fMRIPrep tutorial: A practical guide



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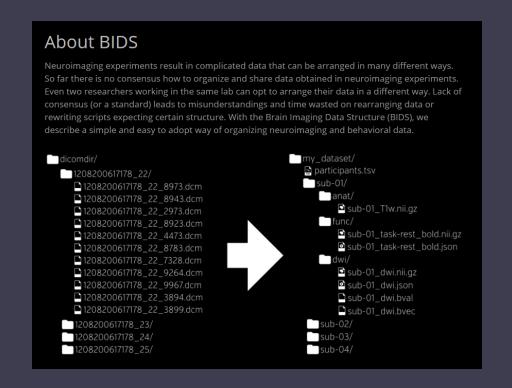
- 1 What is fMRIPrep, and what does it do
- 2 The inputs and outputs of fMRIPrep
- 3 Running fMRIPrep in a container (local)
- 4 Running fMRIPrep on HPC (Compute Canada)
- 5 Tips for running fMRIPrep on HPC
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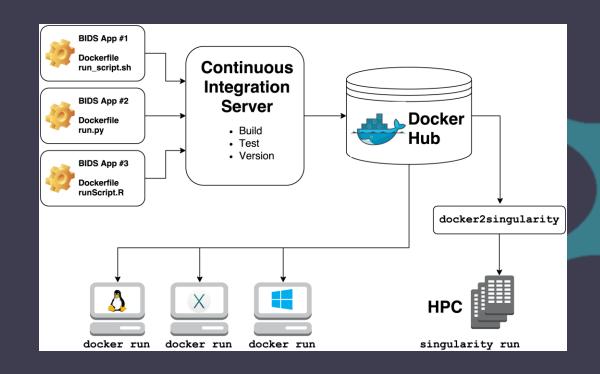




NI Processing: BIDS and BIDS App

BIDS is way of organizing NI data with community consensus.





https://bids.neuroimaging.io/

https://docs.google.com/document/d/1Wwc4A6Mow4ZPPszDIWfCUCRNstn7d_zzaWPcfcHmgl4/edit#heading=h.9146wuepclkt Gorgolewski KJ, et al. (2017). PLoS Comput Biol 13(3): e1005209. https://neuroimaging-core-docs.readthedocs.io/en/latest/pages/choropleths.html



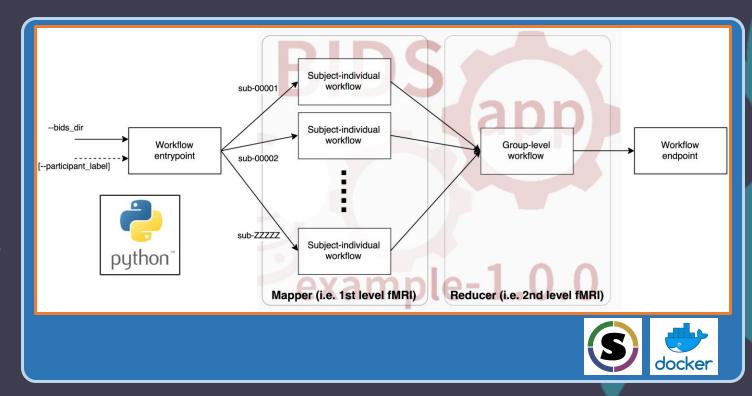


BIDS App: The basics

A BIDS App is a container image capturing a neuroimaging pipeline (most of the time, nipype wrapped) that takes a BIDS-formatted dataset as input.

Containers

- Docker: building, hosting and running containers locally (Windows, Mac OS X or Linux)
- Singularity: running containers on HPCs



Running a BIDS App

BIDS_App(container image) bids_dir(input) derivative_dir(output) \
group/participant(--participant_label xxx)(analysis_level) \
confs(configuration for the BIDS APP)

