TRANSLATIONAL DIFFUSION OF NUCLEAR SPINS IN POROUS MEDIA: A COMPUTATIONAL PHYSICS APPROACH TO UNDERSTAND NMR DATA

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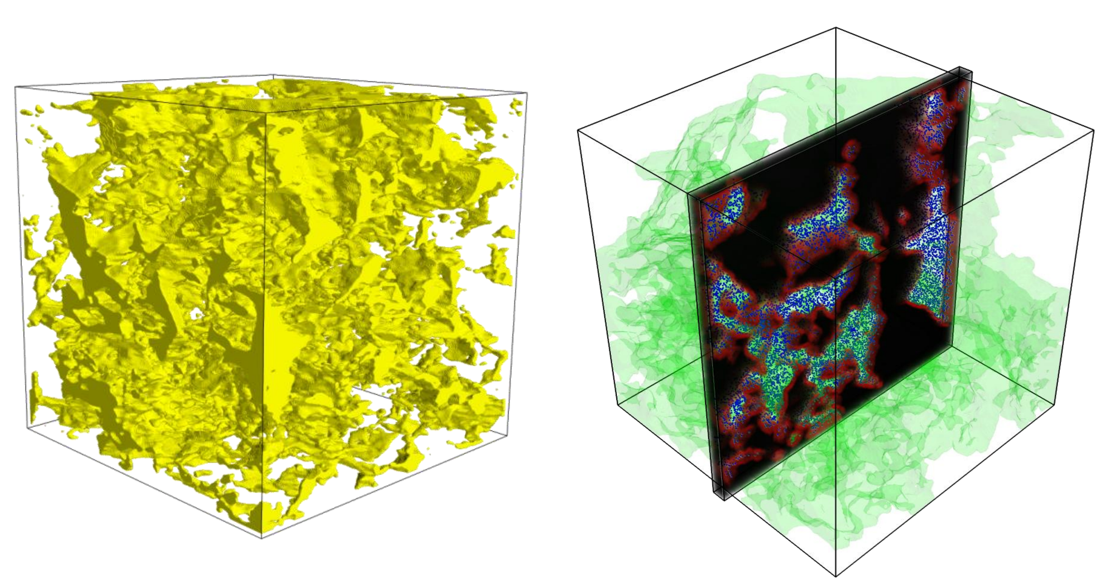
Abstract: Fluid dynamics in porous materials is an important issue in different areas, such as scientific and technological, especially in oil exploration. Several NMR studies are being developed to elucidate fluid dynamics in porous media and estimate properties such as permeability, tortuosity and characteristic lengths. In order to understand, computationally, the correlation between NMR data and the fluid dynamics restricted in porous media is necessary to develop techniques for both physical phenomena. Using a random walk method in position and phase space, we developed a software to obtain the T_2-distribution based in the intrinsic diffusion of the fluid molecules in the porous media reconstruct by microCT images. This computational physics model is able to simulate information obtained by one and two-dimensional NMR techniques.

This work combines two random walk approaches, over the space and phase-space, in order to simulate the relaxation behavior of fluids within porous media, taking into account the dephasing due the interactions of the nuclei with the pore walls and among themselves. The relationship between T_2 distributions and pore properties, *e.g.* morphology and ratio distribution (S/V), can be analyzed under slow and fast translational diffusion regimes with the Brownstein and Tarr Model. The pore morphology is computationally represented by a 3D voxel-based description, in which both real (obtained by x-ray microtomography) and virtual idealized models can be used as boundary conditions.

