Exploring Transverse Relaxation Mechanisms by Simulation at the Nano Scale: Introduction of a High Speed Monte Carlo Algorithm

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Introduction: Monte Carlo (MC) modeling of spin package diffusion in an inhomogeneous field generated by perturbers has been used to simulate field-inhomogeneity-induced transverse relaxation in studies of iron-rich tissues, iron overload diseases, and superparamagnetic iron oxide (SPIO) particles [1, 2]. Most previous studies carried out simulations on the ~10μm cellular scale (e.g. beads [3] or cells containing high-level ferritin/hemosiderin [2]). However, intracellular iron distribution is inhomogeneous with cluster sizes in 0.1μm range [4], critically affecting the observed transverse relaxation rate [5]. Unfortunately, the traditional MC algorithm is $O(n^5)$. Thus a 100-fold increase in spatial resolution will be amplified to a 10^{10}-fold increase in computing time, which makes sub-cellular simulation a forbidding task. Here, we introduce a novel high-speed MC algorithm (the 'field profile algorithm') based on 1D diffusion on the field profile as an effort to solve this problem.

Methods: Inspection of the traditional MC algorithm reveals that most computational resources are occupied by repeatedly calculating the magnetic field from the positions of spin packages and perturbers in 3D space. The underlying assumption of our new method is that spin package diffusion about perturbers in 3D space is equivalent to 1D 'jumps' on the field profile. Thus, we can speed up the traditional MC algorithm by omitting redundant calculations of magnetic field (Fig 1). Instead we compute the 3D ΔB_0 field only once in a small universe, and calculate the field profile as a histogram of ΔB_0. Spin package diffusion is then modeled as 'jumps' between bins of field profile governed by a probability matrix P (Fig 2), whose elements p_{ij} are the probabilities for spin packages to 'jump' from the i^{th} bin of field profile to the j^{th} bin within one step. The P matrix is computed by counting all possible steps in the universe. The field profile algorithm was implemented in IDL (ITT, Boulder, CO, USA) on a Windows PC (64bit 1.74GHz processor and 1GB RAM).

As an example, the dependence of T_2 on the water self diffusion constant D was calculated for D values ranging from 0.50 to 2.00 $\mu m^2/ms$, with 1,000 spin packages, spatial resolution 33nm, maximal T_E 50ms, and universe size 100^3. Other parameters used in this simulation include: perturber volume fraction f = 0.174%, B_0 = 1.5T, and susceptibility difference $\Delta\chi = 2.2\times10^{-4}$ (cgs unit). 500 bins were used for the field profile since we found that stable estimations of field profile are obtained for bin-numbers larger than 200 (data not shown).

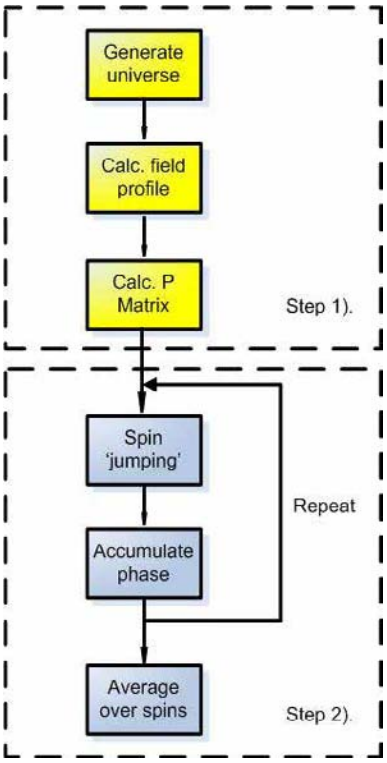

Fig 1. Algorithm flow chart. The field profile algorithm is composed of two independent steps: 1). Calculating field profile and P matrix; and 2). 1D 'jump' of spin packages.

Results: In most cases, field profiles can be estimated accurately from a small universe so that step 1) in Fig 1 only occupies an inferior portion of the total computing time. Since the only requirement on the universe is that it should carry a representative field distribution, step 1) is O(1) with respect to spatial resolution. Thus, computational complexity of the field profile algorithm is determined by step 2) as $O(n^2)$. It takes 6 to 12 hours to accomplish a simulation of 1,000 spin packages per parameter set. Conversely, a similar calculation with traditional MC algorithm took more than 48 hours before the calculation was finally aborted by the researcher. Simulated T_2 values follow a linear relationship with D as predicted by the outer sphere theory (Fig 3).

Discussion and Conclusion: Our example study demonstrated the superior speed of the field profile algorithm. The speed of the algorithm can be further improved by using faster languages such as C or FORTRAN, and by adopting parallel computing concepts. We estimate that with all these improvements, simulations for 1,000 spin packages with spatial resolution in ~10nm range can be accomplished within an hour. An additional advantage of the field profile algorithm is its flexibility, e.g. Maxwell equations can be used to compute the field for interacting perturbers. In summary, this algorithm provides researchers a powerful tool to investigate transverse relaxation mechanisms on sub-cellular (~0.1 to 1μm) to nano (~10nm) scale, which was not previously achievable by traditional simulation techniques.

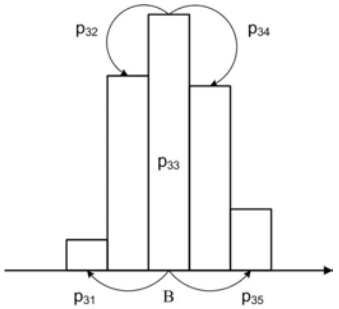

Fig 2. Rationale of the field profile algorithm: spin-package diffusion can be modeled as 1D 'jumps' on the field profile governed by a probability matrix $P = (p_{ij})$

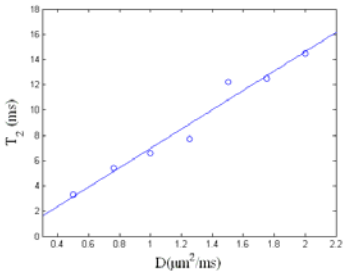

Fig 3. D-T_2 curve. T_2 values simulated on nano scale linearly increase with D, which is predicted by the outer sphere theory.

References:

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