SpinWalk, a GPU accelerated framework for Monte-Carlo simulation of spins random walk

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Purpose: Monte Carlo simulation is a powerful computational technique to model spin dynamics and predict the resulting MR signal, particularly in a microvascular network. It involves a large number of iterations over several tens of thousands of spins, and therefore is computationally intensive. For MRI sequences, in which a steady-state magnetization is desired, several repetitions of the sequence are required prior to the actual image acquisition to reach steady-state magnetization, further increasing the computational demands. To address this, we introduce *SpinWalk*, an open source MR simulator for Monte-Carlo simulation of spins with random walk (https://github.com/aghaeifar/SpinWalk).

Method: The simulator is programmed in C++ and leverages CUDA technology to execute on a GPU, allowing for a massive parallelization across spins. If an HPC cluster with multiple GPUs is accessible, the simulation will be distributed to available devices which enhance the speed of the simulation even further.

Initially, spin-packages are distributed randomly throughout the entire volume, although predefined spatial positions are also permissible. A vascular network mask can be utilized to prevent spin-packages from being positioned inside a vessel or passing through it during the random walk. All spin-packages begin in equilibrium with a magnetization of M = [0,0,1], but it is possible to specify any starting magnetization. The simulator requires the utilization of one or more pre-calculated field maps, to account for the spin-packages' dephasing during their random walk. Random walk in 3D was calculated from a Gaussian distribution ($\mu = 0, \sigma = \sqrt{6D\Delta t}$, where D is the diffusion coefficient) for every time-step (Δt). The presented *SpinWalk* has the capability to dynamically update the perceived field to accommodate temporal variations in off-resonance, such as those caused by an increase in CBF or CBV.

The simulation's output includes the resulting magnetization vector at the echo time, with the possibility of multi-echo acquisition, as well as the final spatial position of the spin-packages after their random walk. The resulting outputs can be utilized as input for subsequent simulations.

The simulation and sequence parameters can be conveniently adjusted through a configuration file. Additionally, multiple configurations can be provided to the simulator for a batch run. The impact of the size of randomly orientated vessels on BOLD fMRI using GRE, SE, bSSFP and GRASE sequences is exemplarily examined. Sequence parameters are provided in Table 1.

Table 1: Simulation and sequence parameters

Δt=50μs, Spins=100K, D=1.0um^2/ms, BV=2%, B_0=9.4T				
Sequence	TE/TR(ms)	FA	T1/T2(ms)	Prep. Scans
GRE	20/40	90°	∞/∞	0
SE	20/40	90°-180°	∞/∞	0
bSSFP	5/10	16°	2200/41	1000
GRASE	5:10:200/200	90°-180°(10x)	2200/41	0

Results and Discussion: With the utilization of a single NVIDIA RTX A4000 GPU device, it is possible to simulate GRE or SE sequence for 30 distinct vessel sizes, spanning from 0.5μm to 1 mm, with oxygenation levels of Y=77 % and Y=85 %, all within two seconds. Similarly, the simulation of bSSFP can be accomplished in less than 8 minutes. On a HPC cluster with four NVIDIA Quadro RTX 5000 devices, GRE and bSSFP are simulated 1.4x and 2.5x faster, respectively. Relative BOLD signal changes $(1 - Y_{77\%}/Y_{85\%})$ in percent as a function of vessel size for these simulations are shown in Figure 1.

One challenge that arises is the limited GPU memory, as *SpinWalk* necessitates keeping the fieldmap in GPU memory. In our simulation, the field map size of 1024x1024x1024 was manageable; however, increasing the resolution to a finer level may present a challenge in terms of memory capacity.

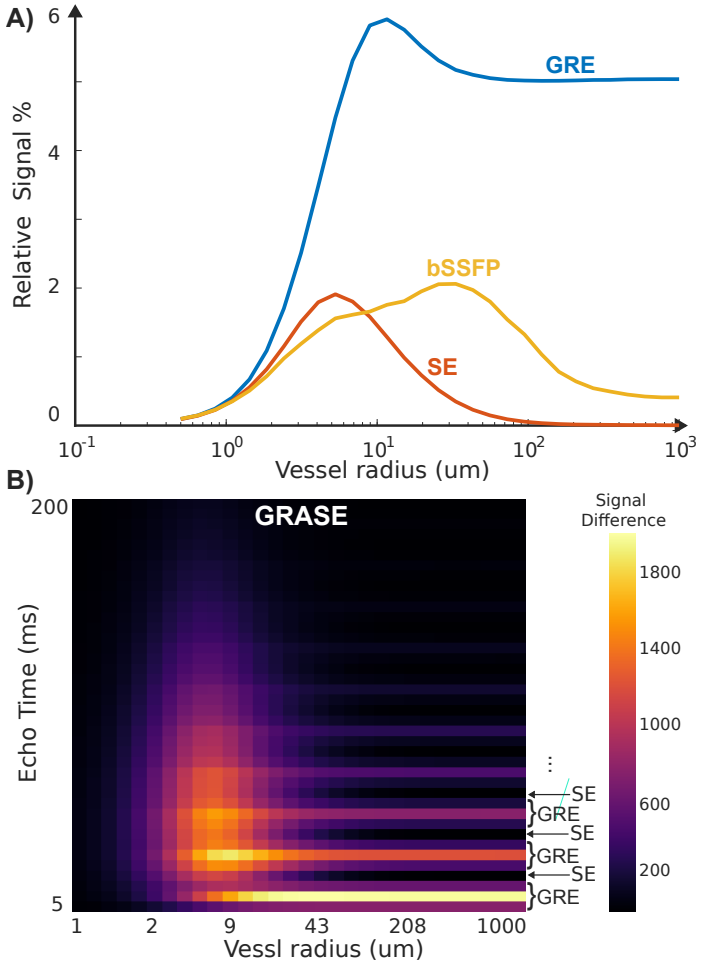

Figure 1: The simulation results produced by SpinWalk. A) Comparison of relative BOLD signal change in GRE, SE, and bSSFP sequences as a function of vessel radius. B) BOLD signal change $(Y_{85\%} - Y_{77\%})$ in GRASE sequence for 10 SE and 30 GRE.