Sample (Berea)

Binary Image

3D Representation to Pore Media:



Block of Porous Media — Particles within Pore

Reconstruction with Burn Method:

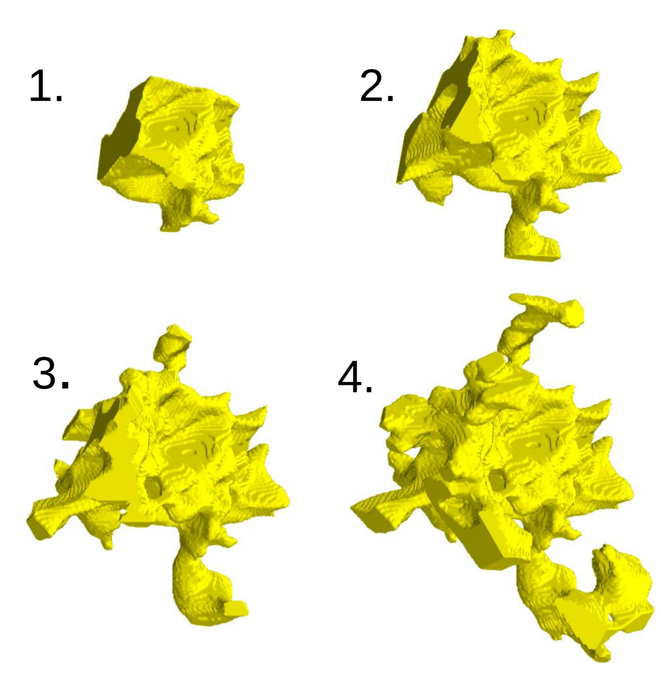
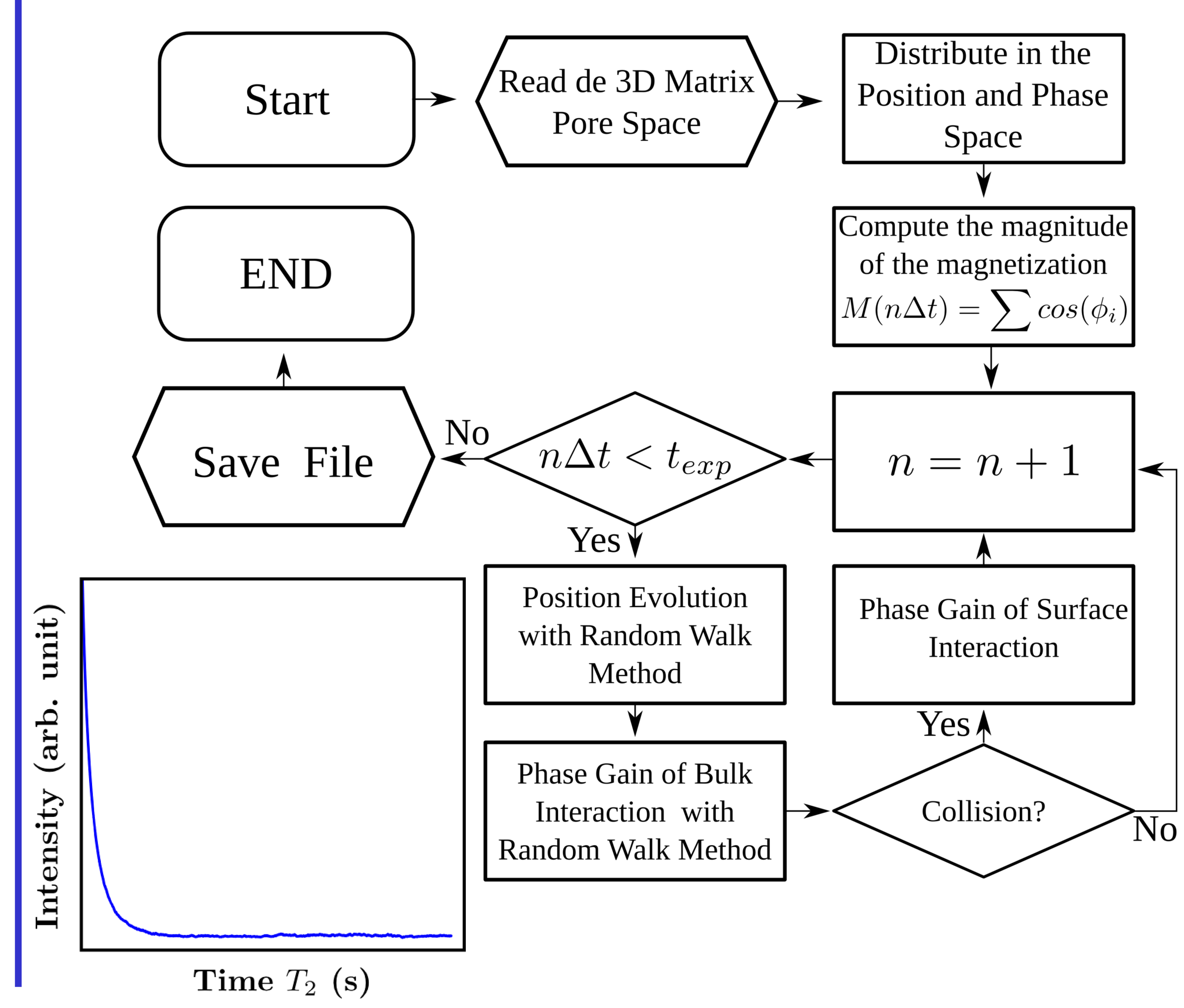
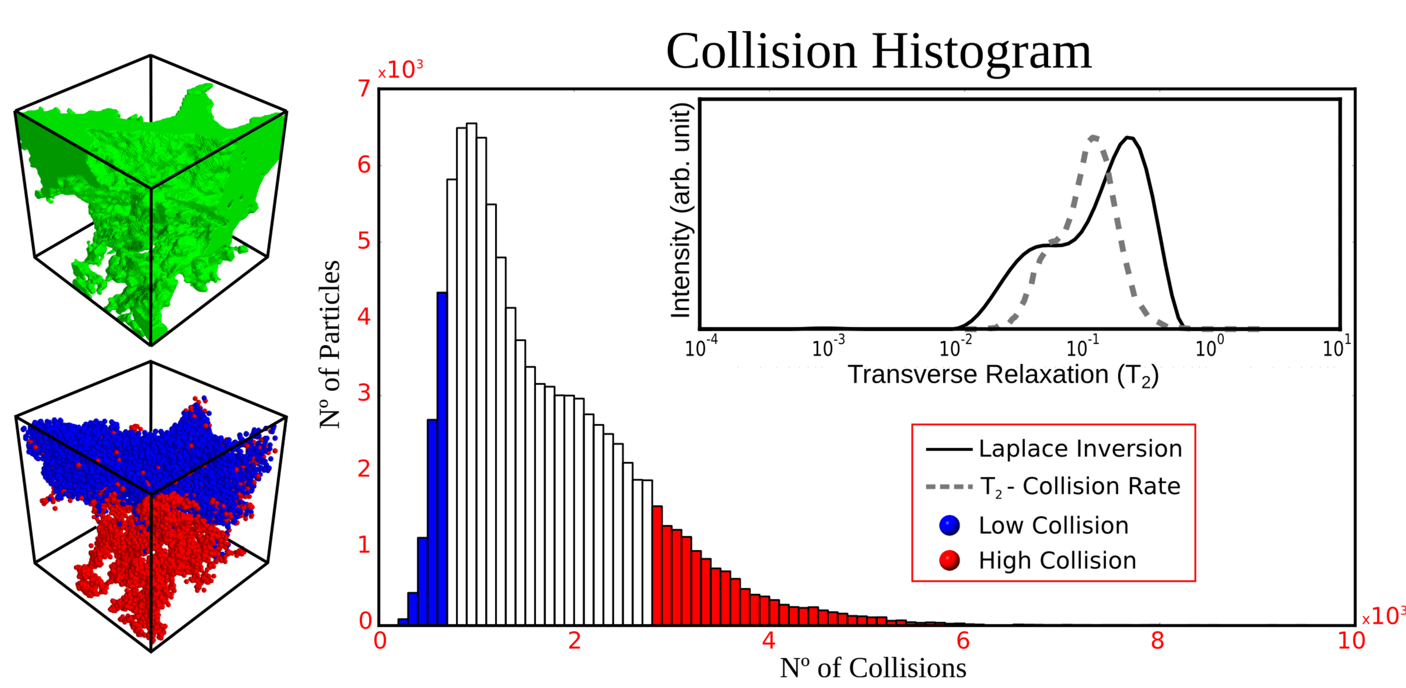


