

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

Ali Aghaeifar¹, Sebastian Mueller¹, and Klaus Scheffler^{1,2}

¹High-field MR Center, MPI for Biological Cybernetics, Tübingen, Germany.

MPI für Biologische Kybernetik

Introduction

- ► 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.

Method

- ► The simulator is programmed in C++ and leverages CUDA technology to execute on a GPU, allowing for a massive parallelization across spins.
- ➤ Within an **HPC** cluster with multiple GPUs, the simulation will be distributed to available devices which enhance the speed of the simulation even further.
- ► How **SpinWalk** operates and its capabilities:
 - |-spins are distributed randomly in the volume (predefined spatial positions are allowed) |-a vascular mask -> prevent spins from being positioned in or passing through a vessel |-spins begin in equilibrium magnetization (specifying starting magnetization is possible)
 - |- random walk in 3D is calculated from a Gaussian distribution ($\sigma = \sqrt{6D\Delta t}$)
 - |- multiple predefined field maps can be lined up for simulation in a queue
 - -- accommodate temporal variations in off-resonance (e.g., increase in CBF or CBV)
 - |- multiple RF excitation can be defined
 - |-- FA, phase, and start time can be adjusted
 - |- multiple echo can be recorded
 - |- batch run over different sequence types and parameters is possible
- ► For the purpose of demonstration, simulations are performed on GRE, SE, bSSFP, and GRASE sequences using the following parameters:

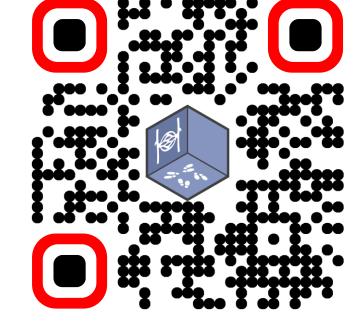
Δt=50μs, Spins=100K, D=1.0um2/ms, BV=2%, B0=9.4T				
Sequence	TE/TR (ms)	FA	T1/T2(ms)	Prep. Scans
GRE	20/40	90	∞/∞	0
SE	20/40	90-180	∞/∞	0
bSSFP	5/10	16	2200/41	1000
GRASE	5:5:200/200	90-180(10x)	2200/41	0

Source Code



https://github.com/aghaeifar/spinwalk

The community's feedback and contributions are warmly encouraged and appreciated.



Results & Discussion

- ➤ Simulation of **GRE** or **SE** sequence for **30** distinct vessel sizes, spanning from **0.5um** to **1mm**, with oxygenation levels of **Y=77**% and **Y=85**%, all within **2** seconds. Simulation of **bSSFP** can be accomplished in less than **8** minutes. This timing is obtained with utilization of a single NVIDIA RTX A4000 GPU device. Relative signal change between two oxygenation levels for these simulations is plotted in Figure 1.
- ► The result of **multi-RF** and **multi-echo** acquisition is depicted in Figure 2 for **GRASE** sequence. The image shows signal difference between two oxygenation levels.

