





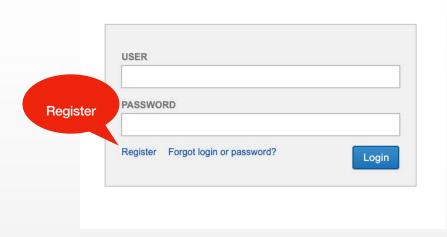


XNAT CLUSTER AWS

The MRI Research program provides NYSPI users the framework to preprocess supported fMRI, DTI, and anatomical data. This is a tutorial on how to access and utilize the resources.

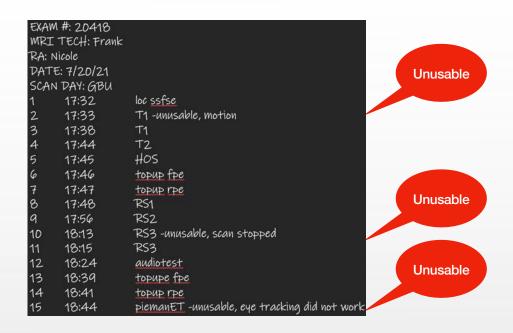
- XNAT stores the raw DICOM images acquired during a scan. XNAT can also convert raw MRI data into BIDS format and provide mriqc outputs through the XNAT webpage.
- The cluster can be accessed through a terminal and provides a program which pulls all BIDS data and supported non-BIDS data from XNAT and validates those data for processing pipelines.
- AWS is accessed though a website that launches the available processing pipelines to process the validated BIDS data.

XNAT account creation



- XNAT accounts are created by visiting
 https://xnat.nyspi.org/ and registering for an account.
- For access to a protocol to be granted, the user must email the PI of the study, cc'ing <u>Matthew.Riddle@nyspi.columbia.edu</u> requesting access to the protocol on XNAT.

Taking Notes at Scan Time



- It is crucial to take notes during the acquisition of MR data.
- Each MR scan has an associated and unique exam number that is created by the MR console.

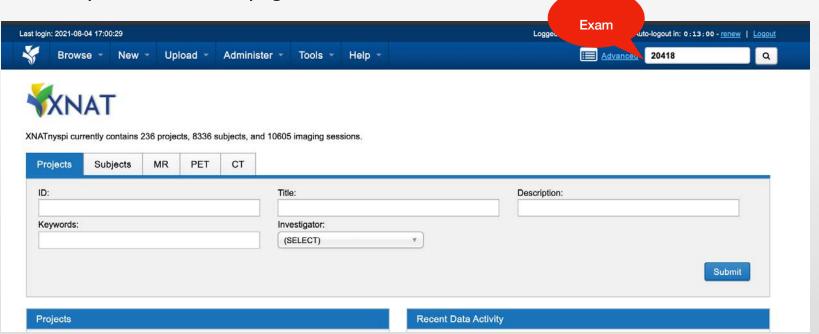
These notes should include:

- date
- exam number in addition each series should be noted. In the above example, Series 2, Series 10, and Series 15 are unusable. If the data going into processing pipelines is bad it could lead to errors in processing or bad data coming out.

XNAT Interface

- Once you have your notes and your exam number, we can now find and update your exam on XNAT. There are many ways to navigate on the XNAT website. The easiest way to find your data is by using your exam number.
- Data is automatically transferred to XNAT from the MRI console within 2 days of acquisition.

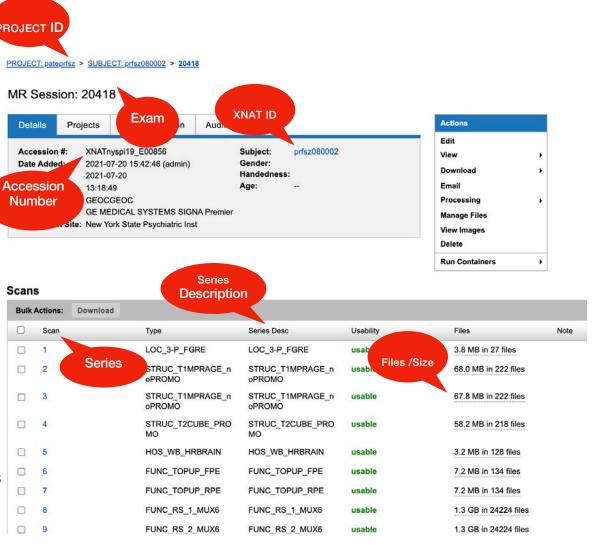
 Enter the exam number into the search bar on XNAT to go to your MR Session page



XNAT Session Page

Before using the XNAT interface to qc download or proceed with data flow, it is important to familiarize yourself with the following XNAT terms.

