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Monte Carlo Simulations of the T_2 relaxation induced by exotic-shaped superparamagnetic nanoparticles

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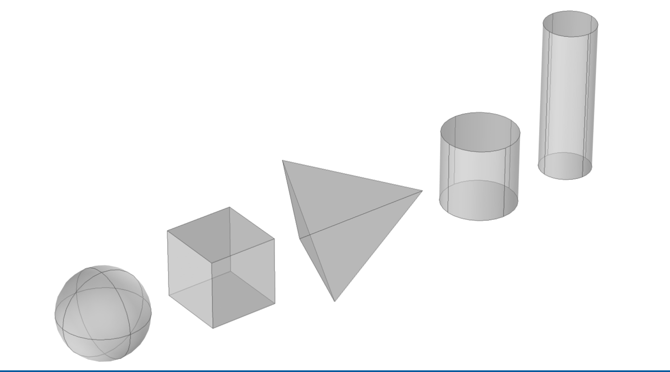
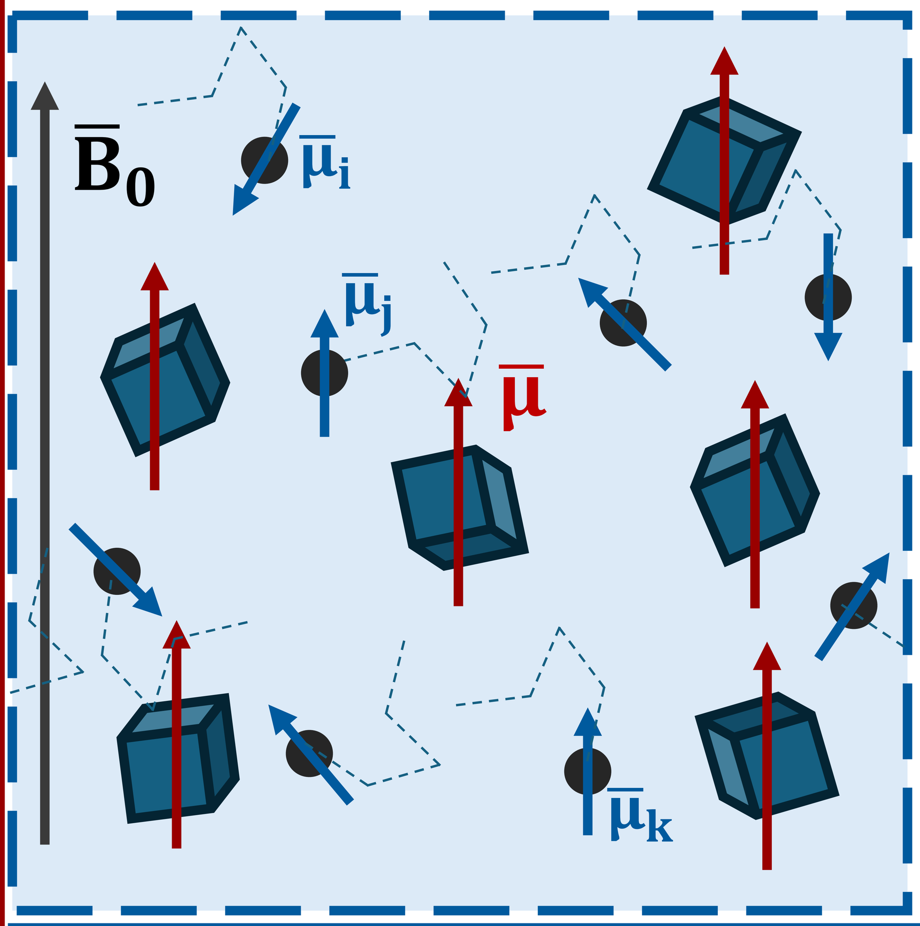
I. Introduction and research context



The transverse relaxation ($R_2 = 1/T_2$) of water protons induced by *exotic-shaped superparamagnetic nanoparticles* (NPs), used as negative contrast agents in MRI, was studied using **Monte Carlo simulations** under a high static magnetic field (B_0). Comparison with the spherical case, at equal volume, reveals **deviations from the expected relaxation** within the *Motional Average Regime*. **Analytical Stray Field analysis** supports these findings and provides an alternative approach for computing relaxation times of exotic-shaped NPs.

II. Monte Carlo Methodologies

II. a. Diffusion Setup [1]



- $1'500$ Magnetite NPs, $\bar{\mu}$
- $10'000$ Water Protons, $\bar{\mu}_i$
- Static Magnetic Field $\bar{B}_0$

- CPMG Sequence ($T_E = 0.25 - 0.5 - 1$ ms)
- Constant volume fraction ($f = 3.14\ 10^{-6}$) $\Leftrightarrow$ ($C = 0.211$ mM)
- Periodic Random Walk Diffusion ($D_{water} = 3.10^{-9}\ m^2 s^{-1}$)
- Relaxation stems from the **Larmor precession of proton spins** around the **local stray field** (**NPs** + $\bar{B}_0$).