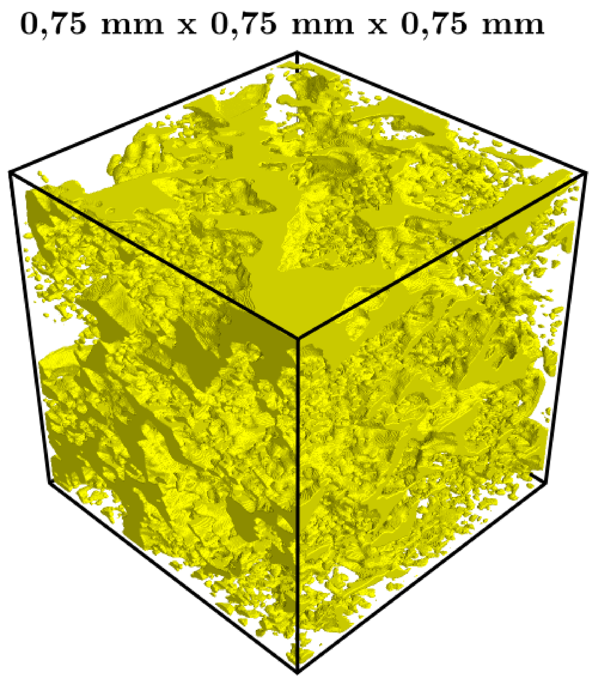
Diagram Software:



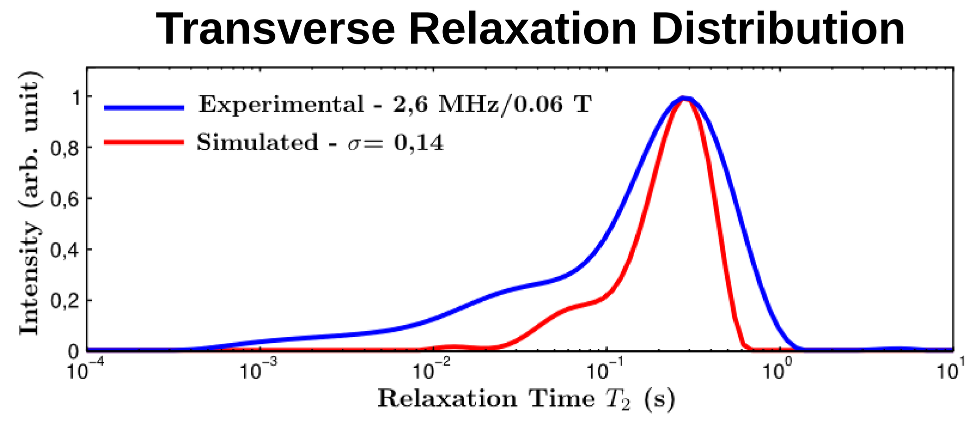
Transverse Relaxation: Experimental and Simulated Data