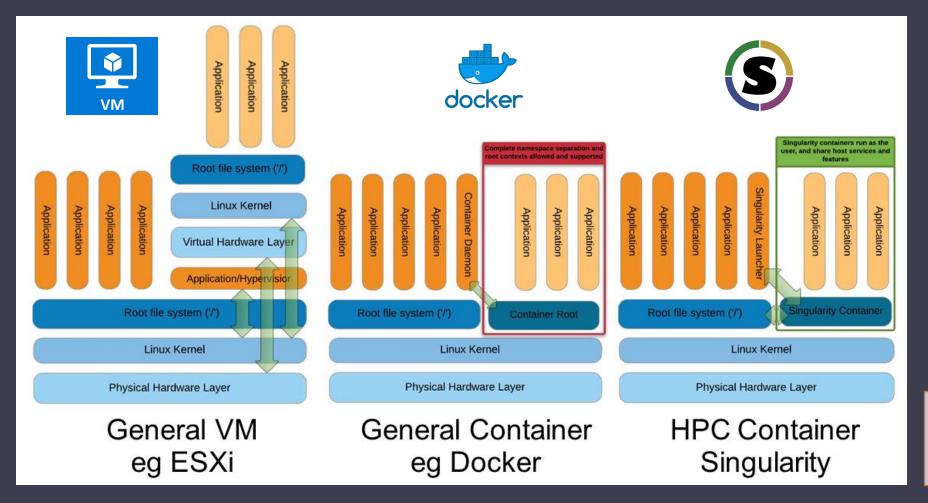
https://bids.neuroimaging.io/ https://github.com/BIDS-Apps

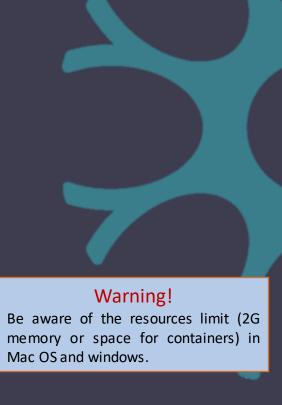
Gorgolewski KJ, et al. (2017). PLoS Comput Biol 13(3): e1005209.





Containers: A "vm" like wrapped-env for pipelines





https://tin6150.github.io/psg/blogger_container_hpc.html





Containers: Instead of installation and dependencies

Build containers (root needed)

- sudo docker pull poldracklab/fmriprep:latest
- sudo singularity build fmriprep_latest.simg docker://poldracklab/fmriprep:latest
- sudo docker build --no-cache -t your container name -f your dockerfile .



RUN a docker container

```
sudo docker run -it -p host_port:cont_port \
-v host_bids_dir:cont_bids_dir:ro \
-v host_derivates_dir:cont_derivates_dir \
... \
poldracklab/fmriprep:latest(docker_container:version)
\ cont_bids_dir cont_derivates_dir --participant_label
\ xxx (group) -w work dir(conf)
```

RUN a singularity container

```
singularity run --cleanenv
-B host_bids_dir:cont_bids_dir:ro \
-B host_derivates_dir:cont_derivates_dir \
... \
fmriprep_latest.simg (singularity container) \
cont_bids_dir cont_derivates_dir \
--participant_label xxx (group) -w work_dir(conf)
```

Solve the mounting point err

```
docker run -v /var/run/docker.sock:/var/run/docker.sock \
-v ~{HOME}/container_dir:/output \
--privileged -t --rm singularityware/docker2singularity -m
"container dir you need to add" container name
```

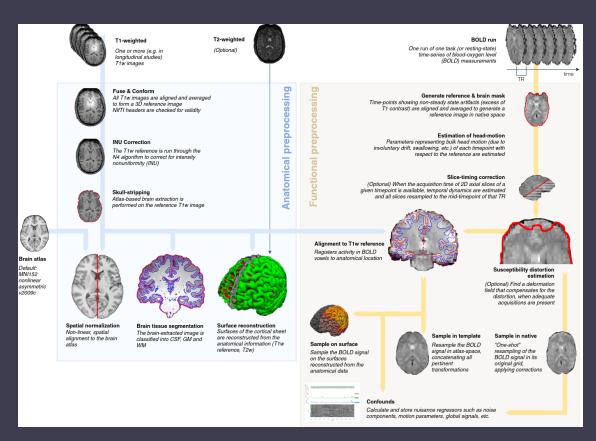
https://www.docker.com/ https://sylabs.io/singularity/ https://hub.docker.com/ https://github.com/singularityhub/docker2singularity