- XNAT ID
 - Provided to MRI operator via Metal Screener.
 - Must be BIDS formatted (no special characters or spaces)
- XNAT PROJECT ID
 - Shorthand project ID automatically assigned in XNAT
- EXAM number
 - Unique session ID automatically assigned by scanner
- ACCESSSION ID
 - Unique session ID automatically assigned by scanner
- SERIES / SERIES DESCRIPTION
 - Each exam is comprised of several Series, determined in the protocol for each project. Each Series has a Series Description assigned by Feng.
- FILES / SIZE
 - The number of files and their size should be the same for each series type.



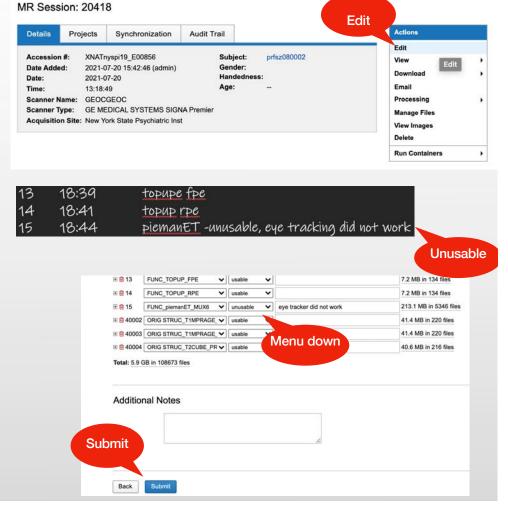
XNAT Series Usability

PROJECT: pateprfsz > SUBJECT: prfsz080002 > 20418

- The first step in managing your data on XNAT is to indicate which Series, if any, are unusable so that they may be excluded from data flow.
- IMPORTANT: Verify that your subject ID is COMPLETELY accurate in XNAT and that your exam is in the correct XNAT project. DO NOT continue if either of these are incorrect, contact Matt Riddle:

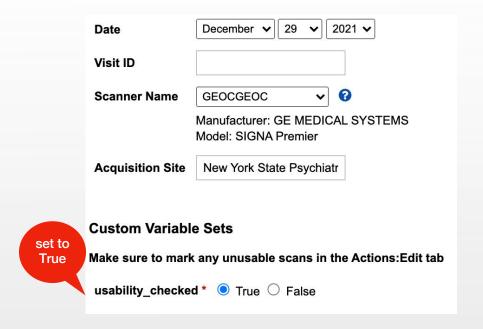
Matthew.Riddle@nyspi.columbia.edu

- From The MR Session page select the Edit tab.
- For example, from the Scan notes, it is clear that Series 15 needs to be marked as unusable
- Select unusable from the dropdown menu for Series 15 and fill in any notes.



XNAT Series Usability cont.

- IMPORTANT: Once you are done confirming the usability of each series and marking any unusable series as "unusable", you need to set the "usability_checked" variable to "True" for the exam session.
- This step MUST be done whether the exam is all usable series or has any unusable series.
- Marking this variable "True" will flag the exam as being ready for further processing in the supported pipelines.
- To do this, find the radio button for the "usability_checked" variable on the Edit page and be sure it is set to True, and finally hit Submit at the bottom of the page.



XNAT Series Usability cont.

In addition to the hardware failure indicated in the previous example of usability, there are other factor which may cause a series to be deemed unusable.

- 1. If the subject had to go to the bathroom and interrupted a Series
- 2. If the MR tech had to restart a Series (they should always indicate this)
- 3. If the Head Movement was severe
- 4. If the reconstruction of the Series failed (Hardware)

TIPS!