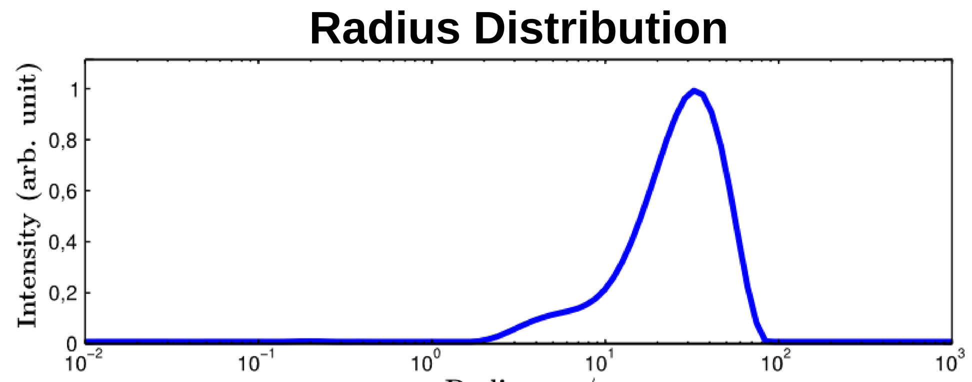
Dimensions:
0,75 mm x 0,75 mm x 0,75 mm



Transverse Relaxation Distribution

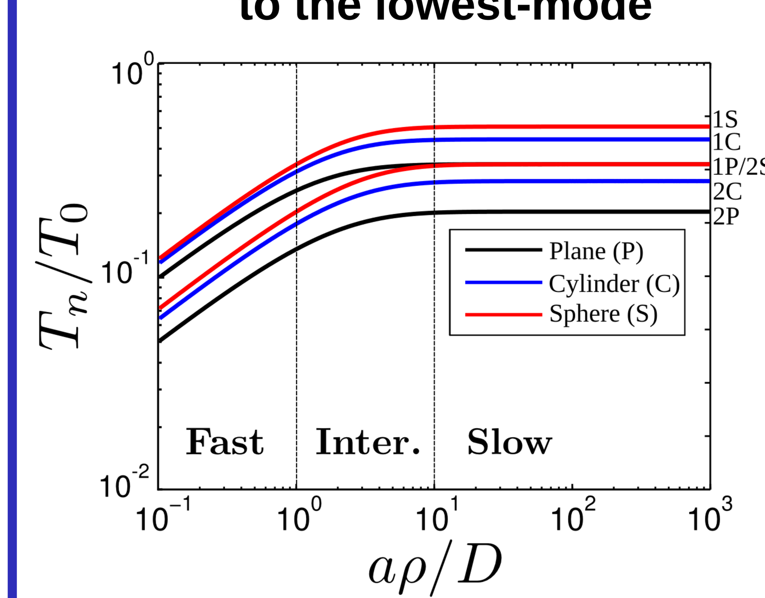


Radius Distribution