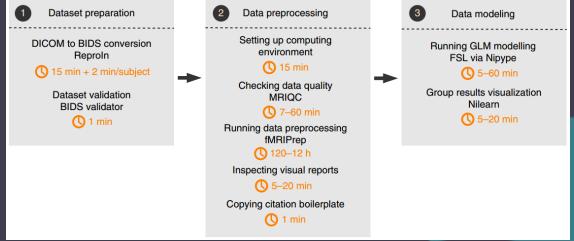




fMRIPrep: A BIDS App for robust anat & func MRI preprocessing

fMRIPrep is a containerized anat & func MRI preprocessing pipeline with the best tools for each step





- •<u>FSL</u> (version 5.0.9)
- •ANTs (version 2.2.0 NeuroDocker build)
- •<u>AFNI</u> (version Debian-16.2.07)
- •<u>C3D</u> (version 1.0.0)
- •<u>FreeSurfer</u> (version 6.0.1)
- •<u>ICA-AROMA</u> (commit e8d7a58, post v0.4.4-beta)
- •bids-validator (version 1.4.0)
- •connectome-workbench (version Debian-1.3.2)

Warning!

Very narrow FoV images and very special study groups (infants or non-human brains) are challenging for any standard pipeline including fMRIPrep.

https://fmriprep.org/en/stable/index.html https://github.com/poldracklab/fmriprep

Esteban, et al. (2019) *Nature Methods*, 1(16): 111–16. https://doi.org/10.1038/s41592-018-0235-4. Esteban, et al. (2020) *Nature Protocols*, 7(15): 2186–2202. https://doi.org/10.1038/s41596-020-0327-3.





fMRIPrep: Basic inputs

Standard BIDS App inputs:

```
input (bids_dir)
output (derivative_dir)
analysis_level (participant)
```

Filtering BIDS

```
--participant_label 001
--bids-filter-file ses-2.json
--skip_bids_validation
-t, --task-id rest
--anat-derivatives
```

Specific options for sub-modules

```
--anat-only --output-spaces <SPACE>[:cohort-
<label>][:res-<resolution>][...]
--fs-license-file --fs-subjects-dir --cifti-
output
--force-bbr --use-aroma --return-all-components
--skull-strip-template --skull-strip-tlw --use-
syn-sdc
```

Workflow and env confs

```
-w, --work-dir
--resource-monitor
-v/-vvv increase log and debug level
--nprocs, --omp-nthreads, --mem, --low-mem
```

Preprocessing task	Included with fMRIPrep	
Anatomical T1-weighted brain extraction	antsBrainExtraction.sh (ANTs)	
Anatomical surface reconstruction	recon-all (FreeSurfer)	
Head-motion estimation (and correction)	MCFLIRT (FSL)	
Susceptibility-derived distortion estimation (and unwarping)	3dqwarp (AFNI)	
Slice-timing correction	3dTshift (AFNI)	
Intrasubject registration	bbregister (FreeSurfer), FLIRT (FSL)	
Spatial normalization (intersubject co-registration)	antsRegistration (ANTs)	
Surface sampling	mri_vol2surf (FreeSurfer)	
Subspace projection denoising (e.g., independent or principal component analysis)	MELODIC (FSL), ICA-AROMA	
Confounds	In-house implementation	
Detection of non-steady states	In-house implementation	

