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CREATE CHANGE

NeuroDesk

Reproducibility anywhere at anytime - An interactive session
introducing NeuroDesk

Steffen & Saskia Bollmann

The University of Queensland

Acknowledgement of Country

The University of Queensland (UQ) acknowledges the Traditional Owners and their custodianship of the lands on which we meet.

We pay our respects to their Ancestors and their descendants, who continue cultural and spiritual connections to Country.

We recognise their valuable contributions to Australian and global society.



Declaration of Financial Interests or Relationships

Speaker Name: Saskia and Steffen Bollmann

I have the following financial interest or relationship to disclose with regard to the subject matter of this presentation:

Company Name: Oracle Cloud

Type of Relationship: Cloud credits to support NeuroDesk container hosting and development platform. If you are interested in taking part in Cloud Credit Program: contact Research Advocate, Peter Winn (peter.winn@oracle.com)

Company Name: Siemens Healthineers

Type of Relationship: Previous Employment (Steffen, 2019) + joint grants (ARC Linkage + ITTC) + joint patents

How we organize the talk



A researcher
using
NeuroDesk

One of the
NeuroDesk
developers



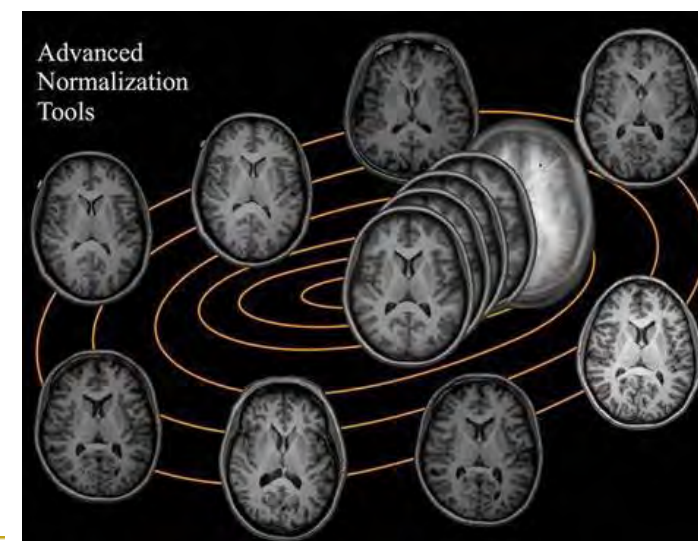
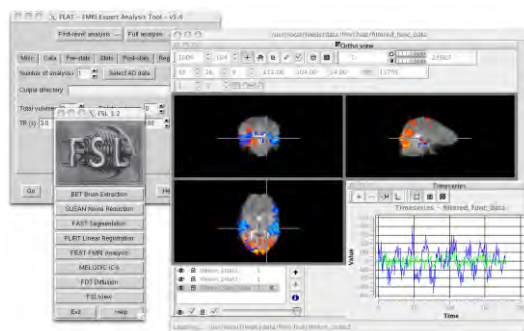


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Motivation

Large ecosystem of scientific software ...



Dependencies for specialised tools

Development has been first inspired from the VMTK toolbox, but as of today the script has and is currently being actively revamped. It is currently used on Linux and MACOS. The dependences are:

- ITK ≥ 4.9 , < 5.0 (do not forget to set ITK_DIR)
- python 2.7 (not tested with 3.5 and higher) with numpy, dipy, scikit-image (non exhaustive list)
- ANTs (<https://github.com/ANTsX/ANTs>). ITK 5.0 will be installed during ANTs compilation; ignore this version
- cmake + cmake-gui
- MACOS: realpath

```

RUN apt-get update -qq \
&& apt-get install -y -q --no-install-recommends apt-utils bzip2 \
    ca-certificates curl wget locales unzip cmake g++ gcc git cmake \
    cmake-curses-gui make pigz zlib1g-dev libboost-all-dev \
    bash /src/install_scripts/install_itk.sh > log_00_itk
&& apt-get clean \
    bash /src/install_scripts/install_boost.sh > log_01_boost
&& rm -rf /var/lib/apt/lists/* /tmp/* /var/tmp/* \
    bash /src/install_scripts/install_braincharter.sh > log_02_braincharter
&& sed -i -e 's/# en_US.UTF-8 UTF-8/en_US.UTF-8 UTF-8/' /etc/locale.gen \
    bash /src/install_scripts/install_afni_fsl.sh > log_03_afni_fsl
&& dpkg-reconfigure --frontend=noninteractive locales \
&& update-locale LANG="en_US.UTF-8" \
&& chmod 777 /opt && chmod a+s /opt