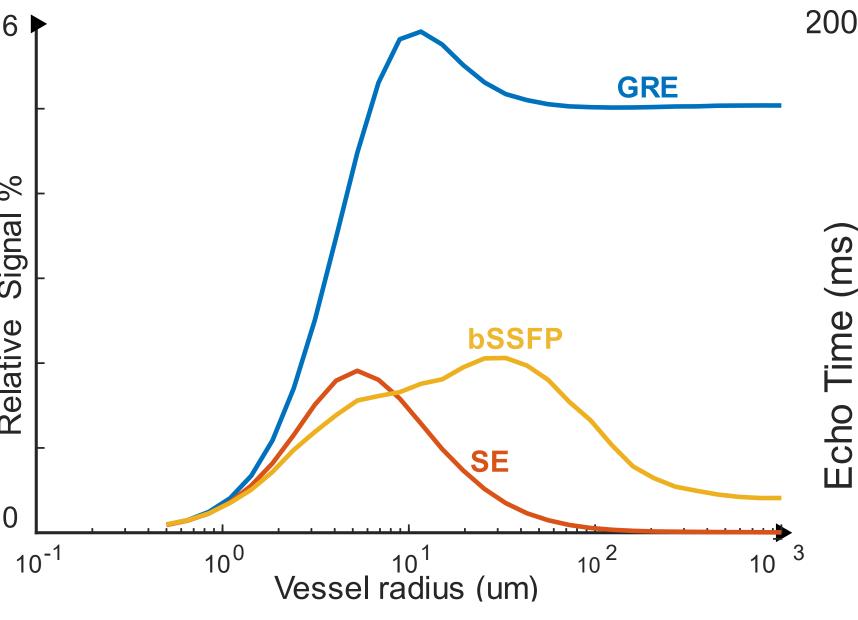


Figure 1. The change in extravascular BOLD signal using GRE, SE, bSSFP imaging methods was investigated in relation to vessel radius. We presumed blood oxygenation levels of 77% for the resting state and 85% for the activated state. These simulations were conducted with randomly oriented cylinders at field strength of 9.4T. GRE demonstrates consistent sensitivity to vessel sizes exceeding approximately 50 μm . SE demonstrates specificity for vessel radii ranging from 2 to 10 μm . The bSSFP profile closely resembles the SE profile; however, its sensitivity to larger vessels remains nonzero.

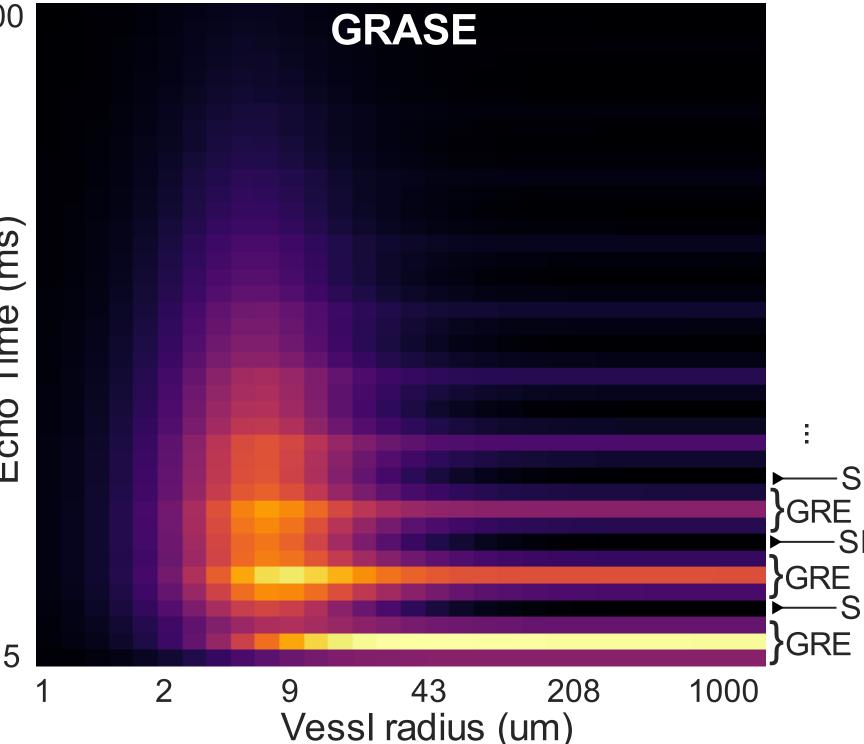


Figure 2. BOLD-related signal changes as a function of vessel size along GRASE echo trains for echo-spacing of 20 ms. The refocusing pulses employed were ideal 180° pulses. Note signal change shown in the image is not relative.

► The influence of vessel orientations on BOLD signal, considering a range of vessel sizes, and exploring various FAs and TRs within the bSSFP sequence, is investigated using SpinWalk in simulations. The outcomes of these investigations are illustrated in Figure 3.