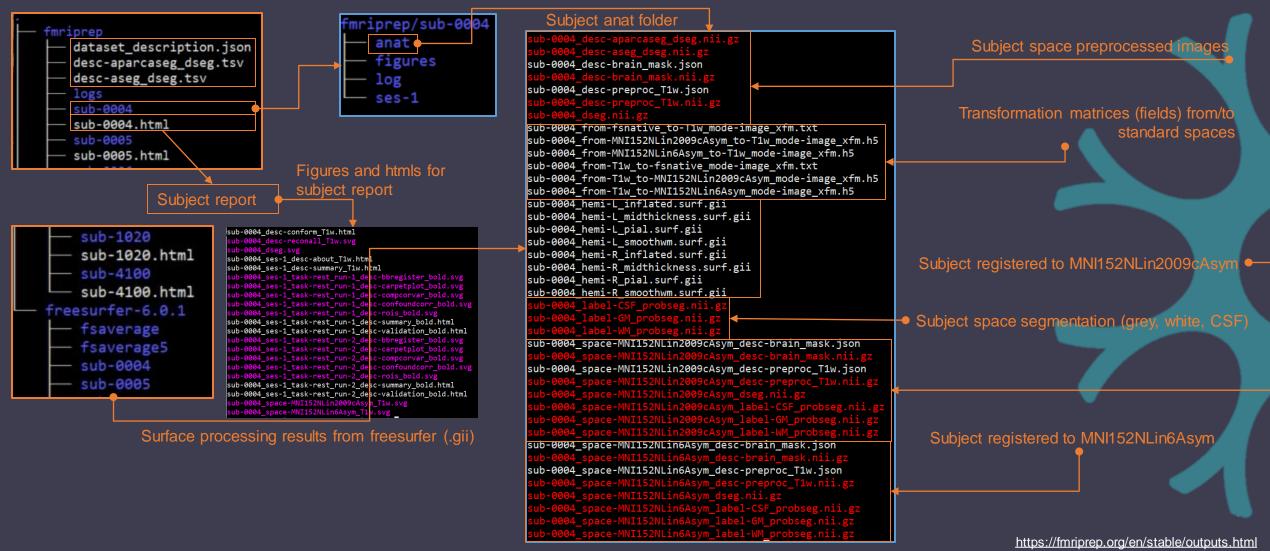
https://fmriprep.org/en/stable/usage.html

Esteban, et al. (2019) *Nature Methods*, 1(16): 111–16. https://doi.org/10.1038/s41592-018-0235-4. Esteban, et al. (2020) *Nature Protocols*, 7(15): 2186–2202. https://doi.org/10.1038/s41596-020-0327-3.





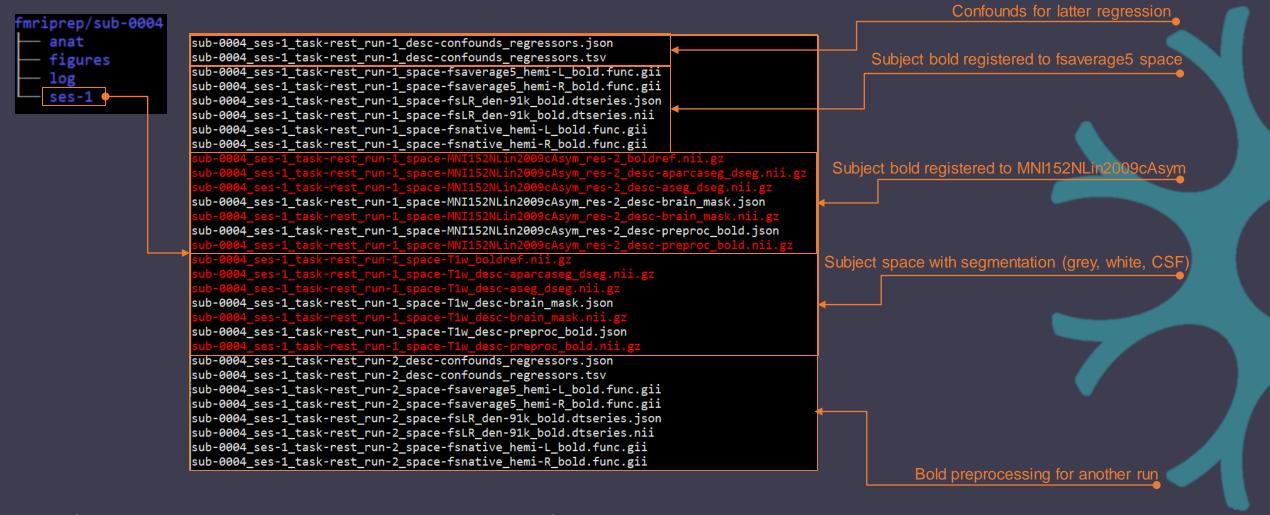
fMRIPrep: Basic outputs (anat)







fMRIPrep: Basic outputs (func)



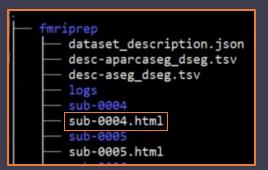
Confounds (or nuisance regressors) are variables representing fluctuations with a potential non-neuronal origin.

