UMMRIS - Particle-based MR Simulation Framework

T. Kober¹, D. Gembris¹, and R. Männer¹

¹Institute for Computational Medicine, University of Mannheim, Mannheim, Germany

Introduction: Computer simulations allow for predicting and interpreting the outcome of NMR and MRI measurements. A survey of existing solutions prompted us to develop an easy-to-use software for more realistic simulations of diffusion tensor imaging (DTI), that could be used to support MR based fibertracking. The aim was to be able to model microscopic structures that result in deviations from the single tensor model, e.g. observed in HARDI measurements. Validation of diffusion tensor imaging (DTI) results and new methods of diffusion modeling in different geometries remains challenging. Suitable and parametrizable phantom datasets are required but currently rarely available. Therefore, the University of Mannheim MRI Simulator (UMMRIS), a flexible particle-based Bloch equation simulation framework has been developed using an object-oriented approach (C++).

Theory: Particle diffusion is modeled as a random walk process, i.e. the particles make successive steps in a random direction. Using the equation for the mean displacement d of homogeneous, isotropic diffusion as the variance for the probability density function P_D , the three-dimensional diffusion vector is generated by randomly sampling P_D for each vector component r_i :

$$d^{2} = 2D\Delta t , \qquad P_{D}(\vec{r}_{i,0} \mid \vec{r}_{i}, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(r_{i} - r_{i,0})^{2}}{4D\Delta t}}$$

If a particle crosses a body boundary, it is reflected (angle of inflection = angle of reflection).

A temporally discretized Bloch equation is used to compute the change of the magnetic vectors of the isochromats and their Larmor frequency in the momentary time step. For this purpose, the discretized Bloch equation is solved considering the current magnetic field which is experienced by the corresponding isochromat. Only differences to the basic Larmor frequency $\omega_0=\gamma B_0$ are considered, because working with the absolute Larmor frequencies would necessitate very high sample rates. The total magnetization resp. signal is generated by summing up the contributions of all isochromats. Spatial filters may be defined in order to obtain signal only from a subset of isochromats.

Methods: The framework has an easy-to-use graphical user interface for defining and previewing geometries and experimental parameters as well as for displaying imaging or raw signal output. The resulting images are generated by simulating the signal of moving or non-moving particles which experience particular magnetic fields, defined by a user-specified MR sequence. The simulation space is defined as a volume of a certain size experiencing the homogeneous main magnetic field B₀. Body objects define the model geometry. Besides the possibility of creating arbitrary bodies, several standard geometries like cubes, cylinders and y-shapes are predefined in the program package. One ore more bodies can be arranged freely inside the experiment volume. Each body contains an arbitrary amount of particles, which are regarded as a cluster of spin ensembles, the *isochromats*. These isochromats are the building block of the physical simulation. Each of them comprises a position and a magnetic vector, as well as a spin density value. Physical parameter sets, the *substances* and the *nuclei*, are associated with each isochromat, e.g. defining the diffusion coefficient D.

One can either make use of already existing sequences like the echo-planar-imaging (EPI) or diffusion-weighted (Stejskal-Tanner) sequence or by designing arbitrary sequence objects: These objects arrange basic sequence building blocks on the



<u>Figure:</u> Results for the simulation of an EPI measurement of a phantom: a) Diagram of the particle distribution in a y-shaped geometry, b) diagram of the raw signal and c) k-space (left) and image space matrix of the simulated y-shape object.

experimental time axis, like gradient lobes of different shapes or RF pulses. In order to increase simulation speed, pulses are phenomenologically modeled, i.e. only the effect of the pulses on the isochromats is simulated.

Conclusion: The simulation has been successfully validated using different geometries. On standard PCs, computation time is, e.g., for 64x64 EPI sequences with up to 10.000 particles in the order of minutes. The software is currently being tested for solving the inverse problem of reconstructing geometric structure on a sub-voxel scale, including the analysis of diffusion time dependence. **References:**

- 1. T. H. Jochimsen et al., "ODIN object-oriented interface for NMR.", J Magn Reson, 2004 (170), 67-78
- 2. H. B: Cattin et al., "The SIMRI project: a versatile and interactive MRI simulator.", J Magn Reson 2005 (173), 97-115
- 3. W. B. Blanton et al., "BlochLib: a fast NMR C++ tool kit.", J Magn Reson 2003 (162), 269-283
- 4. B. Pütz et al., "Edge enhancement by diffusion in microscopic magnetic resonance imaging.", J Magn Reson 1992 (97), 27-53