- It is important to check that the size of the series is consistent and accurate. The same Series will usually have the same number of files and total size from run to run, as seen on the right of the XNAT session page.
- It is often helpful if the person who ran the scan and collected the MRI data also does the usability check on XNAT!
- Being mindful of recording these Series errors is crucial for avoiding problems with data flow.

XNAT BIDS and mriqc

The XNAT platform has the ability to produce BIDS and run mriqc.

- This must be requested for each protocol by sending an email to <u>Juan.Sanchez@nyspi.columbia.edu</u> cc'ing the protocol PI.
- BIDS data are automatically generated from XNAT exam sessions that have had their series Usability Checks completed and the XNAT variable "usability_checked" marked "True" in the XNAT session page. Data will usually process within a few hours of being marked depending on system utilization.
- Once the BIDS data has been generated, you will be able to run mriqc on the exam session.

Introduction to mriqc

Quality control of MRI data

Here, we propose MRIQC for the assessment of the acquired (unprocessed) data. We also recommend specifying clear exclusion criteria before assessment. To our knowledge, there is no consensus on a data curation protocol; laboratories currently address the problem by applying their internal know-how and subjective assessments, or by skipping the data-curation step altogether. An ultimate curation protocol remains the subject of active discussion in the field. Describing such a protocol to check the quality of unprocessed data is beyond the scope of this article.

https://www.nature.com/articles/s41596-020-0327-3

XNAT mriqc usage

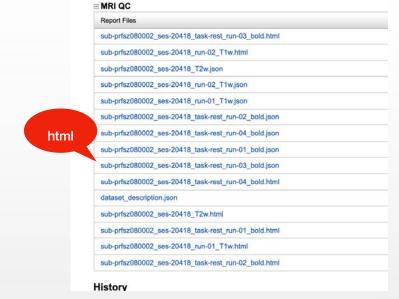
After XNAT generates BIDS data for your session, you may run mriqc.

- 1. From the Session page, select the Run Containers Tab.
- 2. ONLY AFTER dcm2bids completes can you launch mriqc.
- 3. You will receive email confirmation once mriqc completes (up to an hour).



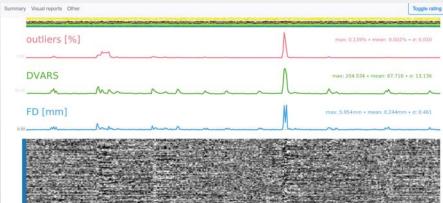
XNAT mriqc usage cont.

 After MRIQC is run you will be able to access the outputs as html files on the MR Session Page





- Mriqc provides Visual reports for anatomy
- Mriqc provides FD DVARS and visual reports for BOLD



Running XNAT BIDS Manually

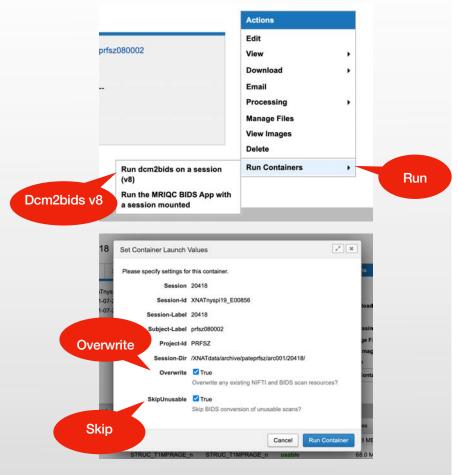
Running the XNAT BIDS pipeline on a session manually is supported in circumstances where BIDS data needs to be

corrected

1. From the Session page, select the Run Containers Tab.

- 2. IMPORTANT: Only run one exam through the BIDS pipeline at a time in order to limit resource utilization on the XNAT system.
- 3. Select "dcm2bids" v8:
 - Once selected make sure to select Skip Unusable and Overwrite, unless you don't need to reconvert existing bids data.
- 4. You will receive email confirmation once dcm2bids completes (up to an hour).
- 5. NOTE: If you are NOT an "owner" for the project, please contact Juan or David to rerun dcm2bids on a session for you as you will not have permissions to update the session information.

David.Semanek@nyspi.columbia.edu



Preparing your data for post processing on the CLUSTER

Once your data has been stored, marked useable and unusable, and converted to BIDS format on XNAT, The MRI computing cluster will provide the infrastructure for preparing your data for pre-processing.

