

Diffusion microstructure modelling using a modular and extensible GPU accelerated toolkit

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INTRODUCTION: Large multi-shell high angular resolution dMRI datasets are increasingly used to estimate models of brain white matter that include either multiple fiber directions in each voxel³ or microstructural information such as axonal density, diameters and/or dispersion^{1,2,7}. Microstructural compartment modelling is a computationally expensive operation, particularly when the aim is to combine it with modelling of multiple fiber directions and more realistic models that include, e.g. (anisotropic) orientation dispersion or axonal diameter distributions. Previous work⁸ has shown that graphics processing unit (GPU) based acceleration can speedup a single dMRI model by 100x. However, a single specific model implementation does not easily allow further model development, exploration and comparison. Here, we present a new GPU accelerated open source python toolbox for flexible and very fast microstructure compartment analysis of dMRI datasets.

METHODS: The toolbox is completely written in Python and OpenCL. The object oriented design (Fig. 1) abstracts microstructure compartment models, noise models and optimization and sampling routines, such that each can be interchanged. Using the toolbox one can build complex models by combining compartment models in a tree-like compartment hierarchy using the python specification language. For model inversion by Markov Chain Monte Carlo sampling one can then add (per parameter) a prior and proposal function. For scalar parameter estimates by model optimization one can add a parameter transformation function (parameter space to optimization space) to modularly handle parameter constraints.

```
(S0(),
  ((Weight('w_iso'),
    Ball().fix('d',1.7e-9)),
  '*'),
  (Weight('w_ani'),
    Stick().fix('d',1.7e-9)),
  '*'),
  '+'),
  '*')
```

Fig. 2: The Ball&Stick model expressed in the microstructure modelling language.

Microstructure modelling language: We developed a microstructure model specification language to generate complex hierarchical multi-compartment models with tree structure. These compartment models are combined using basic math operators. For instance: (Ball(), Stick(), '+'). To fix or initialize parameters to specific values one can use the fix command with either a constant or with previously calculated results (constants or per voxel). For a complete example of a Ball & Stick model see Fig. 2.

RESULTS: We illustrate the use of the toolbox on the estimation of three commonly used models on suitable high resolution whole brain datasets: the diffusion tensor (DTI), multi-direction CHARMED^{2,4} and NODDI⁷. We optimize the models using a cascade where we initialize similar parameters with the results of a previous model. We optimize all models twice with a median smoothing step of each parameter map in between. Examples were run on an AMD R9 280x. For the DTI example 1.5mm isotropic single shell dataset was used with b-val 1000s/mm², 30 directions and 5 b=0 measurements acquired on a Siemens Prisma^{FTT}. The principle DT direction was initialized from a Ball&Stick fit. The total run time (including fitting Ball&Stick first) was 6 minutes. Fig. 3 (left) shows calculated FA and MD maps. For the CHARMED model a 2mm isotropic dataset with max b-val=6000 s/mm², Δ=45.9ms, δ=29.4ms, TE=94ms, #dirs=45) and 6 b0's acquired on a Siemens Prisma^{FTT} was used. We estimated the CHARMED model by first fitting Ball&{1,2,3}Sticks with and initializing CHARMED with these orientations. Total runtime: 55 minutes. Fig. 3 (middle) shows calculated hindered FA and FR maps. For the NODDI example we used the dataset accompanying the Noddi Matlab toolbox, a two-shell dataset with 24 b-val 700s/mm², 48 b-val 2000s/mm², and 9 b0 measurements. For fitting we fixed the principal angles of the intra and extra axonal compartment models to a previous Ball&Stick fit. Total run time: 35 minutes. Fig. 3 (right) shows calculated hindered NDI and ODI maps.

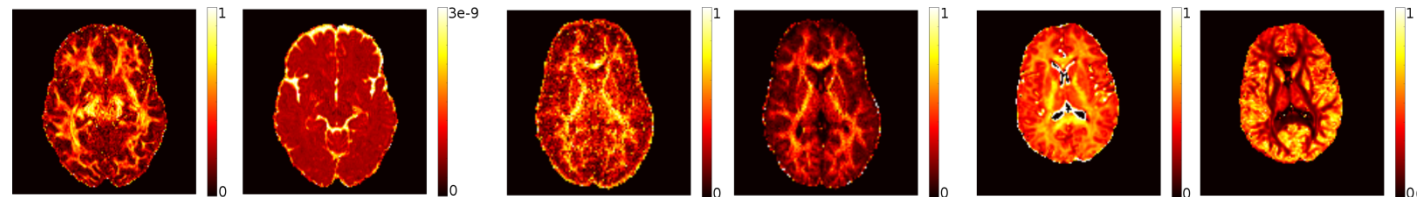


Fig. 3 (Left): DTI fit 1) fractional anisotropy (FA), 2) mean diffusivity (MD), (Middle): CHARMED fit 1) hindered FA, 2) restricted fraction (FR), (Right): NODDI fit, 1) neurite density index (NDI), 2) orientation dispersion index (ODI)

DISCUSSION: We present a GPU accelerated modular and extensible toolbox for diffusion microstructure modelling. The toolbox is open source, python scriptable and compatible with other packages, such as Camino, DiPy, BrainVoyager and FSL. Due to its speed and flexibility this toolkit is highly useful for the model developer in prototyping and testing models. Moreover, its speed is essential in large group or population studies where one needs to process tens to thousands of datasets. Finally, due to the modular and object oriented structure of the toolkit all routines can easily be extended to accommodate computations for different modalities, for example light microscopy or genetics data. For availability of the toolkit, please email Robbert Harms (r.ohbert.harms@maastrichtuniversity.nl). The toolbox is expected to be publicly released Q1-2015.

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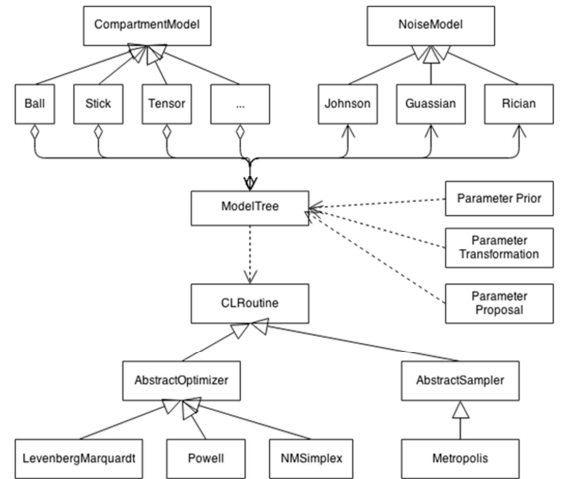


Fig. 1: The object oriented structure