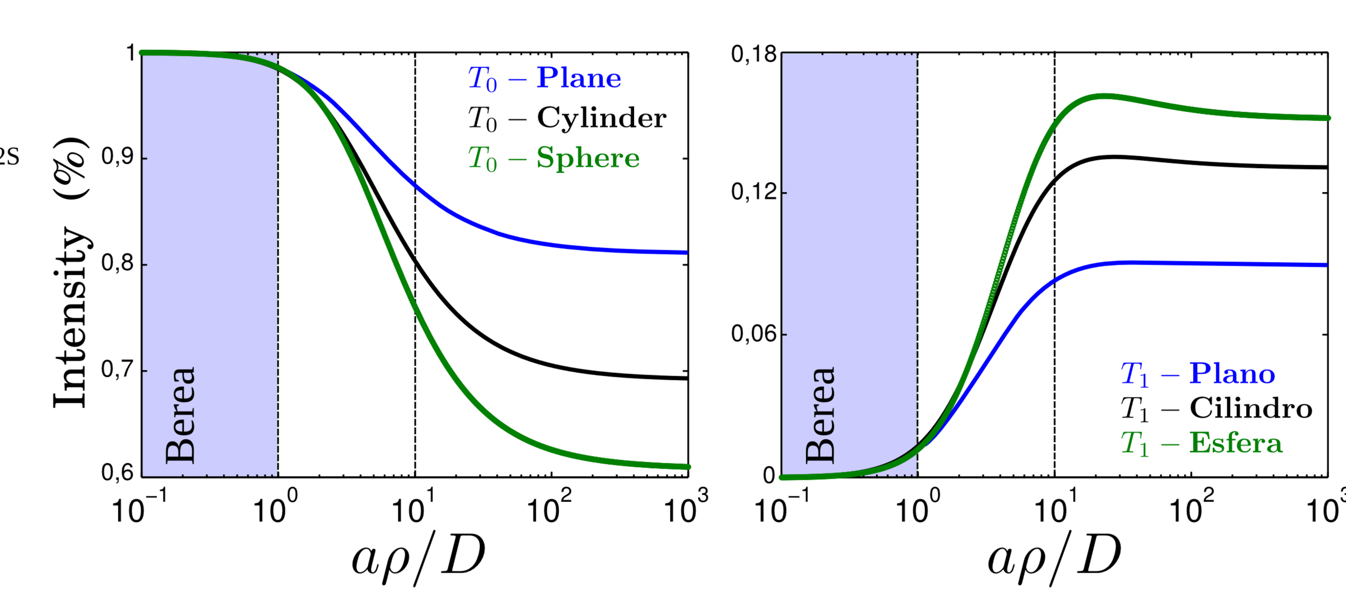


Surface Relaxivity and Length Scale on Porous Media: Brownstein e Tarr Model

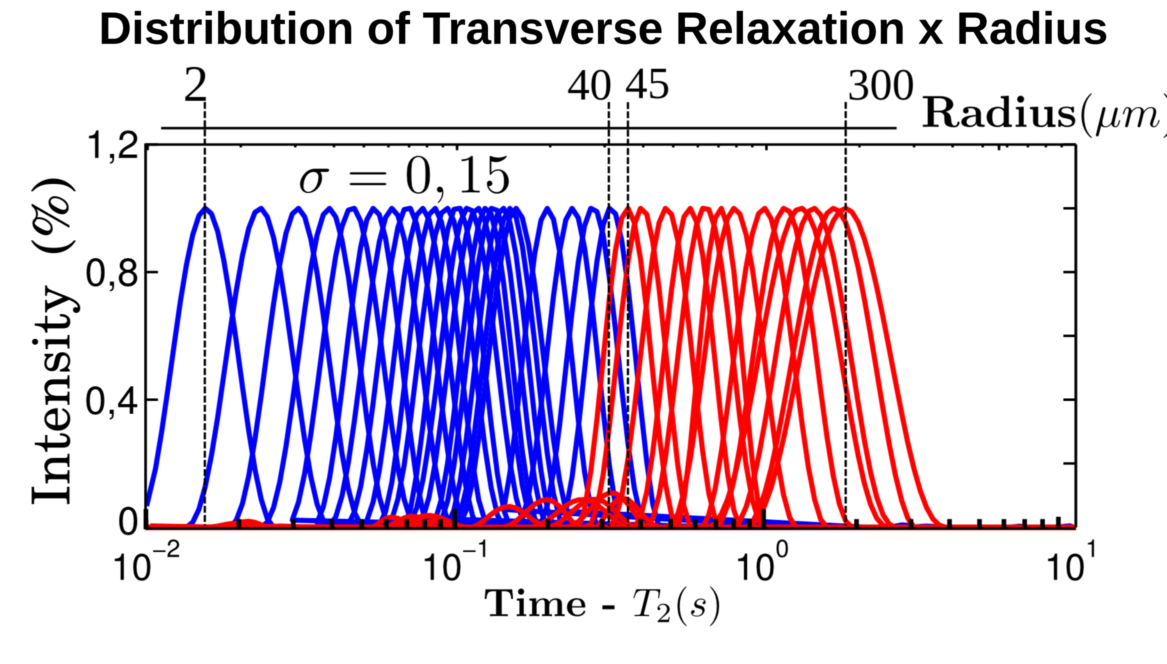
Ratio of the *n*th mode decay time to the lowest-mode



