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Monte Carlo Simulation for Magnetic Resonance Diffusion Measurements

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Magnetic resonance imaging (MRI) is widely used as a non-invasive diagnostic technique to visualize the internal structure of biological systems. MRI has limited spatial resolution and the microscopic behaviour within an image voxel cannot be visualized with qualitative images. Quantitative analysis of molecular diffusion provides insights into the microscopic structure beyond the MRI image resolution. It is challenging to analytically derive the MR diffusion signals for complex microscopic environments, particularly with susceptibility effects. In this work, an easy to use open-source Monte Carlo algorithm has been developed to simulate MR diffusion measurements under arbitrary conditions.

The self diffusion of water molecules can be described by Brownian motion. The Monte Carlo method was applied to simulate the Brownian motion in a user-defined microscopic environment. The fast simulation can be performed on any MRI experiments with user-defined magnetic field distribution. The method has been applied to predict nanoparticle configuration. Magnetic nanoparticles, serving as biosensors, distort the local magnetic field leading to changes in the MR diffusion signals. The simulation agreed with the experimental results. The nanoparticle concentration in water can be determined with MR diffusion measurements.

We have developed an efficient, easy to use algorithm for rapid diffusion simulation in different microscopic environments with arbitrary magnetic fields. This simulation will be employed to optimize the nanoparticle biosensor systems for a wide range of targets, including cancer cells and COVID virus.

Authors: Mr PARASRAM, Tristhal (University of Windsor); Dr LU, Rongsheng (Southeast University); XIAO, Dan (University of Windsor)

Presenter: Mr PARASRAM, Tristhal (University of Windsor)

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