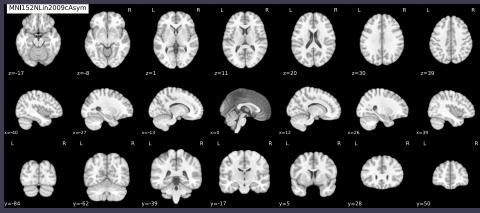
https://fmriprep.org/en/stable/outputs.html

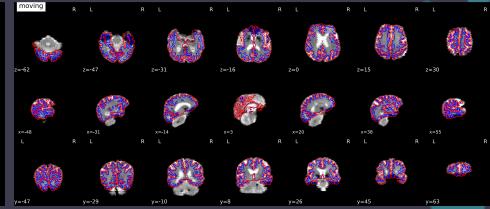




fMRIPrep: Basic outputs (report)







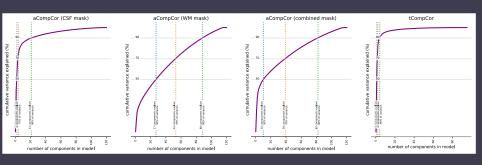
Summary

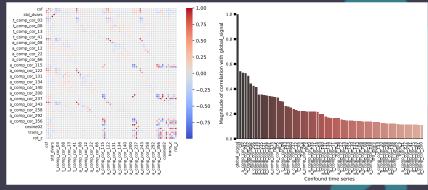
- Subject ID: 0004
- Structural images: 1 T1-weighted (+ 1 T2-weighted)
- Functional series: 2
 - Task: rest (2 runs)
- Standard output spaces: MNI152NLin2009cAsym, fsaverage, MNI152NLin6Asym
- Non-standard output spaces: anat, fsnative
- FreeSurfer reconstruction: Run by fMRIPrep

Anatomical

Anatomical Conformation

- Input T1w images: 1
- Output orientation: RAS
- Output dimensions: 192x256x256
- Output voxel size: 1mm x 1mm x 1mm
- Discarded images: 0





https://fmriprep.org/en/stable/outputs.html





fMRIPrep: working with local container

Warning!

If you have only limited number of subjects, running fMRIPrep locally might be a good idea, or if you would like to investigate the container. I ran MRIQC locally more often.

```
Create out and temporal dir
                           fmriprep.sh
#!/bin/bash
mkdir -p data_fmriprep_20.1.1
mkdir -p data fmriprep work
                                            To be safe with container path
echo "" > data_fmriprep.log
echo "Start fmriprep QC..."
unset PYTHONPATH
singularity run -B $HOME:/home/fmriprep --home/home/mrigc --cleanenv
    -B ${HOME}/project/data BIDS:/data:ro\
     -B ${HOME}/project/data_fmriprep_20.1.1:/out
     -B ${HOME}/project/data_fmriprep_work:/work\
     -B ${CODE_DIR}:/codes\
    -B ${HOME}/project/templateflow:/templateflow\
     -B ${LOCAL_FREESURFER_DIR}:/fsdir\
     ${HOME}/container_images/fmriprep_v20.1.1.simg/data/out
participant --participant-label sub-0002 -w /work --output-spaces \
MNI152NLin2009cAsym:res-2 anat fsnative fsaverage5 --bids-filter-file \
/codes/ses-1.json --fs-subjects-dir/fsdir\
--fs-license-file/home/fmriprep/.freesurfer/license.txt\
--cifti-out 91k --return-all-components --write-graph \
```

```
#!/bin/bash
mkdir -p data_mriqc_0.15.2
mkdir -p data_mriqc_work
echo "" > PD_mrigc.log
echo "Start group N participants QC..."
unset PYTHONPATH
singularity run -B $HOME:/home/mrigc --home /home/mrigc --cleanenv
    -B ${HOME}/project/data_BIDS:/data:ro \
    -B ${HOME}/project/data_mrigc_0.15.2:/out \
    -B ${HOME}/project/data_mrigc_work:/mrigc_work \
    -B ${HOME}/project/templateflow:/templateflow \
    ${HOME}/container_images/mriqc_v0.15.2.simg /data /out participant
    --participant-label sub-0002 ... sub-1020 -w /mrigc
echo "Start group QC..."
singularity run -B $HOME:/home/mriqc --home /home/mriqc --cleanenv \
    -B ${HOME}/project/data_BIDS:/data:ro \
    -B ${HOME}/project/data mrigc 0.15.2:/out \
    -B ${HOME}/project/data_mriqc_work:/mriqc_work \
    -B ${HOME}/project/templateflow:/templateflow \
    ${HOME}/container_images/mriqc_v0.15.2.simg /data /out group
    -w /mrigc work --verbose-reports
```