- Pulling all BIDS data from XNAT and creating a BIDS-compliant, "rawdata" folder structure
- Editing the json sidecars for proper use of FieldMaps
- Editing multi volume field map acquisitions
- Validating BIDS data
- Pulling some non-BIDS data from XNAT to the cluster

*The cluster refers to the array of different computers that work together to allow for parallel processing and is accessed though a single managing computer called "the doctor"

CLUSTER account creation and access

```
SSH juan—juan@doctor:~—ssh juan@10.20.193.112—80×24

Last login: Wed May 13 09.26:19 on ttys002

[juan@Juans-MacBook-Pro ~ % ssh juan@10.20.193.112

[juan@10.20.193.112's password:

Last login: Wed May 13 12:29:19 2020 from 192.168.12.197

[juan@doctor ~]$
```

- CLUSTER accounts are created by emailing Juan.Sanchez@nyspi.columbia.edu
- Once your account has been created you will have a username and password associated with your "cluster account"
- To access the cluster from your computer open terminal and ssh into "the doctor" (ip 10.20.193.112) using your username and password.
- A basic knowledge of terminal is needed to navigate the cluster as there is no graphical user interface available.
 - https://www.youtube.com/watch?v=BMGixkvJ-6w
- A basic knowledge of vi is needed to manage text files
 - https://www.youtube.com/watch?v=HMpB28l1sLc

BIDS Directory Structure on cluster

 Once you have access to the protocol, you can navigate to your project's home directory.

[juan@doctor ~]\$ cd /MRI_DATA/nyspi/xnatprojectname

- The project name can be found on the MR Session page
- IMPORTANT: Do not create any new, arbitrary folders within a BIDS directory as this can disrupt the supported pipelines!
- The directory structure on the cluster is in BIDS format and will have no MR data (yet).
 - rawdata will be the destination for all BIDS data pulled from XNAT.
 - derivatives will be the destination for all post processing outputs and non-BIDS compliant data.
 - Abcd, neuromelanin, fmriprep, ciftify ... etc
 - scripts will be the location of the xnatproject_working.lst file, which you will populate with the XNAT exam numbers for the data you wish you pull to the cluster.

BIDS SPEC explanations

https://bids-specification.readthedocs.io/en/stable/01-introduction.html

https://bids-specification.readthedocs.io/en/stable/02-common-principles.html#source-vs-raw-vs-derived-data

Using the sub-xgrab program to prepare data for post processing

- BIDS data downloading and preparation is performed through the sub-xgrab program on the cluster.
- Before running the program, it is necessary to populate the xnatproject_working.lst for any subjects that need to be prepped.
- The program reads the xnatproject_working.lst present in the "scripts" directory list which the user populates in vi using data from XNAT.

/MRI_DATA/nyspi/patensasc/scripts/patensasc_working.lst

```
20286
20071
20185
20218
20126
```

- Each row on this list will represent a single subject session that needs to be prepped.
- The only information needed for sub-xgrab to find the data on XNAT is the unique exam number for the session.

Running the sub-xgrab program

- Now that the xnatproject_working.lst list is populated we can use the sub-xgrab program, which will run on all sessions in the list.
- The program is accessed through terminal and can be run from any location on the doctor:

```
[semanekD@doctor ~]$ sub-xgrab -d department -p project_id -a arguments -u username_for_xnat
```

- In order to use the program, 4 arguments must be passed after the above command
 - -d directory in MRI_DATA where your project lives (if acquired at NYSPI, -d will always be nyspi)
 - -p the XNAT project name
 - -a the arguments that you want to run to prepare your data
 - -u vour XNAT username

 While -d and -p will always be the same for your project, -a can be any of these options

sub-xgrab arguments for BIDS data converted on XNAT

You can input any of the single three arguments to run on the exams in the working list. You can also combine them.

-a pull

 Downloads converted BIDS data from XNAT to "rawdata". This argument by itself will release the terminal and run in the background so you can continue to use your SSH session. It's best for situations where you are pulling several exams from XNAT as this step takes some time to run. Logs can be checked using sub-xmanage (more on this in the next slide).