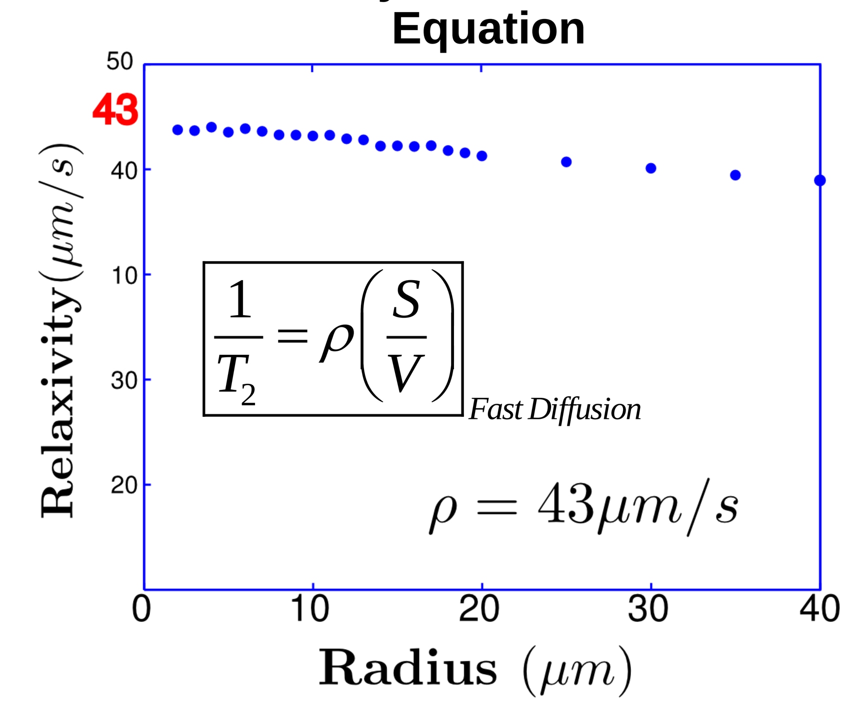
Relative Intensity of the *n*th mode decay time



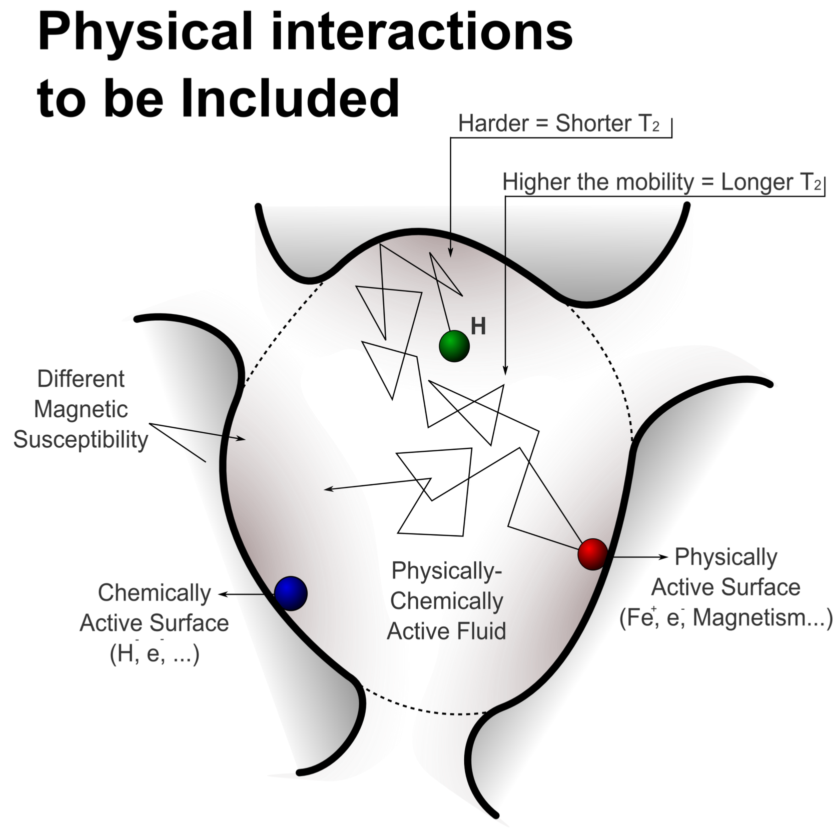
Distribution of Transverse Relaxation x Radius