```

Trying out new versions and keeping things consistent

Advantages of cortical surface reconstruction using submillimeter 7 T MEMPRAGE

Natalia Zaretskaya^{a,b,c,d,*}, Bruce Fischl^{d,e,f}, Martin Reuter^{d,e,f,g}, Ville Renvall^h,
Jonathan R. Polimeni^{d,e,i}

Recon with native submillimeter resolution

See also [HighFieldRecon](#)

This page describes how to run the [FreeSurfer](#) recon-all for data with voxel sizes less than 1mm³ at native resolution. Several [FreeSurfer](#) binaries have been fixed to enable this feature. The pipeline is still [under development, so please use with caution](#).

Required FreeSurfer version

[dev version built after August 2015](#) or [FreeSurfer 6](#)

Note on the voxel size

The method works well for voxel sizes 0.75 mm³. It should work with voxel between 1mm³ and 0.75mm³. Inputs with 0.5 mm³ voxels or below will have a brainmask failure (we are working on it!), but if you fix the brainmask manually, the rest of recon-all should work well. We haven't tested the stream for inputs with anisotropic voxels.

Freesurfer 6 release downloads and setup: [here](#).

Important Note: When processing a group of subjects for your study, it is essential to process all your subjects with the same version of FreeSurfer, on the same OS platform and vendor, and for safety, even the same version of the OS. While we continue to work to ensure that results match across platforms, there are none-the-less system-level libraries that are OS dependent. An exception to this rule is that you may view and edit files across any platform or version, and run some post-processing tools (outside the recon-all stream) if you check with us first (for instance you may run the longitudinal processing with newer versions).

GLIBC 2.5 vs 2.18

Reproducibility of neuroimaging analyses across operating systems

Tristan Glatard^{1,2}, Lindsay B. Lewis¹, Rafael Ferreira da Silva³, Reza Adalat¹, Natacha Beck¹, Claude Lepage¹, Pierre Rioux¹, Marc-Etienne Rousseau¹, Tarek Sherif¹, Ewa Deelman³, Najmeh Khalili-Mahani¹ and Alan C. Evans^{1}*

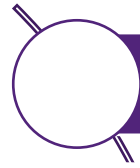
- glibc 2.5 vs 2.18 deliver different floating-point results
- leads to significant differences in long pipelines

```
expf(1.540518522262573242187500000000)  
=4.6670093536376953125000
```

```
expf(1.540518522262573242187500000000)  
=4.6670098304748535156250
```



... creating problems for researchers:



Most tools require Linux

... creating problems for researchers:

Most tools require Linux

Tools are not available in standard package systems

```
(base) uqsbollm@uqsbollm-7952:~$ sudo apt install freesurfer
[sudo] password for uqsbollm:
Reading package lists... Done
Building dependency tree
Reading state information... Done
Package freesurfer is not available, but is referred to by another package.
This may mean that the package is missing, has been obsoleted, or
is only available from another source

E: Package 'freesurfer' has no installation candidate
```

... creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare

Then run `cmake ..` and set `CMAKE_INSTALL_PREFIX` to be the desired directory as the above `cmake` command is ignoring the setting.

```
make -j 4
```

This will fail configuring `beast`.

Edit `/home/564/sb1053/minc-toolkit-v2/minc-toolkit-v2/BEaST/CMakeLists.txt`
and comment out `FIND_PACKAGE(NETCDF)` (in two places).

run `make -j 4` again.

This will fail to compile `/home/564/sb1053/minc-toolkit-v2/minc-toolkit-v2/minctools/progs/mincdump/mincdump.h`
Edit this file and replace `enum` with `#define`:

... creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare
- Conflicting dependencies

```
freeview.bin: error while loading shared libraries:  
libpng12.so.0: cannot open shared object file: No  
such file or directory
```

... creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare
- Conflicting dependencies
- Reinstalling tools on different platforms takes time

... creating problems for researchers:

- Most tools require Linux
- Tools are not available in standard package systems
- Compiling from source often a nightmare
- Conflicting dependencies
- Reinstalling tools on different platforms takes time
- Differing results between software versions

The organic solution ...