• -a split

 Edits multivolume field maps if applicable, produces two field map series for each multivolume field map, with the data from each encoding direction in a separate series.
 This argument runs quickly, even on multiple exams, in the foreground of the terminal and prints its log information in the terminal's normal outputs.

-a intend

• Populates fieldmap json sidecars with information linking them to their corresponding bold data. This argument runs quickly, even on multiple exams, in the foreground of the terminal and prints its log information in the terminal's normal outputs.

-a check

• Runs a check of sessions in the working list against session folders in rawdata. The script will report any missing sessions or confirm all sessions exist in rawdata. This is useful if you have pulled many sessions and want to confirm they have all transferred, or if split or intend report a missing session and you want to find if there are any other sessions missing. You can also put all your session numbers for your project in your working list and run a comprehensive report of what sessions are available on the cluster.

Combinations

- -a pulltosplit
- -a pulltointend (unlike "pull" by itself, the combined commands will run in the foreground of the terminal, and could take fair amount of time if you are pulling multiple exams)
- -a splittointend

Managing sub-xgrab workflows with sub-xmanage

- When submitting jobs that include the -a pull argument, you can check on the progress and troubleshoot any errors from the logs by using sub-xmanage.
- In this example we ran the following command:
 sub-xgrab -d nyspi -p spanint -a pull -u semanekD
- You can check on the progress and see the output by typing the following in the terminal from any location: sub-xmanage.
- After entering this command, you will see the following screen. NOTE: You MUST use sub-xmanage to remove your sub-xgrab job after it is done as the cluster only allows one job per user on the system (you may of course run multiple exams from the same XNAT project in a single job).
- You will see the Active status replaced with Inactive when the sub-xgrab program has completed.
- If you need to troubleshoot any errors, you can look at the log files by typing 1.
- Make sure to
 Remove the
 job once
 completed by
 entering 3!

Job status

```
CURRENT ACTIVE & INACTIVE XGRAB JOBS FOR USER semanekD

Status Job Name
Active --> sub-xgrab_semanekD

Available management options:

1) Check xgrab Log 3) Remove xgrab Job 5) Exit
2) Save xgrab Log 4) Refresh
(Press Ctrl+C to abort)

Select an option:
```

BIDS validation and data correction

- Once the data are prepped, they must be validated.
- All subjects/exams in "rawdata" will be validated regardless of who is in the working list.
- To validate your data run the following command in the terminal from any location: validate xnatprojectname

```
[semanekD@doctor ~]$ validate spanint
          bids-validator@1.8.9
          bids-specification@disable
          (node:1) Warning: Closing directory handle on garbage collection
WOO HOO!
          (Use `node --trace-warnings ...` to show where the warning was created)
          This dataset appears to be BIDS compatible.
                  Summary:
                                          Available Tasks:
                                                                   Available Modalities:
                  46 Files, 2.41GB
                                          FUNC MUX6 GNG
                                                                   MRI
                  2 - Subjects
                                          FUNC MUX6 Resting
                  2 - Sessions
                                          FUNC MUX6 SST
                  If you have any questions, please post on https://neurostars.org/tags/bids.
```

• If the BIDS subject ID for a session needs to be changed, we offer subxfix_modbidsid with the following usage:

sub-xfix_modbidsid [-d department -p project_id -s BIDS_session_number -n new_ID]

sub-xgrab and non-BIDS compatible DICOM data

sub-xgrab can pull some supported DICOM-only data from XNAT for data that cannot be converted to BIDS using the XNAT tool. Currently, the cluster supports the pulling of neuromelanin series using the following argument:

• -a nm

 Downloads neuromelanin DICOM data for exams on the working list (in the "scripts" folder) from XNAT to the /derivatives/neuromelanin folder in your project folder on the cluster in "{exam_number}_{series_number}.tar.gz" format. This argument by itself will release the terminal and run in the background so you can continue to use your SSH session. Logs can be checked, and jobs managed using sub-xmanage, the same as for -a pull, and only one job can be run at a time. Please remove your job after it completes.