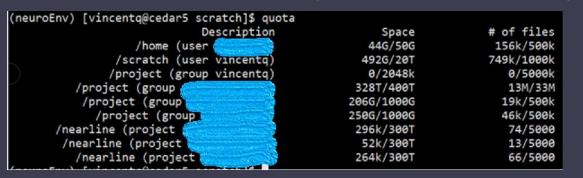


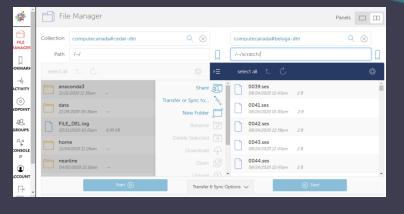
mriqc.sh

fMRIPrep: HPC Basics (Compute Canada)

Things you need to get ready before running codes (containers) on HPC

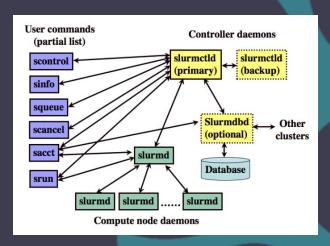
- 1. An account for HPC (Refer to Lex's pinned document in slack channel #uk_biobank);
- 2. The document for HPC, Compute Canada docs: https://docs.computecanada.ca/wiki/Getting_started
- 3. Cluster management and job scheduling system docs (SLURM for Compute Canada), https://slurm.schedmd.com/documentation.html,
- 4. Get ssh client ready for remote terminal (ssh for linux, Bitvise SSH Client for Win...);
- 5. Get Globus ready for data transportation, https://globus.computecanada.ca/, ftp tool is ok for small files;
- 6. Get your data, codes and containers ready uploaded on HPC.
- Tip1: Use quota to make sure you have enough space/N_files for your computation.
- Tip2: scratch is the place where you should have all your computation.
- Tip3: sq/scancel to check the job status and cancel job.





Warning!

Always use Globus for data transportation, especially inter-cluster data transportation, it is faster and safer.









fMRIPrep: running on HPC (Compute Canada), preparation

fmriprep.sh

```
#!/bin/bash
DATA NAME= (${@:1:1})
echo ${DATA NAME}
WD DIR=${HOME}/scratch
DATA DIR=${WD DIR}/${DA<u>TA NAME}</u>
BIDS DIR=${DATA DIR} BIDS
CODE DIR=${WD DIR}/src
CODE SLURM=${CODE DIR}/fmriprep.slurm
CODE COLLECT=${CODE DIR}/fmriprep.format
SUB LIST=${CODE DIR}/${DATA NAME} fmriprep preopt.list
CON IMG DIR=$ {WD DIR}/container images/fmriprep v20.1.
OUT DIR=${DATA DIR} fmriprep anat 20.1.1
LOG DIR=${DATA DIR} fmriprep anat.log
SLURM LOG DIR=${DATA DIR} fmriprep anat slurm log
WORK DIR=${DATA DIR} fmriprep anat work
FREESURFER LICENSE="${WD DIR}/container images"
TEMPLATEFLOW HOST HOME=$HOME/scratch/templateflow
RUN ID=$(tail -c 9 ${LOG DIR})
if [ -z $RUN ID ]; then
 echo 'no previous run found...'
  echo "previous run $RUN ID found, deleting logs..."
  rm fmriprep vince-${RUN ID}*.out
  rm fmriprep vince-${RUN ID}*.err
rm -rf ${OUT DIR}
rm -rf res/${OUT DIR}.tar.gz
rm -rf res/${OUT DIR} freesurfer.tar.gz
rm -rf ${WORK DIR}
rm -rf ${SLURM LOG DIRDIR}
rm -rf res/${SLURM LOG DIR}.tar.gz
rm -rf ${SUB LIST}
```

```
chmod +x ${CODE SLURM}
chmod +x ${CODE COLLECT}
awk -F"\t" '{print $1}' ${BIDS DIR}/participants.tsv >> ${SUB LIST}
sed -i '1d' ${SUB LIST}
echo "Step1: subjects list created!"
mkdir -p ${OUT DIR}
                                                      Submit to cluster •-
mkdir -p ${WORK DIR}
mkdir -p ${SLURM LOG DIR}
if [ -d ${TEMPLATEFLOW HOST HOME} ]; then
     echo "Templateflow dir already exists!"
    mkdir -p ${TEMPLATEFLOW HOST HOME}
    python -c "from templateflow import api; api.get('MNI152NLin2009cAsym')"
    python -c "from templateflow import api; api.get('OASIS30ANTs')"
echo "Step2: starting fmriprep!"
sbatch ${CODE SLURM} ${DATA NAME} ${CON IMG DIR} >> ${LOG DIR}
```

```
fmriprep_anat.format
fmriprep_anat.sh
fmriprep_anat.slurm
pre_opt.json
```