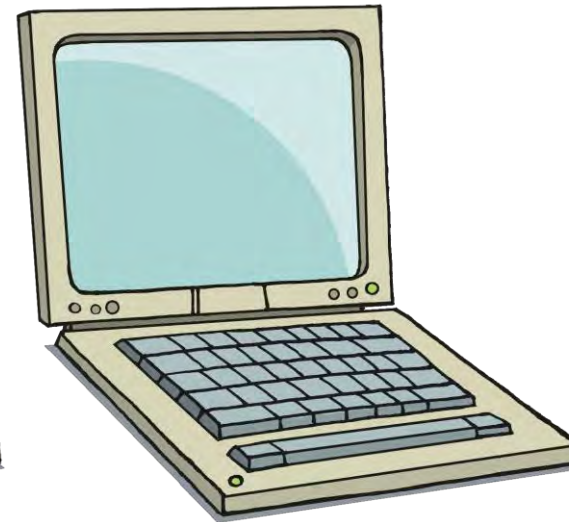
Use this one when
you do the
'normal' analysis



This has the 'high-
resolution' version
installed



This one is for the
study running since
1999
DO NOT TOUCH



This is the only one
where we managed
to get minc
compiled





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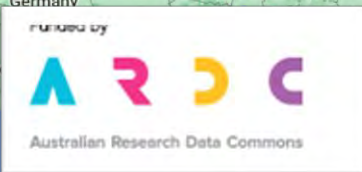
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NeuroDesk Architecture

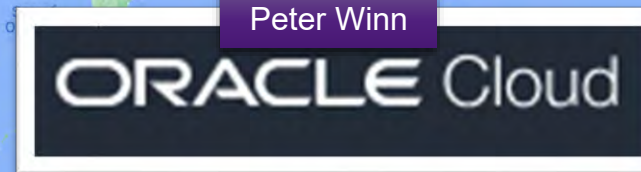
**Australian Research Container
Orchestration Service (ARCOS)**



Martin Grignard



Peter Winn



Jakub Kaczmarzyk

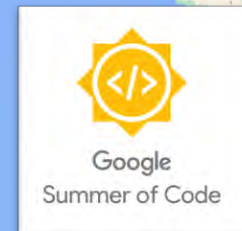
Niruhan Viswarupan

Dao Thanh Thuy

Will Woods

Aswin Narayanan

Yorguin Jose Mantilla



Tom Johnstone

David White

Oren Civier

Paris Lyons

Steffen Bollmann

Angela Renton

Thomas Shaw

Megan Campbell

Ryan Sullivan



What exists already and how can we combine efforts?