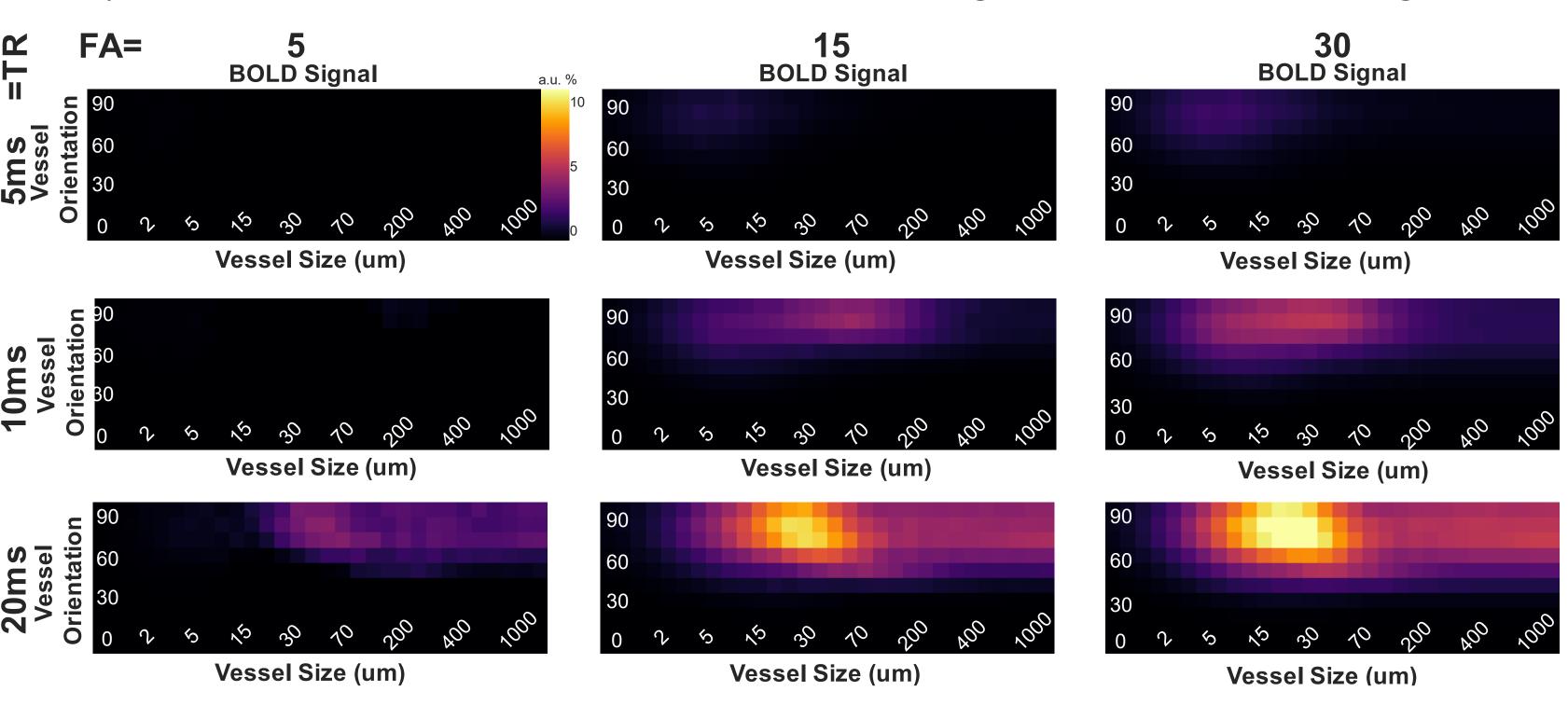


Figure 3. The alteration in BOLD signal in relation to the orientation of a cylinder-like vessel with respect to the BO was examined for the. This investigation encompassed various vessel radii. The simulations used parallel cylinders positioned at a specific angle relative to the BO direction. The bSSFP sensitivity to larger vessels was observed to intensify with an increase in TR and higher FA.

²Department for Biomedical Magnetic Resonance Imaging, University Hospital Tübingen, Germany.