

General-Purpose Diffusion simulation for any sequence using Monte Carlo approach optimized for parallel and multi-core processors

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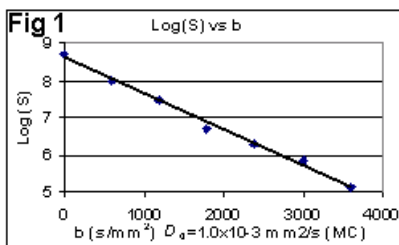
Introduction Our aim in this work is to extend a general-purpose integrated MR simulation / MR console environment (1) to include diffusion-weighting. An important requirement of this general-purpose simulator is that it works directly on any pulse-sequence, so that any sequence written for the MR console is also available for simulation without additional simulation programming or expertise required of the user. In this mode the simulator acts as a virtual experiment. The console/simulator architecture is waveform-based, so that the input to the simulator is the pulse sequence waveforms. Simulation of diffusion effects is important in a number of applications including DWI, microscopy and hyperpolarized gas imaging.

Monte Carlo: From these requirements we investigated Monte Carlo (MC) stochastic methods which directly simulate the underlying spin dynamics of the phantom and do not require explicit identification and tracking of individual coherences. The Monte Carlo approach has the merit of imposing few restrictions but has high computational demands. The diffusion process was simulated by applying a *random walk* to the underlying spins (i.e. spin isochromats). The random displacements ($\Delta x, \Delta y, \Delta z$) each spin moves in time interval Δt are drawn from a Gaussian distribution random numbers with 0 mean and σ variance given by: $\sigma = \sqrt{2D_0\Delta t}$. This simulates isotropic diffusion with constant diffusion coefficient D_0 . Only isotropic diffusion was

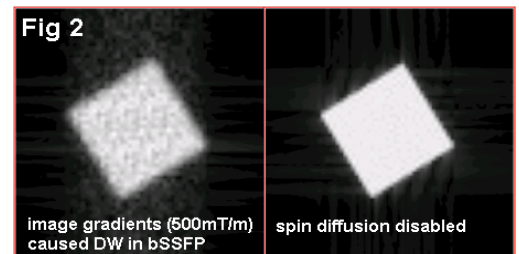
implemented for demonstration purpose. Anisotropic diffusion will need more complicated handling (2). This algorithm was then incorporated into our existing general-purpose isochromat summation based simulator.

Computational Implementation: The random numbers were generated using Intel @ Math Kernel Library 9.1 for Linux which provides satisfactory performance due to the use of the SSE (Streaming SIMD Extensions) instruction set. The simulation was optimized for multi-core CPU architecture by using POSIX threads. This allows its performance to automatically scale with the number of cores used in the computer (it will instantly support an 80-core processor without reprogramming). Each thread handles a single partition of the phantom. A unique seed is given to each thread to avoid correlations in the random numbers. PVM (Parallel Virtual Machine), an inter-process communication library, is further utilized to parallelize simulation across a high performance computer cluster, to reduce the simulation time to a practical level.

Results: The approach was validated with a Stejskal-Tanner SE sequence (4). The phantom is square shaped, consisting of 150x150 isochromats. $\log(S)$ vs b plot (Fig 1) shows good agreement. To demonstrate the generality of the approach which takes into account all the gradients (i.e. readout, PE, etc.), an EPI DW simulation was run. To amplify the contribution from imaging gradients, readout and PE was increased to 500 mT/m level by reducing FOV. The MC method correctly predicted the weighting compared with the analytic values (3) while the simplified Stejskal-Tanner (ST) equation deviates by a large amount (table below). This generality is further demonstrated in Fig 2, which shows a balanced SSFP sequence (with many coherences) with strong imaging gradients. MC diffusion simulation resulted in intensity attenuation equivalent to a b value of 100 mm²/s.



b-ST (s/mm ²)	MC (s/mm ²)	Analytic (s/mm ²)
0	550	500
20	740	600
50	790	670
100	970	760
200	1130	900
400	1350	1160



Discussion: Although impacting simulation speed, spin position randomization with a large number of spins per voxel offers two advantages: reduction of noise, blurring and ghosting image artifacts in diffusion simulation, and prevention of spurious refocusing in the presence of strong gradients (1). Simulation performance therefore is considerably slower than the real experiment, by a factor of 100 or more. In a simulation experiment above, we've measured 400 sec simulation time, for a 7-seconds EPI DW sequence, with a 22,500 isochromats phantom (quad-core dual-processor Dell PE1855 1.6GHz; 8 cores in total). We estimate by spawning the simulation across a 28-node cluster, a five-fold reduction in simulation time will be achieved.

Conclusion: We have demonstrated that Monte Carlo method can reliably produce diffusion weighting for any pulse sequence. Although computationally demanding, optimization for multi-core processors means that performance will improve as industry makes new CPUs available. The general-purpose nature of this user-friendly approach make it a good diagnosis and experimental design tool.

References (1) Sharp-JC et al. Proc ISMRM p.1351 (2006) (2) Farnell-L, et al. Journal of Computational Physics 198, 65-79 (2004) (3) Bihan-DL, et al. Diffusion and perfusion magnetic resonance imaging: applications to functional MRI (1995) (4) Stejskal-EO et al. The Journal of Chemical Physics 42, 288-292 (1965). Acknowledgements: IBD MR Technology Group (Winnipeg, MB)