 CONDA®

 NeuroDebian



 nectar

 docker



CVL

Characterisation
Virtual Laboratory

Funded by



Australian Research Data Commons



Design principles for NeuroDesk

Linux, Mac, Windows

- Docker

Scale to HPC

- Singularity

Interactive

- Full Linux desktop interface

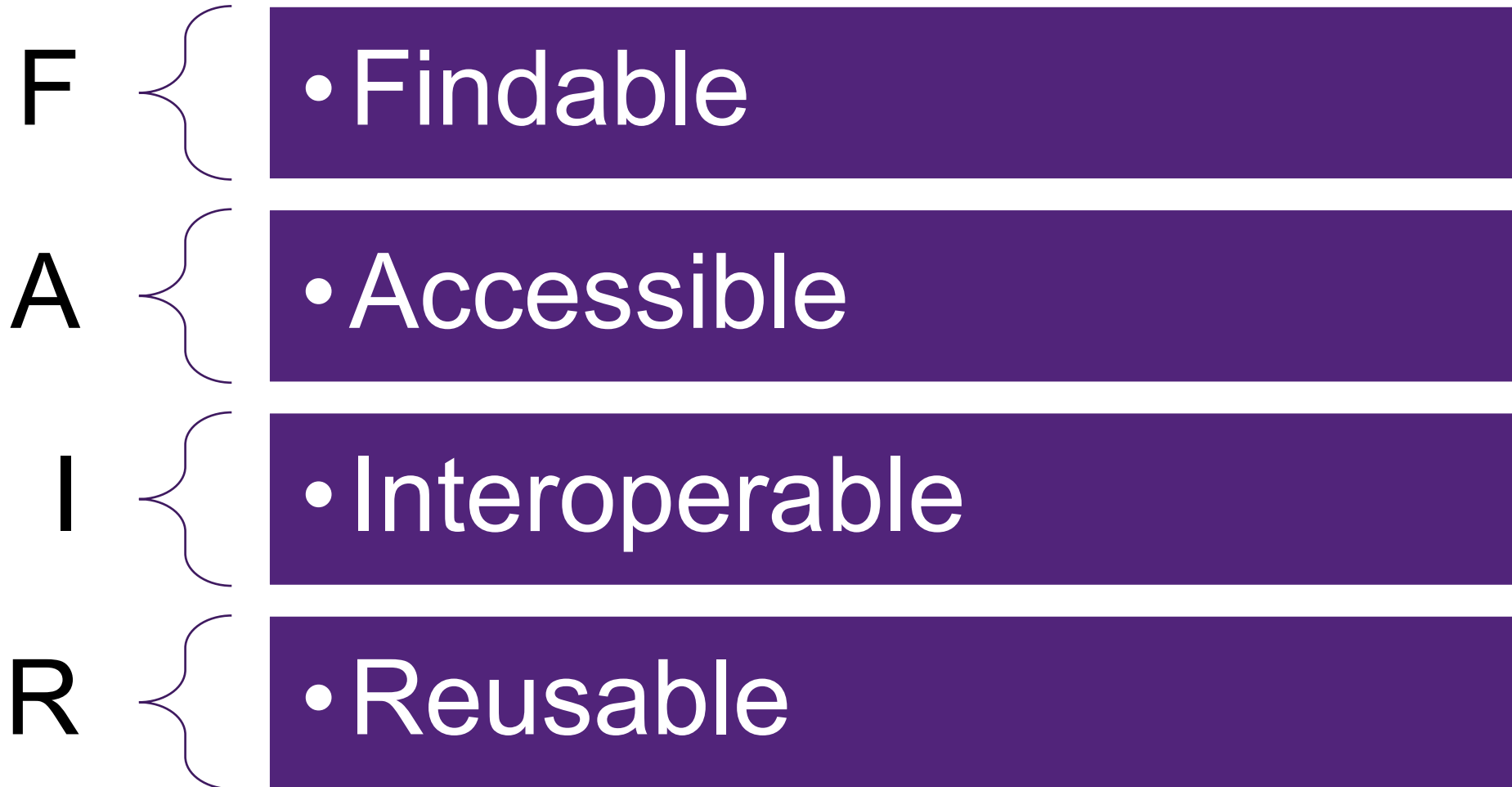
Lightweight

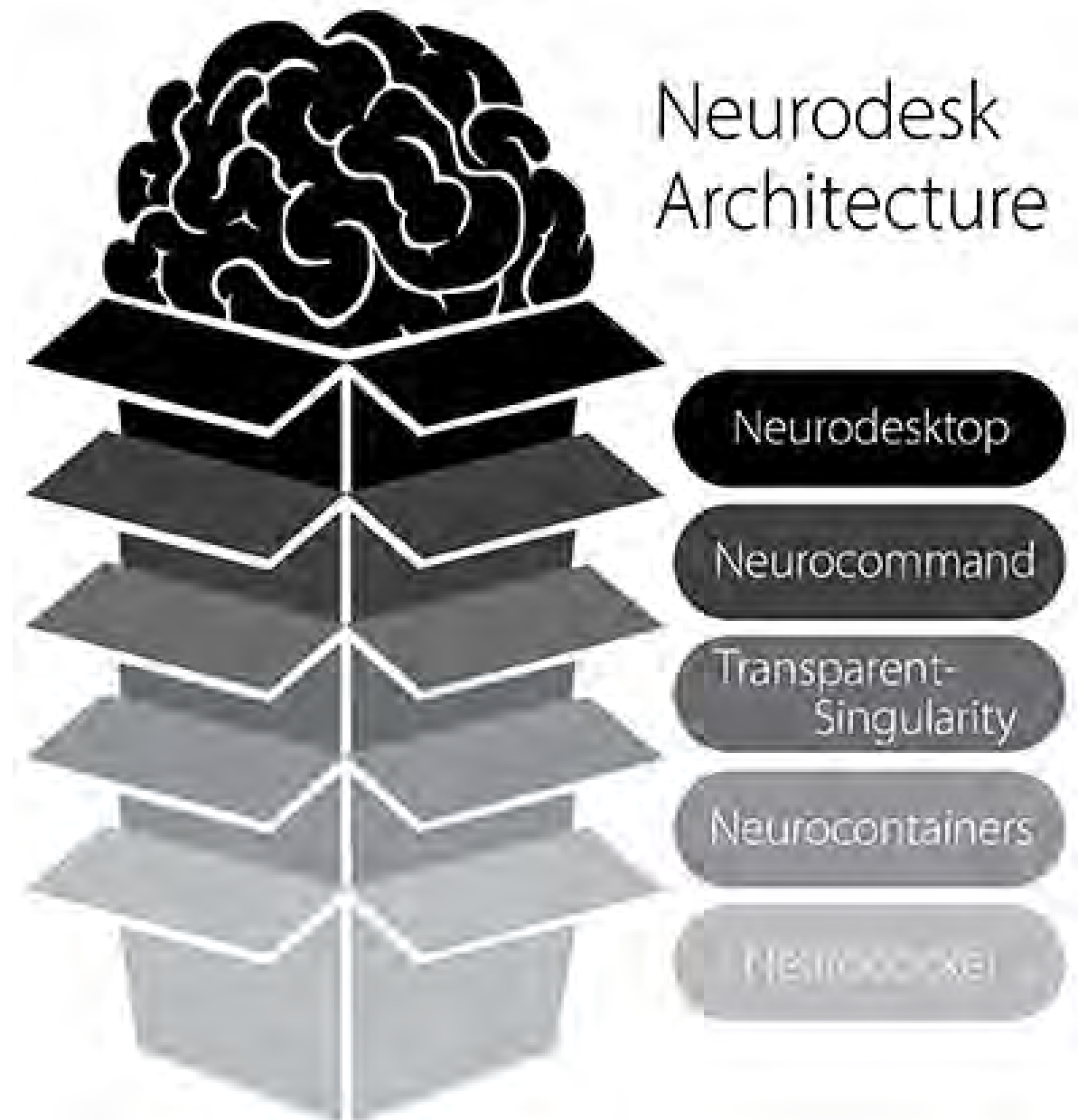
- Tools are installed on demand

Re-use existing tech

- NeuroDebian, conda, NeuroDocker

Neurodesk makes imaging analyses ...





Advanced users
directly using
Docker/Singularity



Neurocontainers –
Automated Container
building

Advanced Users
on HPC/Linux



Neurocommand –
Integrating our containers
on any Linux OS

Researchers on Windows,
Mac, Linux



Neurodesktop –
Lightweight Linux
Desktop with everything
installed



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NeuroDesktop on Windows


<http://neurodesk.github.io/>


NEURODESK


Documentation GitHub Search this site...


Get started with Neurodesk


A flexible, scalable, and easy to use data analysis environment for reproducible neuroimaging


 Linux


 Windows

 Mac

 HPC

 Cloud

 Demo





Neurodesktop

Fully featured desktop in a container

[Read more ...](#)



Neurocommand

Core installer

[Read more ...](#)



Neurocontainers

Software container library

[Read more ...](#)

