Smoothed Particle Hydrodynamic (SPH) simulation of diffusion in realistic neural tissue models

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Introduction In principle, the sensitivity of MRI to the diffusion of water in neural tissues provides a method for inferring local characteristics of the tissue structure and physiology by sampling the spatial (diffusion tensor imaging, DTI [1]) and spectral (q-space imaging [2]) variations of the diffusion weighted imaging (DWI) signal and relating this to a model of the signal behavior generated by a specific pulse sequence. Unfortunately, in practice the complexity of neural tissues precludes the formulation of analytical solutions for the DWI signal behavior, making investigation of diffusion in real neural tissues problematic. A promising approach to the problem is to numerically simulate the DWI experiment, including the construction of the tissue, the diffusion of water through the permeable membranes, and the influence of the pulse sequence. To date, this methodology has been primarily confined to analytical tissue models and grid based (i.e., finite difference) simulations [3]. Unfortunately, analytical tissue models have difficulty capturing the complexity of realistic neural tissues, and the simulation of fluid motion within more complex geometries by traditional grid-based methods is complicated by the computational complexity caused by the non-conformity of the tissue boundaries (individual fiber walls, inter-fiber spaces, cells, etc) and the computational grid. In this paper we describe a novel approach using Smoothed Particle Hydrodynamics (SPH) [4] in combination with ray tracing and complex tissue generation using parametric curves. Initial results in a standard geometry is shown to be consistent with theory.

SPH Theory SPH is a particle based method for solving the Navier-Stokes equations that simplifies the equations by assuming that particles have a limited region of influence that is described by an interpolating function $W(x,h)$ that allows the description of any function $A(x)$ in terms of its values at a set of arbitrary points defined by the neighboring particles: $A(x) = \int A(x')W(x-x',h)dx'$. The interpolating function is typically a Gaussian: $W(x,h) = (2h^2)^{-1/2} e^{-x^2/h^2}$ where the variance *h* defines the spatial scale of particle-particle interactions. Defining functions in terms of an interpolation kernel allows the construction of a differentiable interpolant function from its values at the neighboring particles. Our implementation is capable of solving the Navier-Stokes equations, each term in the N-S equations can be turned on or off separately, allowing investigation of separate effects (e.g., just diffusion) or the inclusion of additional physiological effects such as driven intercellular fluids. For the present study, however, we employed only a simplified diffusion model $x(p) = p \bullet x + v(p)t$ where the velocity $v(p)$ is that of Brownian motion.

Tissue Creation Octrees were employed to create hierarchically structured ellipsoidal "cells", within which are recursively generated additional internal structures that represent intercellular constituents. Ellipsoidal cross section "fibers" hierarchically organized into fiber "bundles" with user defined cross sectional area and fiber density. Fibers are generated using parametric curves using De Casteljau's algorithm which gives a numerically stable method of calculating the position along a Bezier spline. Parametric curves allow efficient generation of complex paths without the need for difficult triangle generation for individual surfaces. Moreover, they facilitate ray tracing complex geometries with little storage. An example is shown in Fig 1. The boundaries of the cells and fibers are permeable to a degree chosen by the user, as are the intra- and extra-cellular diffusion coefficients.

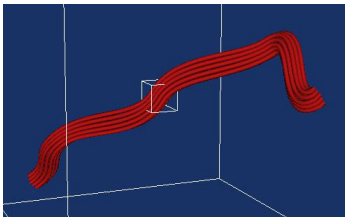

Fig1: Fiber bundle generation along parametric curve

SPH Implementation Particles are stored in an octree to speed up the evaluation of the SPH kernels and allow neglect of intersections of distant surfaces. SPH simulation within this neural tissue model is complicated primarily by the requirement of satisfying the boundary conditions for permeability imposed by the complex geometry. The permeability is defined as the probability that a particle will pass through a surface of permeability *P* and normal ***n***. The necessity of determining how each particle's trajectory intersects with a functionally defined surface was solved using the methods of ray tracing which allows that particle path, defined by its velocity, to be traced and thus determine its intersection with an arbitrary boundary in a similar fashion as the simulation of light through a dielectric.

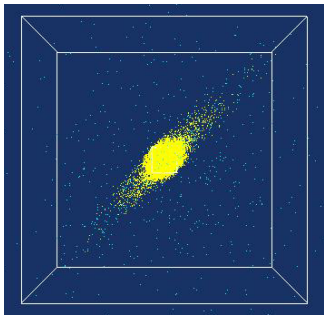

Fig 2: SPH simulation in straight fiber (not Fig 1)

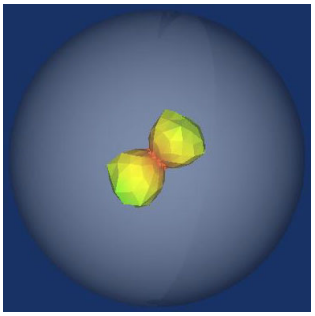

Fig 3: Peanut shape ADC consistent with theory

Pulse sequence simulation and MR signal generation The user interface allows the choice of all diffusion imaging parameters (e.g., gradient strength, diffusion gradient sampling pattern, b, Δ, δ,), the imaging parameters (e.g., voxel size, SNR), the pulse sequence (e.g., spin echo). The phase of each particle generated by its motion along applied gradient directions is tracked and the resulting projection through the voxel generates the signal. The resulting signal is mapped onto the gradient sampling pattern to allow construction of the angular variations in ADC (relative to a reference sphere of b=0 [Fig 3]), which is then available to our DTI analysis routines.

Results and Conclusion The final particle distribution from an SPH diffusion simulation in a straight fiber bundle in a spin echo experiment with G=4G/cm, b=8300, Δ=100 ms, δ=10 ms is shown in Fig 2. The calculated ADC (Fig 3) from 162 diffusion encoding directions determined from spherical tessellations matches closely the "peanut" expected from anisotropic, single fiber diffusion [5], suggesting the efficacy of the SPH approach to the effecient and accurate simulation of diffusion in realistic neural tissue models.

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