Running MCs for NIH

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# Rotation and segmentation

## Rotation

* We use the *sub\_neurologicalHighRes.nii* files for each subject
* This first needs to be rotated so that it lands on close to an axial orientation for NIH – not true for Gates - Vince’s script does the final rotation after that.
* *MRI\_Rotate.sh* does this first rotation, but you need to change three things:
  1. The subject list
  2. The working directory
  3. The -rotate x y z amount. It can be negative to allow rotation the other direction.
* This will need to be done on an individual basis for all participants, then we can move to the next step.

## Segmentation

* We need to do this in two steps (for NIH) - one is to remove the background noise, the other is to strip the skull
* These can be run as a group
* Turn to the *MRI\_cleanup\_May18.sh* (in the same folder as *autoSegment20190428.sh*) – if running India Gates data the script just has step 6 in it, ignore the in-between ones.
  1. Subjects need to be put in the subject list
  2. Change the working directory
  3. First argument changes the step amount. We probably want step(a-350), but this can be adjusted if needed.
  4. The next two arguments shouldn’t need adjustment - they remove the outside noise, and create ${subj}\_final\_Masked.nii.
  5. We then multiply the image by itself. Check this with Sam - it should be necessary for all NIH kids where resolution is poorer, but this is not necessary for Gates phase 2.
  6. The last line then needs adjustment - shown below. Make sure the wd is correct, then there are two changes you can make: One is the 0.7 below can be adjusted up or down - this is the segmentation parameter. The other is you can add a -a at the end - this uses the other segmentation method (useful if the first one is leaving skull in).

autoSegment20190428.sh -t /Users/administrator/Desktop/test/${subj}\_enhanced.nii -o  
//Users/administrator/Desktop/test/${subj}/ -s 0.7 -c 3 -b -m

autoSegment20190428.sh -t /Users/administrator/Desktop/test/${subj}\_enhanced.nii -o  
//Users/administrator/Desktop/test/${subj}/ -s 0.6 -c 3 -b -m -a

* The end result of this should have no skull, and needs to be checked that it has not cut away part of the brain. Equally there needs to be padded skull all around the brain (although Vince’s script should take care of that). Check previous examples so you know what this means.

# Photon migration simulation preparation

## Individual anatomy

* Once segmented you need to open MATLAB, and navigate to the folder with all the segmented images for that one participant in. You do not need a NIRS or a digpts at this stage.
* Open *AtlasViewerGUI* (by typing the same into MATLAB)
* It will popup with a dialogue box - just hit close or cancel.
* When it opens AV, hit file -> import MRI anatomy
* By default, it should populate the fields - make sure hseg is with segmented head, WM is with white matter, brain is with grey matter, and CSF is with CSF.
* Hit import
* Once this is done, it will ask you to select reference points - hit yes
* These should be the same as for a digitization - NZ, IZ, CZ, LP, RP
* You *MUST* check during this step that the head is aligned with the cardinal left right as given. If not, the rotation and segmentation was not right.
* When this is done it will ask if you want the 10-20 EEG points, hit yes
* When this is done, you can close AV

## Move files

* If you already have an atlas or anatomical (ie template), start here.
* Make a new subfolder for the participant entitled *digitization*
* Copy the anatomical folder, the digpts, the NIRS file, and the HeliumScripts folder into there.
* Use the digpts from that session - if it doesn’t exist, use the template with the same capsize
* NIRS does not need to be from that subject, just the right number of sources/detectors. You need to check if this is right regarding short sources as well.

## Set up probes

* In MATLAB navigate to the digitization folder and open AV
* Go to tools -> register atlas to Digpoints
* Then at the bottom Register Probe to Surface
* Go to Forward model -> set MC Parameters
* Check scattering values with John before going ahead with defaults. These are found in the optical properties excel sheet and can be copied across for NIH and Gates. Change these to what’s specified in the right hand columns.
* Number of photons: 100000000 (thats *8* zeros - count them!)
* Forward model -> Generate MC Input
* Then cancel (don’t run locally on your computer)
* This gives fw …..inp files within the fw folder - check you have the right number
* IF you are running locally to test, you can say ‘file exists, try running now,’ and wait for it to finish. Once that is done you can move to complete steps, below.

# Running MCs

## Transfer files to HPC

* This is only relevant if running on the HPC. Make sure Homer2 versions on HPC match what you have on the computer.
* Copying folder from local destination to HPC, using your ID:

scp -r /Users/administrator/Desktop/sub1002  
taw15kfu@hpc.uea.ac.uk:/gpfs/home/taw15kfu/

* I would then advise using the linux to see them directly (open the HPC app, and hit files). If you prefer to do it remotely, you sign in with:

ssh -XY (id)

* After copying homer2 over, (if not there already - make sure version is the same as the setup computer), set permissions, this allows homer to access the tMCimg file for monte carlo:

chmod 700 /gpfs/home/taw15kfu/homer2/PACKAGES/tMCimg/bin/Linux/tMCimg

* You may also need to make the tMCimg first for the HPC

## Changing paths in files

* We have the fw folder and the HeliumScripts folder (again for HPC use).
* Make changes to the pathnames with the two files, and the subject lists (can do multiple).
* Every single inp file the path needs to be changed
* HeliumScripts folder will be there with all the bsub files
* Also in HeliumScripts, the bsub files need paths to the Headvol to be updated
* *change\_inp.sh* does this, use the backslash vs forward slashes to separate out words, and the second part tells you what each one gets replaced with
* *change\_bsub.sh* does the same thing for the bsub files
* Check that everything is right before proceeding
* If working remotely - use nano to see it in editor instead of bash
* Run these two scripts and check the output.

bash change\_bsub.sh

bash change\_inp.sh

## Running MC

* To run, first edit the subject list in *sub\_job.sh*

bash sub\_job.sh

* Check bjobs, if it has run suspiciously quickly then there is a problem
* Once it’s done, bjobs will show no active jobs
* Then we can transfer everything back to the local destination

## Move back and complete steps

* Once everything finishes, copy folder from HPC to local destination (reverse of the above):

scp -r taw15kfu@hpc.uea.ac.uk:/gpfs/home/taw15kfu/NIRS\_Project/  
/Users/administrator/Desktop

* Do the register atlas to digpts and register probe to surface again.
* After that, you need to cd to the *digitization/fw/* folder of that participant in the terminal and run the following (unless run locally):

touch \*

* This updates the files so they are modified recently. Without this it might say input is newer than output, and wipe the output, or ask you to rerun it.
* If you try to run with Forward model -> Generate MC Input, it will say there is already an input, so hit OK
* *IMPORTANT* if it says anything else hit cancel and check that the fw folder contains the new MC files
* Tick Forward model -> enable sensitivity matrix volume
* Then go to Forward model -> Generate load sensitivity profile
* These will take a while to load. It may ask if the head needs downsampling, if it asks, say yes, and accept the downsampled head.
* This generates a coloured picture which is your sensitivity profile
* Before closing, check that the *Adot* files are in the *digitization/fw* folder