II. b. Stray Field Analysis [2]

- Variation of R_2 induced by NPs at small diameters **[3]**

$$\Delta R_2 \sim \langle B^2_{proj} \rangle$$

- Extrapolation for other shapes

$$\Delta(\Delta R_2) \sim \Delta(\langle B^2_{proj} \rangle)$$

- Analytical Stray Field derived from scalar potential ϕ_m **[4, 5, 6]**

$$\mathbf{B}(\mathbf{r}) = -\mu_0 \nabla \phi_m(\mathbf{r})$$

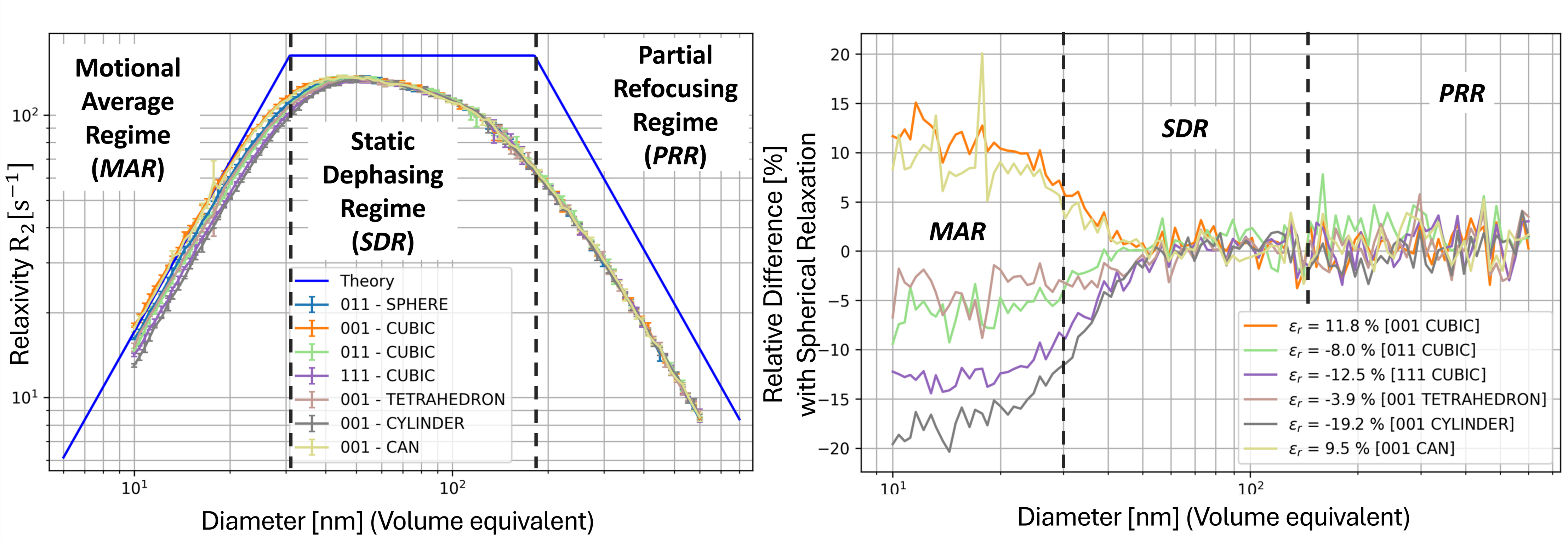
- Using a Monte Carlo Integration,

$$\langle B^2_{proj} \rangle = \frac{1}{V} \int (\mathbf{B}(\mathbf{r} \sim U) \cdot \hat{\mathbf{M}})^2 dV$$

Shape	$\hat{M}$ axis	ϵ_{rel}
Sphere	/	0%
Cubic	111	15%
Cubic	011	−19%
Cubic	001	−29%
Tetrahedron	001	−14%
Cylinder	001	−51%
Can	001	7%

