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

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Summary

This library, `simDRIFT`, provides rapid and flexible Monte-Carlo simulations of diffusion-weighted magnetic resonance imaging (dMRI), which we expect to be useful for dMRI signal processing model development and validation purposes. The primary focus of this library is forward simulations of modular self-diffusion processes within an ensemble of nuclear magnetic resonance (NMR) active nuclei ("spins") residing in complex, biophysical tissue systems. To acheive 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 and Drake (2010)) and supported by a Numba (Lam, Pitrou, and Seibert 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 of the Brownian self-diffusion process have proven useful for developing and validating signal processing models (Chiang et al. 2014; Ye et al. 2020). Existing Monte Carlo simulators typically rely on meshes to discretize the computational domain (see e.g., Panagiotaki et al. 2010; Yeh et al. 2013; Ianuş, Drobnjak, and Alexander 2016; Kerkelä et al. 2020; Rafael-Patino et al. 2020). While this approach does allow for the representation of complex and finely-detailed microstructural elements, creating meshes for the biologically-relevant 3D geome-

tries found in typical imaging voxels can be difficult and may therefore present a barrier to wide use among researchers who lack experience and training in computational mathematics. The software encompassed by `simDRIFT` therefore fulfills a presently-unmet need by allowing for mesh-free Monte Carlo simulations of dMRI that unifies researcher's needs for computational performance and biophysical realism with an easy-to-use and highly-configurable 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. These same traits may also make `simDRIFT` useful for instructors of signal processing or diffusion imaging courses.

Features

Given the coarse-graining of detailed microstructural features (fiber bending, etc…) observed at experimentally realistic diffusion times and voxel sizes (Novikov, Kiselev, and Jespersen 2018), `simDRIFT` represents fibers as narrow cylinders, or "sticks", and cells as isotropic spheres, or "balls" (Behrens et al. 2003). 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 [Figure 1].

Figure 1: Example simulated spin trajectories from an imaging voxel featuring two fiber bundles (red, blue) with various orientations (θ = 0°, 30°, 60°, 90°), along with cells (green)

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 $\mathrm{d}L = \sqrt{6D_0 dt}$. 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.

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