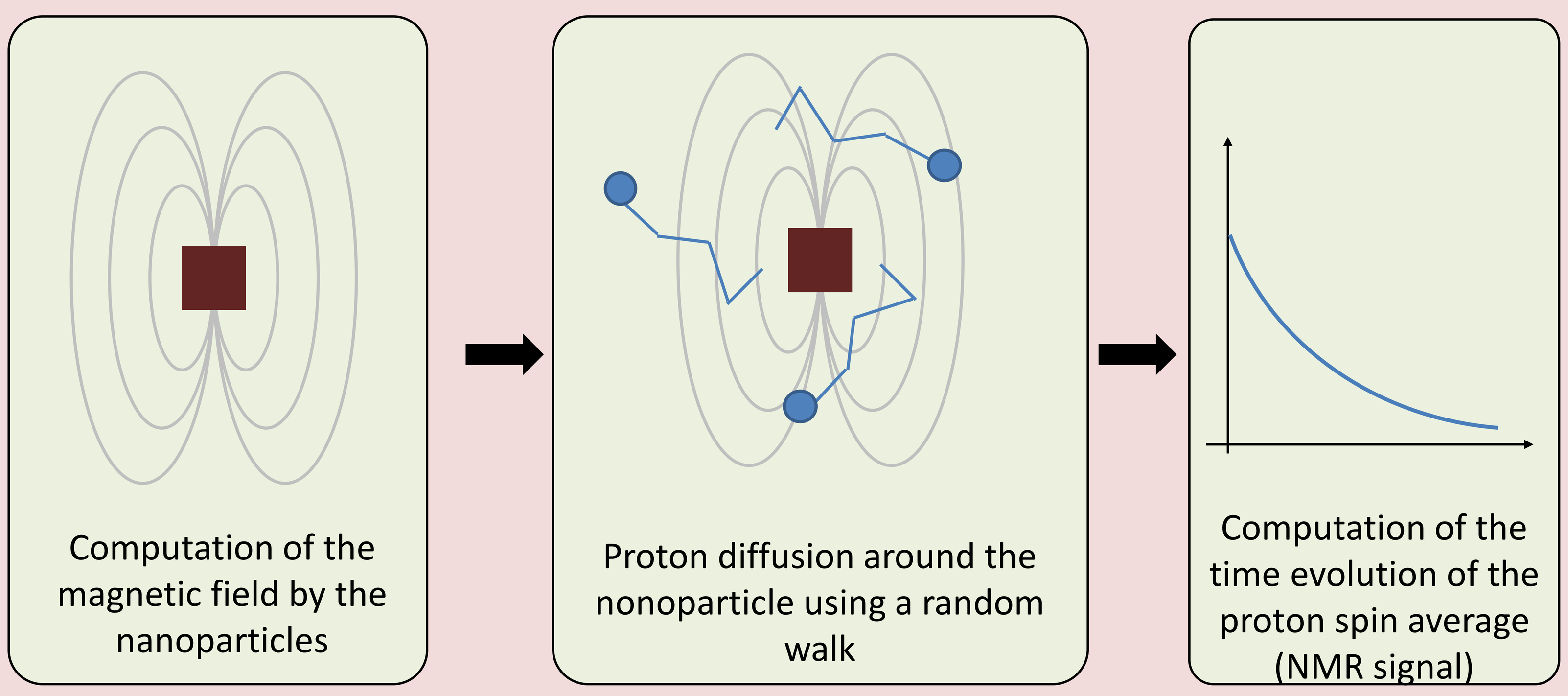


Figure 2 : the three main steps of the simulation of the NMR relaxation induced by IONP

## 3. Results

- The simulation results are presented in Figure 3. The spherical and the cubic cases are shown for comparison.
- The relaxation rates dependence on the IONP size is composed of two well-known regimes [4]: the motional averaging regime (MAR) and the static dephasing regime (SDR).
- From the relaxation point of view, two nanoparticles can be considered equivalent only at equal volume. Abscissa of figure 3 are thus expressed in volume units. Spherical particle radius is also indicated on the graph for information.