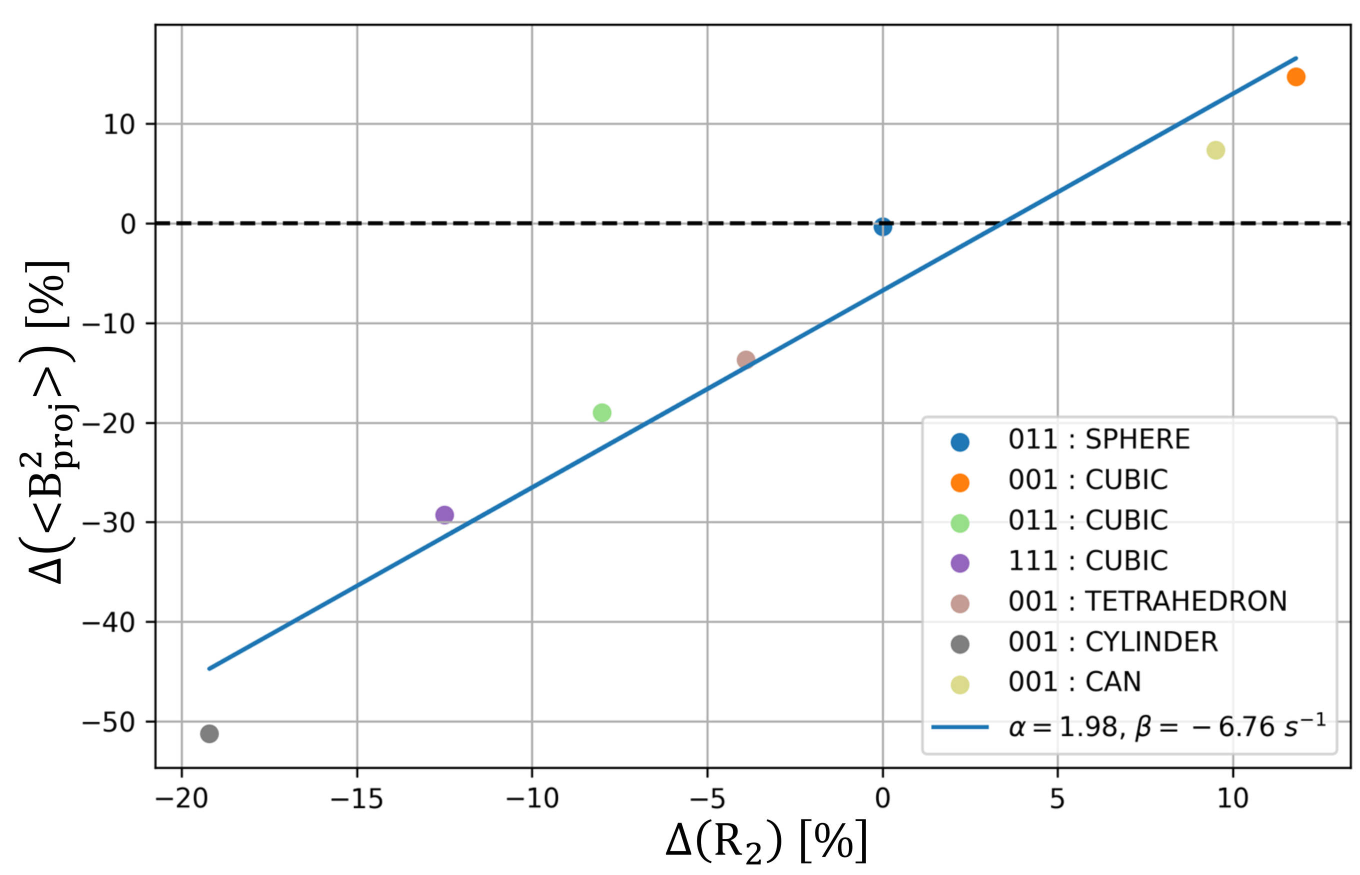
III. Results & Interpretations

III. a. Bell Curves, CPMG at $T_E = 0.5$ms



- Monte Carlo simulations show that significant variations in relaxation times occur at **small NP diameters** (< 40 nm) for all exotic-shaped NP, within the MAR and the lower end of the SDR.
- In addition of particle geometry, we show using cubic-shaped NPs that the **magnetization orientation** can further modulate $\mathbf{R_2}$, with up to a **25% variation** between 001 and 111 orientations.

III. b. Correlation $\Delta R_2 \sim \langle B^2_{proj} \rangle$



- Using the following linear regression :

$$\Delta(R_2) \approx \alpha\, \Delta(\langle B^2_{proj} \rangle) + \beta$$

- We propose an **alternative approach to estimate variations in relaxation times** directly from the **stray field variance**, thus **bypassing diffusion simulations.**

IV. Summary And Future Directions

- **Monte Carlo diffusion simulations** demonstrate that the **nanoparticle (NP) shape** influences the **transverse relaxation** $(\mathbf{R_2})$ for **small particles** (*MAR*), while **larger particles** (*SDR*; and *PRR*) remain unaffected.
- By analysing the **analytical stray field** of various particle geometries, we show that **changes in relaxation** $(\boldsymbol{\Delta}\mathbf{R_2})$ correlate with **variations in the stray field variance** $\langle B^2_{proj} \rangle$.
- This suggests that **analytical stray field analysis alone** may be sufficient to **estimate the gain or loss in transverse relaxation time** $(\mathbf{T_2})$ for exotic-shaped nanoparticles within the *MAR*.
- Future work will explore new geometries (e.g., needles, plates, disks) to further **validate the correlation** between ΔR_2 and $\langle B^2_{proj} \rangle$.

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