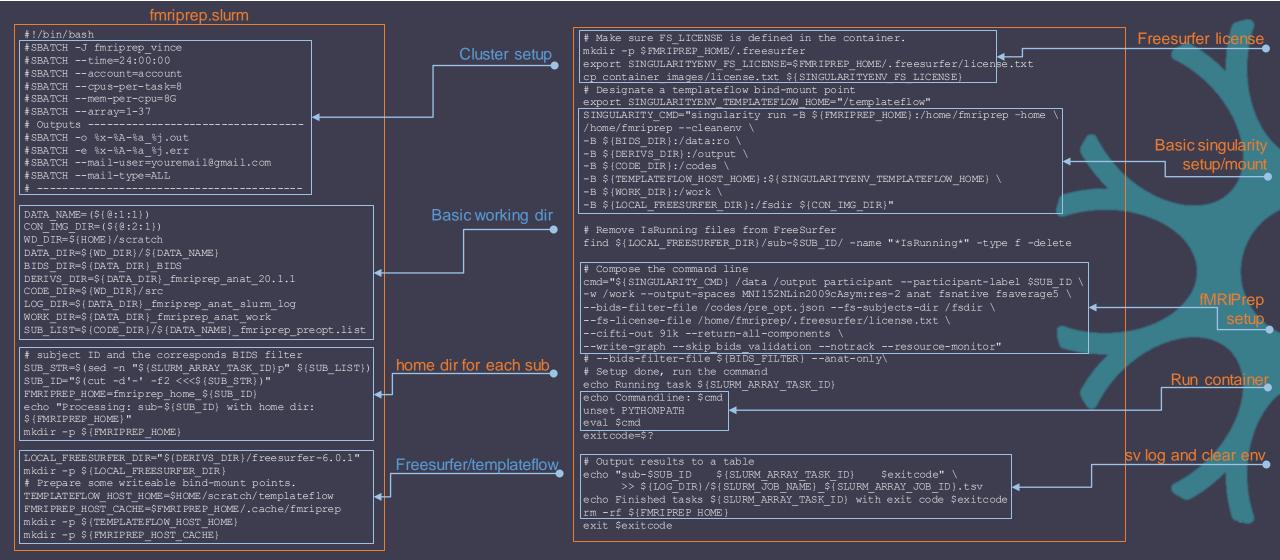
```
fmriprep.format
```

```
#!/bin/bash
DATA NAME= (${@:1:1})
echo ${DATA NAME}
WD DIR=${HOME}/scratch
DATA DIR=${WD DIR}/${DATA NAME}
BIDS DIR=${DATA DIR} BIDS
FMRIPREP VER=20.1.1
DERIVS DIR NAME=${DATA NAME} fmriprep anat ${FMRIPREP VER}
LOG DIR NAME=${DATA NAME} fmriprep anat slurm log
RUN ID=$(tail -c 9 ${DATA NAME} fmriprep anat.log)
mv fmriprep vince-${RUN ID}*.out ${LOG DIR NAME}
mv fmriprep vince-${RUN ID}*.err ${LOG DIR NAME}
#2 collect output
tar -czvf res/${DERIVS DIR NAME}.tar.gz ${DERIVS DIR NAME}/fmriprep
tar -czvf res/${DERIVS DIR NAME} freesurfer.tar.gz
${DERIVS DIR NAME}/freesurfer-6.0.1
tar -czvf res/${LOG DIR NAME}.tar.gz ${LOG DIR NAME}
echo "Step5: fmriprep for ${DATA NAME} Finished"
```