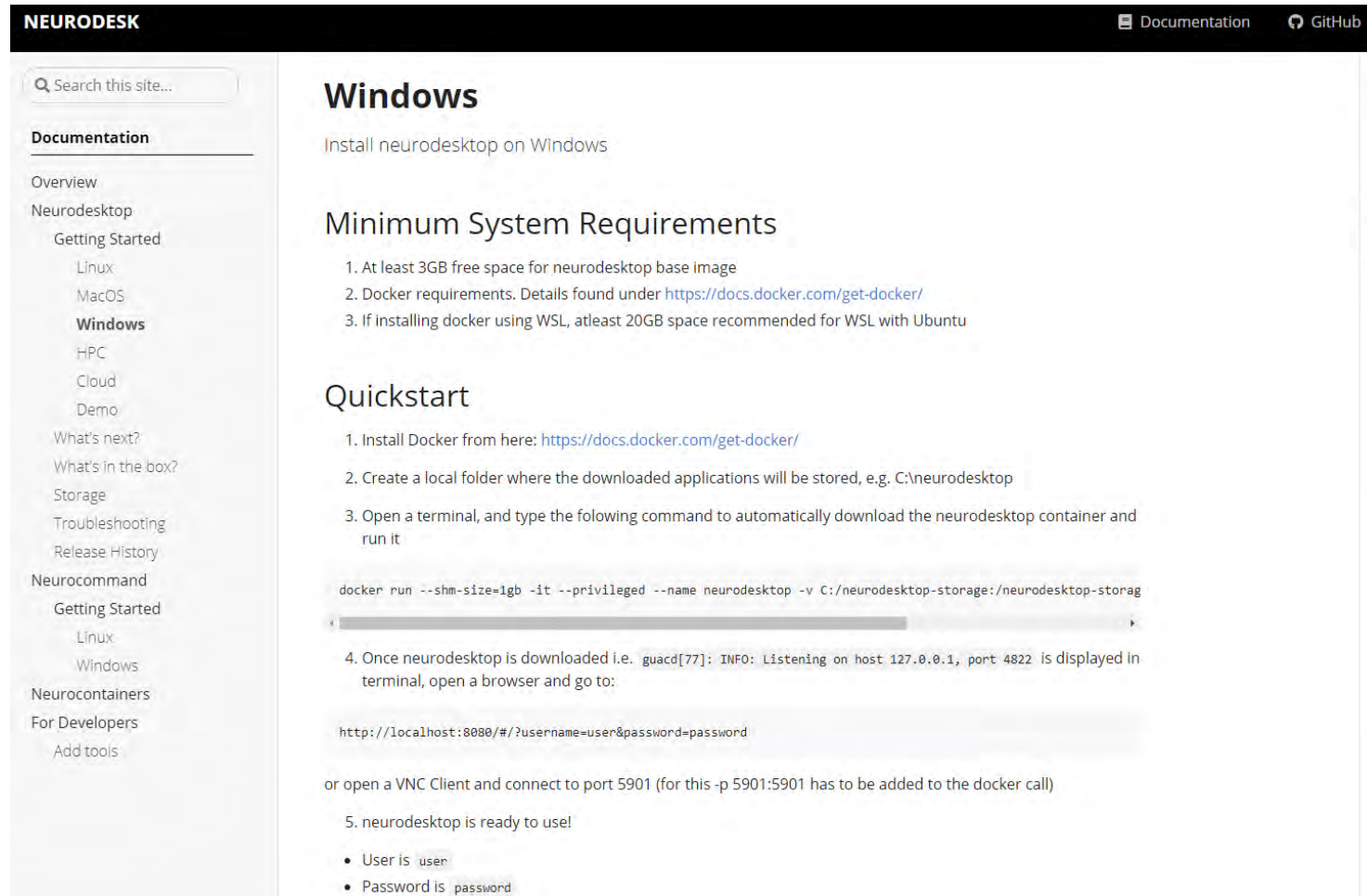


Discussions

Ask questions, suggest new features or raise any issues you have :)

[Read more ...](#)

Start NeuroDesktop



The screenshot shows the NeuroDesk website with a dark header containing the logo and links to Documentation and GitHub. A left sidebar lists navigation options like Overview, Neurodesktop, Getting Started, Linux, MacOS, Windows (highlighted), HPC, Cloud, Demo, What's next?, What's in the box?, Storage, Troubleshooting, Release History, Neurocommand, Getting Started, Linux, Windows, Neurocontainers, For Developers, and Add tools. The main content area is titled 'Windows' and includes a sub-header 'Install neurodesktop on Windows'. It lists 'Minimum System Requirements' (3GB free space, Docker requirements, WSL space) and a 'Quickstart' section with five steps: installing Docker, creating a local folder, running a Docker command (shown in a terminal snippet), accessing the desktop via a browser (URL snippet shown), and opening a VNC client. The final step states 'neurodesktop is ready to use!' with details about the user and password.

NEURODESK Documentation GitHub

Search this site...

Documentation

- Overview
- Neurodesktop
 - Getting Started
 - Linux
 - MacOS
 - Windows**
 - HPC
 - Cloud
 - Demo
 - What's next?
 - What's in the box?
 - Storage
 - Troubleshooting
 - Release History
- Neurocommand
 - Getting Started
 - Linux
 - Windows
- Neurocontainers
- For Developers
 - Add tools

Windows

Install neurodesktop on Windows

Minimum System Requirements

1. At least 3GB free space for neurodesktop base image
2. Docker requirements. Details found under <https://docs.docker.com/get-docker/>
3. If installing docker using WSL, atleast 20GB space recommended for WSL with Ubuntu

