The Journal of Open Source Software

Simulated Diffusion in Realistic Imaging Features of Tissue (Sim-DRIFT)

Jacob Blum [1¶] **and Kainen L. Utt** [1]

1 Washington University in St. Louis, USA ¶ Corresponding author

DOI: 10.21105/joss.05621

Software

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Editor: Jeff Gostick

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Submitted: 25 June 2023
Published: 17 September 2023

Summary

This library, `simDRIFT`, provides for rapid and flexible Monte-Carlo simulations of Pulsed Gradient Spin Echo (PGSE) Diffusion-Weighted Magnetic Resonance Imaging (DWI) experiments, which we expect to be useful for DWI signal processing model development and validation purposes. The primary focus of this library is forward simulations of molecular self-diffusion processes within an ensemble of nuclear magnetic resonance (NMR) active nuclei ("spins") residing in complex, biophysical tissue systems. To achieve a large variety of tissue configurations, `simDRIFT` provides support for n fiber bundles (with user-defined radii, intrinsic diffusivities, orientation angles, and densities) and m cells (with user-defined radii and volume fractions). `simDrift` is written in Python (Python Software Foundation, VanRossum & Drake, 2010) and supported by a Numba (Lam et al., 2015) backend. Thus, `simDRIFT` benefits from Numba's CUDA API, allowing the simulation of individual spin trajectories to be performed in parallel on single Graphics Processing Unit (GPU) threads. The resulting performance gains support `simDRIFT`'s aim to provide a customizable tool for the rapid prototyping of diffusion models, ground-truth model validation, and in silico phantom production.

Statement of need

Monte Carlo simulations are particularly effective at generating synthetic diffusion MRI data from complex, biophysically accurate imaging voxels with known ground-truth microstructural parameters. Consequently, such simulations have proven useful for developing and validating signal processing models (Chiang et al., 2014; Ye et al., 2020). Existing Monte Carlo simulators, such as CAMINO, Disimpy, Realistic Microstructure Simulator, and others rely on meshes to discretize the computational domain Rafael-Patino et al. (2020). While this approach does allow for the representation of complex and finely detailed microstructural features, given the coarse graining of such features (fiber bending, etc…) observed at experimentally realistic diffusion times and voxel sizes (Novikov et al., 2018), `simDRIFT` supplies a reasonable approximation to the relevant self-diffusion processes by parametrizing fibers as narrow cylinders, or "sticks", and cells as isotropic spheres, or "balls" (Behrens et al., 2003). This way, users may readily simulate voxels induced by multiple, oriented fiber bundles and cells without having to re-discretize the computational domain with complex meshes, which scale in size according to the desired feature resolution and size of the simulated image voxel (Panagiotaki et al., 2010).

`simDRIFT`'s superior computational performance represents an important advantage relative to other available open-source software. Comparisons between simDRIFT and Disimpy, a mesh based, CUDA enabled DWI forward simulator known to be faster than CAMINO (Kerkelä et al., 2020), on identical image voxel geometries featuring a 5 μm radius cell, reveals orders of magnitude improved performance, particularly for large resident spin ensemble sizes. Thus, `simDRIFT` is especially useful in a regime where the computational cost of existing software

may be cumbersome or even prohibitive. In particular, `simDRIFT` is able to perform large scale simulations very quickly, therefore benefiting from favorable convergence properties with respect to the diffusion weighted signal. In this context, using just desktop or even laptop level GPU hardware, `simDRIFT` users are able to quickly and easily generate large amounts of synthetic DWI data from a wide variety of voxel geometries.

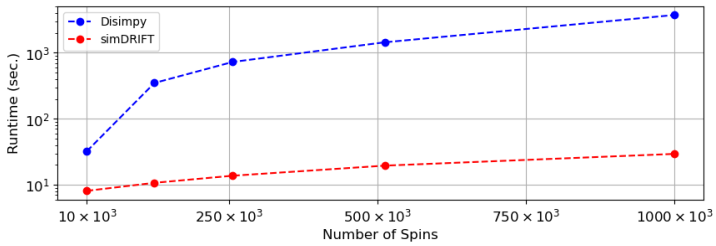

Figure 1: Runtime comparison between simDRIFT and Disimpy, another DWI simulator that runs on the GPU. These simulations were performed on a Windows 10 desktop with an Nvidia RTX 3090 GPU.