fMRIPrep: running on HPC (Compute Canada), the core script







fMRIPrep: running on HPC (Compute Canada), debug

Tip1: Check the %x-%A-%a_%j.out and %x-%A-%a_%j.err to locate the err subject.

Tip2: Go to the DERIVS_DIR/fmriprep/sub-xxxx/log/xxx/fmriprep.toml, and check the log.

Tip3: Go to the fmriprep_work(-w)/fmriprep_wf/single_subject_xxxx_wf, and check the intermediate results with nipypecli crash *.pklz (use the same container and singularity shell).

Tip4: Do a google search and NeuroStars (QA) search.

Tip5: If the problem is still there, just create a new topic with details on NeuroStars or GitHub (@the developer©).

Tip6: Do not forget our #tech-support slack channel ©

```
fmriprep.toml
```

```
[environment] cpu_count = 32
exec_env = "singularity"...
[execution] bids_dir = "/data"...
[workflow] anat_only = false...
[nipype] crashfile_format = "txt"
[seeds] master = 38259...
[execution.bids_filters.tlw]
datatype = "anat"session = "1"
suffix = "T1w"
[execution.bids_filters.bold]
datatype = "func"session = "1"
suffix = "bold"
```

```
_0xe000825ec954f000118ce7296b101b1f.json
        _inputs.pklz
        _node.pklz
        0x0bf71f52b03348f41e67cbbf949c0d6a.json
        inputs.pklz
       _node.pklz
       result_bids_info.pklz
       _0xf83ac98772fabd74cc5ef03c346ecb62.json
       inputs.pklz
       _node.pklz
       result_bidssrc.pklz
        _0xab0de7181360e73d41dda7c2614bc0e1.json
        inputs.pklz
       _node.pklz
       result_ds_report_about.pklz
        _0xa28236e158d9b1a781e7869a00d87e3a.json
       _inputs.pklz
       _node.pklz
       result_ds_report_summary.pklz
       _0xa4a7cc12363b7769849f036835460b64.json
        inputs.pklz
       _node.pklz
       report.html
       result summary.pklz
23 directories, 26 files
```





fMRIPrep: tips for fMRIPrep usage

Tip1: Pre-download the template with templateflow.

python -c "from templateflow import api; api.get('MNI152NLin2009cAsym')"

Tip2: Running quality control (MRIQC) before running fMRIPrep.

I have not solved the synchronization problem on HPC and only took 1 day for about 40 subjects on a local machine (6core, 24G RAM)

Tip3: Skip part of the preprocessing if needed.

```
--skip bids validation --force-no-bbr --skull-strip-t1w skip --fs-no-reconall
```

Tip4: Resources allocation: use batch conf instead of fmriprep conf when running on HPC. recommendation for resources

Tip5: Be careful when you have dramatic anatomical changes between sessions from subjects.

fMRIPrep always assumes that the anatomy won't change between sessions and will estimate a robust anatomical template for a subject from different sessions. This assumption does not hold for pre-and-post operation sessions. However, the brain mask and anatomical registration still work perfectly well for small lesions (ultrasonic thalamotomy).





More resources

- OGs
 - fMRIPrep home page
 - fMRIPrep GitHub
 - BIDS, BIDS App GitHub, BIDS Derivatives
 - NeuroStars (QA)
 - Compute Canada document:
- Tutorials
 - Stanford tutorial
 - Andrew (Jahn)'s Brain Book (with YouTube video)
 - Using fMRIPrep for fMRI data preprocessing by Gelana Tostaeva
 - <u>DartBrains course chapter</u> by Sasha Brietzke & Luke Chang
 - Tutorial: BIDS, fMRIPrep, MRIQC by Saren Seeley
 - Brainlife tutorials
 - <u>Neuroimaging Core Documentation</u> by Dianne Patterson







Thanks