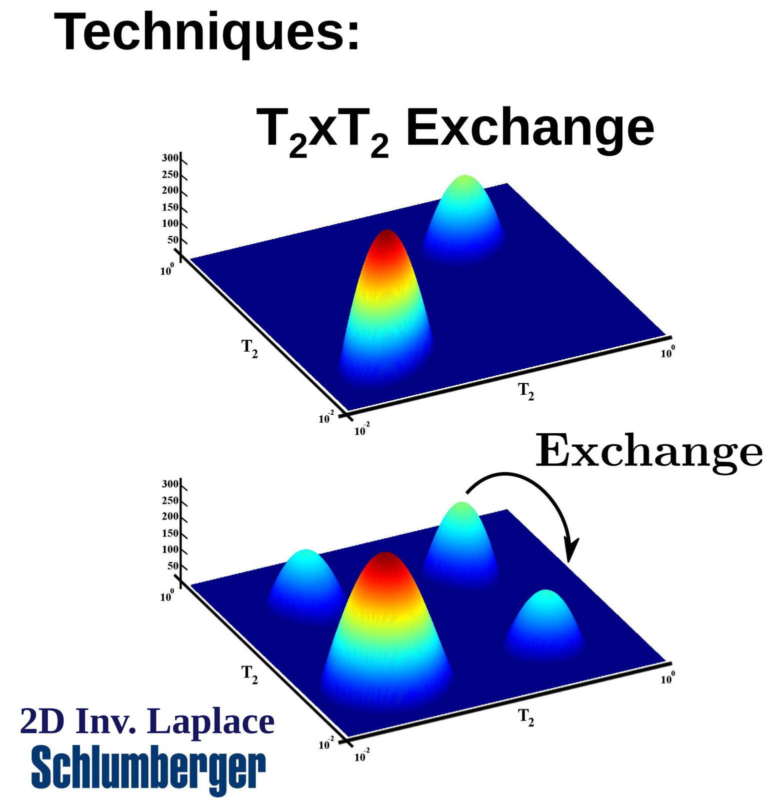
Relaxivity of Fast Diffusion Equation



Physical interactions to be Included



Multidimensional NMR Techniques:



Conclusions and Perspectives:

This computational physics model is able to simulate information obtained by one and two-dimensional NMR techniques, such as CPMG and T_2xT_2 Exchange [1-3], making it possible to identify different diffusion regimes and better understand the spin migration along different sites in the porous space. The next step is include the longitudinal relaxation effects and multidimensional NMR methods to correlate with important properties of porous materials, e.g., permeability and structure factor.

References:

1. Song, Y.-Q. Magnetic resonance of porous media (MRPM): a perspective. Magnetic Resonance, v. 229, n. 0, p. 12-24, 2013.
2. D'Eurydice, M. N. Desenvolvimento de metodologias para o estudo de meios porosos por ressonância magnética nuclear. 174p. Tese (Ph.D.) – IFSC/USP, São Carlos, 2011.
3. Lucas-Oliveira, E. Nuclear spin diffusion in porous media – a computational approach of NMR. 143p. Dissertação (MS) – IFSC/USP, São Carlos, 2015.

Acknowledgments:

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