Therefore, the software encompassed by `simDRIFT` fulfills a presently-unmet need by allowing for mesh-free Monte Carlo simulations of DWI that unify researchers' needs for computational performance and biophysical realism with easy-to-use and configurable open-source software. `simDRIFT` was designed to be used by researchers of all disciplines and focuses who are working with diffusion MRI. Multiple scientific publications which utilize this library are currently in production. The wide customizability, high computational speed, and massively-parallel design will provide avenues for improved model development pipelines and thorough inter-model comparisons, among other potential applications.

Features

The library allows users to construct voxel geometries described by user-defined microstructural and scanning parameters. Specifically, `simDRIFT` simulates the diffusion MRI signal generated from the self-diffusion of water in an isotropic imaging voxel of length L_{voxel} that contains $n \in [0, 4]$ distinct fiber bundles and $m \in [0, 2]$ distinct cells types, according to the user's selection of diffusion imaging protocol, diffusion time (Δ), time-step size $\mathrm{d}t$, and desired free water diffusivity D_{FW}. Within each simulated voxel, the user also has control over the properties of each fiber/cell type. For each fiber bundle, users define the desired orientation (via the angle θ formed between the bundle and the z axis), intrinsic diffusivity (D_i), axonal radius (R_i), and voxel volume fraction V_i/V_{vox}. For each cell type, users similarly define the desired radius R_j and voxel volume fraction V_j/V_{vox}. Examples of such voxel configurations can be seen in 2.

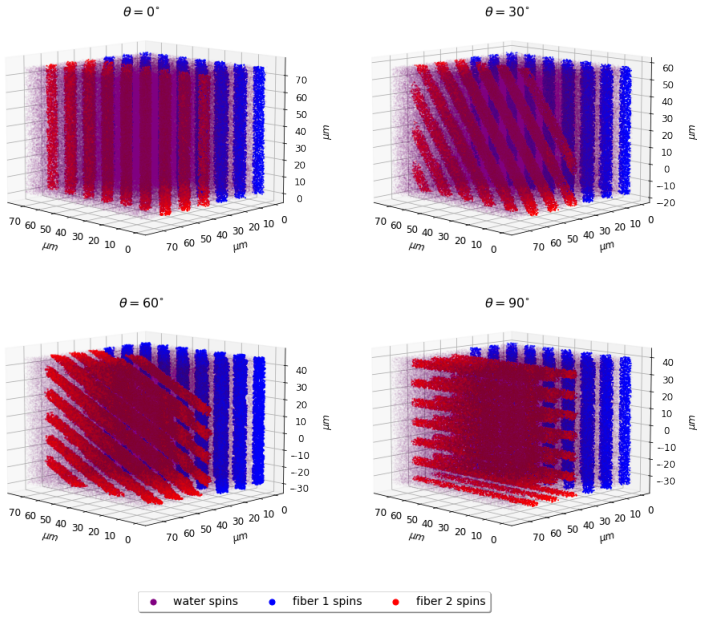

Figure 2: Example simulated spin trajectories from an imaging voxel featuring two fiber bundles (red, blue) with various orientations ($\theta = 0°$, 30°, 60°, 90°), along with extra-fiber spins (purple) .

For each time step $\mathrm{d}t$ in the simulation, each tissue compartment's resident spins are displaced along a randomly chosen direction with a compartment-dependent distance $\mathrm{d}L = \sqrt{6D_0\mathrm{d}t}$. This process is repeated until the target diffusion time of Δ is reached. For diffusion times shorter than the expected pre-exchange lifetime of intracellular water, it is safe to assume no exchange between tissue microstructures. The inter-compartmental exchange of water is computationally forbidden via within-timestep rejection of proposed moves beyond the boundaries of each spin's domain.

Acknowledgments

This work was funded in part via support from NIH NINDS R01 NS11691 and R01 NS047592. The authors would like to acknowledge the early contributions of Chunyu Song and Anthony Wu. We are also immensely grateful for the supportive and clarifying discussions with Professor Sheng-Kwei Song, whose insight helped clarify this project's trajectory.

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