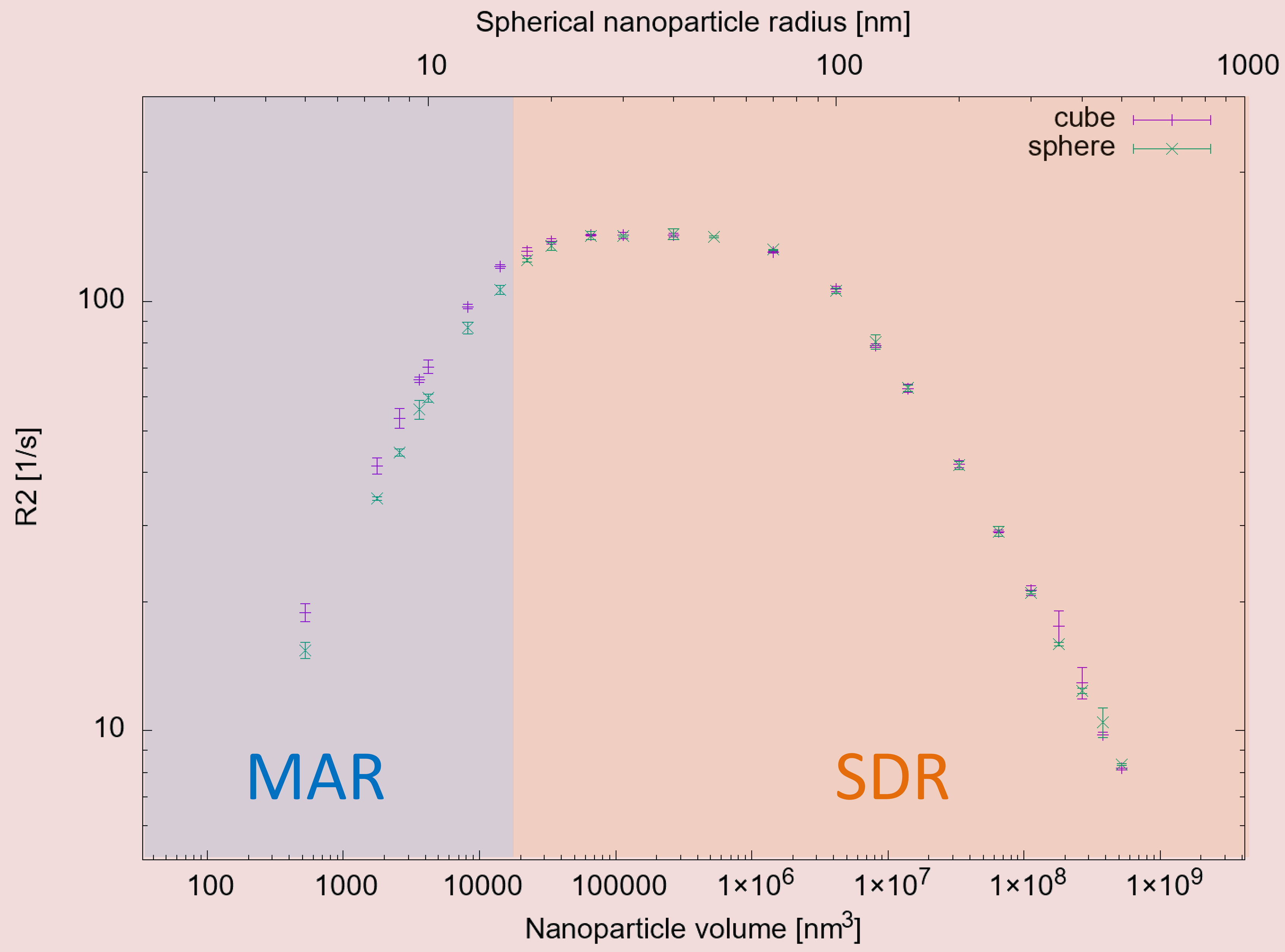


Figure 3: simulation results for spherical and cubic nanoparticles. Abscissa are expressed in volume units for both shapes and in radius units for the sphere case.

- In the **SDR regime, the spherical and cubic results show similar values**: this is expected as, in this regime, only the protons far from the nanoparticles contribute to the relaxation.
- **In the MAR regime, our preliminary results show relative differences of about 15%** which seems to show that the specific cubic nanoparticle shape makes them more efficient than spherical one. However, an optimization of the magnetic field mesh has still to be done to confirm this result.

Future work will consist in testing other NP shapes and determine the shape that will have the greatest impact on the relaxation times.

**References**

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