Managing Your Saved XNAT Password

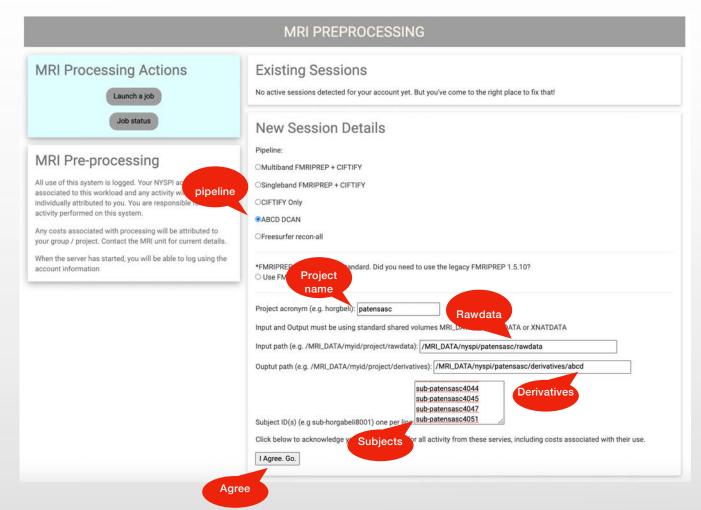
If your XNAT password changes or the logs report an issue connecting to XNAT and you know your account is active and XNAT is reachable, you can reset your own XNAT password on the cluster. The pipeline securely stores your password in an encrypted file that is accessible to the user who owns it. Once removed, sub-xgrab will ask you again to enter your XNAT password. You can run the following command to reset your password:

Post Processing in AWS

- Once you have your account and you have validated all of your raw data you are now ready to run the post processing pipelines by accessing http://mrijob.nyspi.local
- Choose between fmriprep/ciftify , abcd or freesurfer7
- Please be sure to consult with Gaurav.Patel@nyspi.columbia.edu to help decide which pipeline is best for your data.
- In order to launch the post processing pipleines you will need to email juan.Sanchez@nyspi.columbia.edu to create aws account
- The username and password will be the same as your nyspi.columbia.edu email

Post Processing in AWS

- 1. Select your pipeline
- Enter the project acronym or XNAT project
- 3. Enter the input (location of your verified rawdata on the cluster)
- 4. Enter the output (location of the derivatives on the cluster)
 - 1. Abcd requires the abcd directory in the path, fmriprep does not
- 5. Enter the subjects you wish to be processed
- 6. Click I agree



Accessing Post Processed Data

- Once AWS is complete the data will be automatically synced from the cloud to the doctor and in the chosen derivatives directory
- The amount of time to run depends on the pipeline and the size of the data being processed
 - Abcd 6-8 hours
 - Fmriprep 4-6 hours
- You can monitor the status of the job(s) by selecting the Job Status tab
- You are responsible for rsyncing your data if you need it locally
- You may access the data on the cluster using the Virtual Machine
 - If this is your plan you will need to email <u>Juan.Sanchez@nsypi.columbia.edu</u>

ABCD - derivatives organization

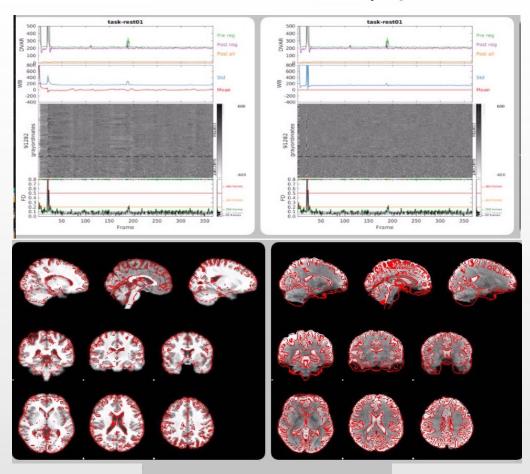
Outputs
The outputs are organized in the following structure:
<pre>output_dir/ sub-id ses-session files </pre>
files
 executive_summary: The .html file within can be opened for quality inspection of pipeline results.
 MNINonLinear: Contains the final space results of anatomy in 164k resolution.
 MNINonLinear/fsaverage_LR32k: Final space anatomy in 32k resolution, where functional data is ultimately projected.
MNINonLinear/Results: Final space functional data.
T1w: Contains native space anatomical data as well as intermediate preprocessing files.
T1w/id: The participant ID folder within T1w is the FreeSurfer subject folder.
task-taskname: These folders contain intermediate functional preprocessing files.

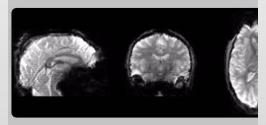
• Please visit the https://www.humanconnectome.org/storage/app/media/documentation/tutorials/Connectome WB Tutorial v1.5.pdf for an in-depth review of file types and how to use workbench to visualize data. In addition for more information on DCAN signal processing please visit: https://github.com/DCAN-Labs/dcan bold processing

ABCD - derivatives MNINonLinear/Results/task/DCAN

	BOLD
Volume MNI	MNINonLinear/Results/task-rest01/task-rest01.nii.gz
Surface fs_LR_32k (HCP Surface Atlas)	MNINonLinear/Results/task-rest01/task-rest01_Atlas.dtseries.nii
Surface Motion Artifact Cleaned	MNINonLinear/Results/task-rest01/DCANBOLDProc_v4.0.0/task-rest01_DCANBOLDProc_v4.0.0_Atlas.dtseries.nii
Surface Motion Artifact Cleaned concatenated (use this for voxelwise RS analyses)	MNINonLinear/Results/task-rest_DCANBOLDProc_v4.0.0_Atlas.dtseries.nii
Surface Motion Artifact Cleaned concatenated and parcellated (use this for parcel wise RS analyses)	MNINonLinear/Results/task-rest_DCANBOLDProc_v4.0.0_Gordon.ptseries.nii

ABCD - Executive Summary/QC





FMRIPREP - derivatives (anatomy)

Anatomical derivatives

Anatomical derivatives are placed in each subject's anat subfolder:

```
sub-<subject_label>/
anat/
sub-<subject_label>[_space-<space_label>]_desc-preproc_T1w.nii.gz
sub-<subject_label>[_space-<space_label>]_desc-brain_mask.nii.gz
sub-<subject_label>[_space-<space_label>]_dseg.nii.gz
sub-<subject_label>[_space-<space_label>]_label-CSF_probseg.nii.gz
sub-<subject_label>[_space-<space_label>]_label-GM_probseg.nii.gz
sub-<subject_label>[_space-<space_label>]_label-WM_probseg.nii.gz
```

FreeSurfer derivatives

A FreeSurfer subjects directory is created in <output dir>/freesurfer , or the directory indicated with the --fs-subjects-dir flag.

```
<output_dir>/
    fmriprep/
    ...
    freesurfer/
        fsaverage{,5,6}/
            mri/
            surf/
            ...
    sub-<subject_label>/
            mri/
            surf/
            ...
    ...
...
```

Please visit https://fmriprep.org/en/stable/outputs.html to learn more details about the fmriprep outputs.

FMRIPREP - derivatives (func)

Functional derivatives

```
Functional derivatives are stored in the func/ subfolder. All derivatives contain task-<task_label>

(mandatory) and run-<run_index> (optional), and these will be indicated with [specifiers]:

sub-<subject_label>/
func/
sub-<subject_label>_[specifiers]_space-<space_label>_boldref.nii.gz
sub-<subject_label>_[specifiers]_space-<space_label>_desc-brain_mask.nii.gz
sub-<subject_label>_[specifiers]_space-<space_label>_desc-preproc_bold.nii.gz
```

Grayordinates files. CIFTI is a container format that holds both volumetric (regularly sampled in a grid) and surface (sampled on a triangular mesh) samples. Sub-cortical time series are sampled on a regular grid derived from one MNI template, while cortical time series are sampled on surfaces projected from the [Glasser2016] template. If CIFTI outputs are requested (with the

```
--cifti-outputs argument), the BOLD series are also saved as dtseries.nii CIFTI2 files:
```

```
sub-<subject_label>/
func/
sub-<subject_label>_[specifiers]_bold.dtseries.nii
```

FMRIPREP - QC

Visual Reports

fMRIPrep outputs summary reports, written to fmriprep/sub-<subject_label>.html">output dir>fmriprep/sub-<subject_label>.html. These reports provide a quick way to make visual inspection of the results easy. Each report is self contained and thus can be easily shared with collaborators (for example via email). View a sample