Quickstart

1. Install Docker from here: <https://docs.docker.com/get-docker/>
2. Create a local folder where the downloaded applications will be stored, e.g. C:\neurodesktop
3. Open a terminal, and type the folowing command to automatically download the neurodesktop container and run it

```
docker run --shm-size=1gb -it --privileged --name neurodesktop -v C:/neurodesktop-storage:/neurodesktop-storag
```
4. Once neurodesktop is downloaded i.e. `guacd[77]: INFO: Listening on host 127.0.0.1, port 4822` is displayed in terminal, open a browser and go to:

```
http://localhost:8080/#/?username=user&password=password
```
5. neurodesktop is ready to use!
 - User is `user`
 - Password is `password`

or open a VNC Client and connect to port 5901 (for this -p 5901:5901 has to be added to the docker call)

```
Using CATALINA_TMPDIR: /usr/local/tomcat/temp
Using JRE_HOME: /usr
Using CLASSPATH: /usr/local/tomcat/bin/bootstrap.jar:/usr/local/tomcat/bin/tomcat-juli.jar
Using CATALINA_OPTS:
Tomcat started.

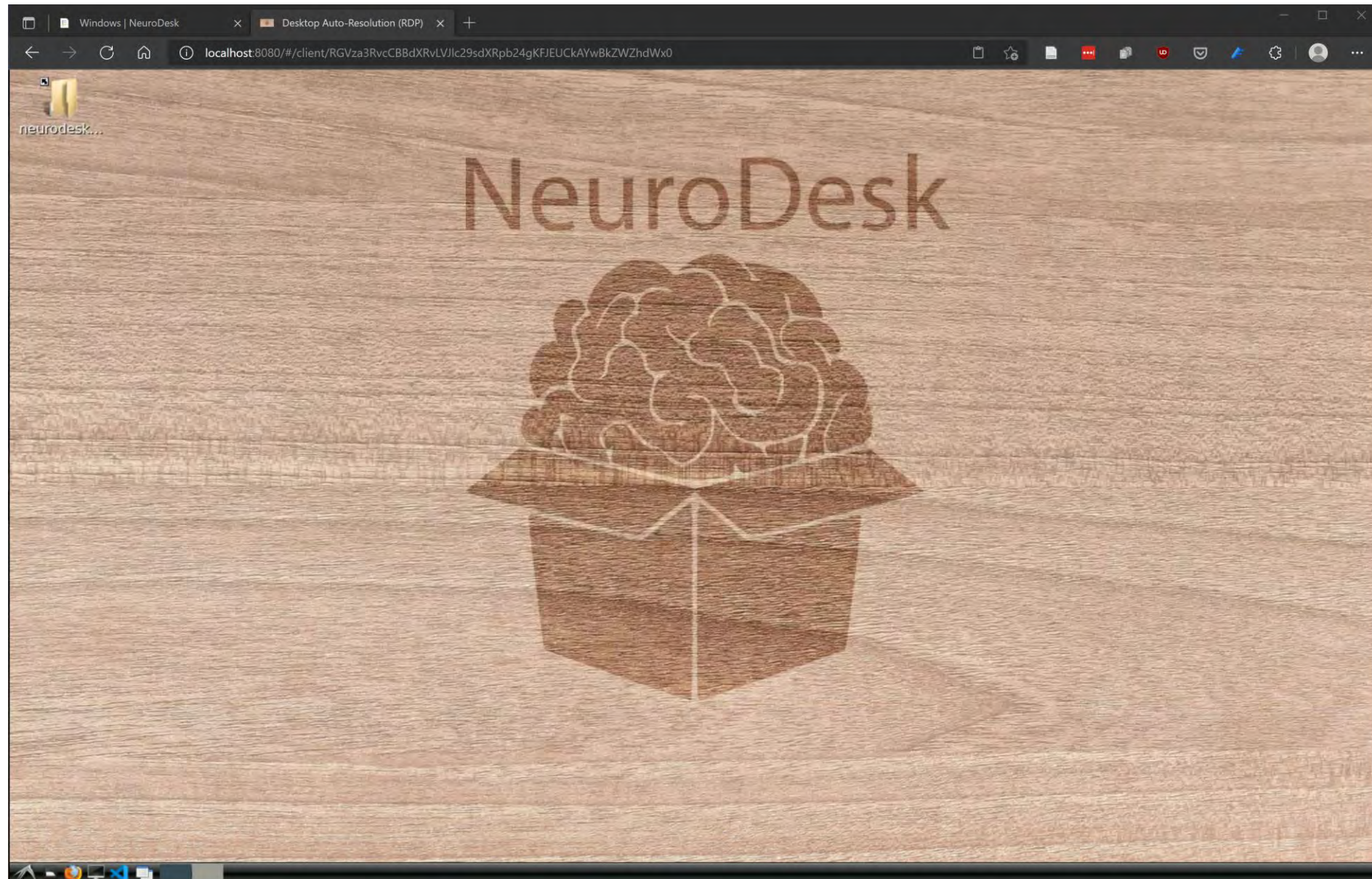
=====
Starting Guacamole Daemon
-----

Use this link for direct Neurodesktop:
!!! http://localhost:8080/#/?username=user&password=password !!!
Once connected to the session, your user info is:
Username: "user"
Password: "password"
-----

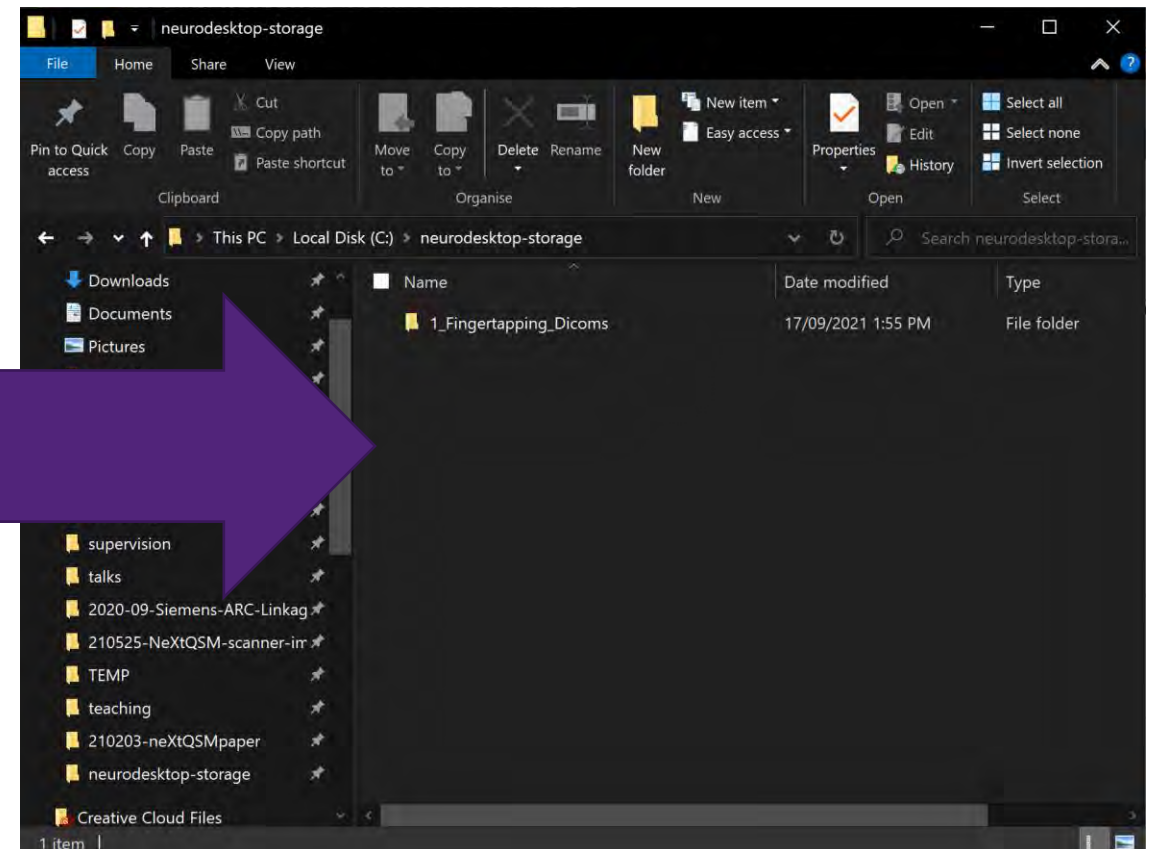
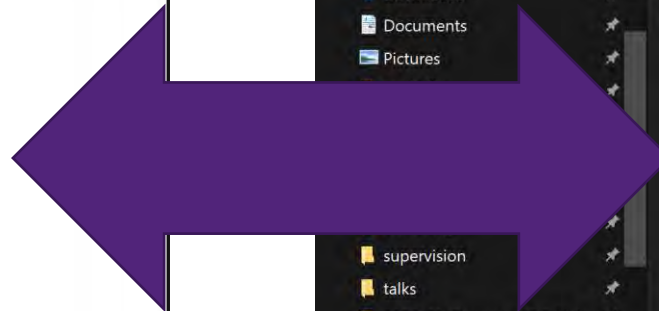
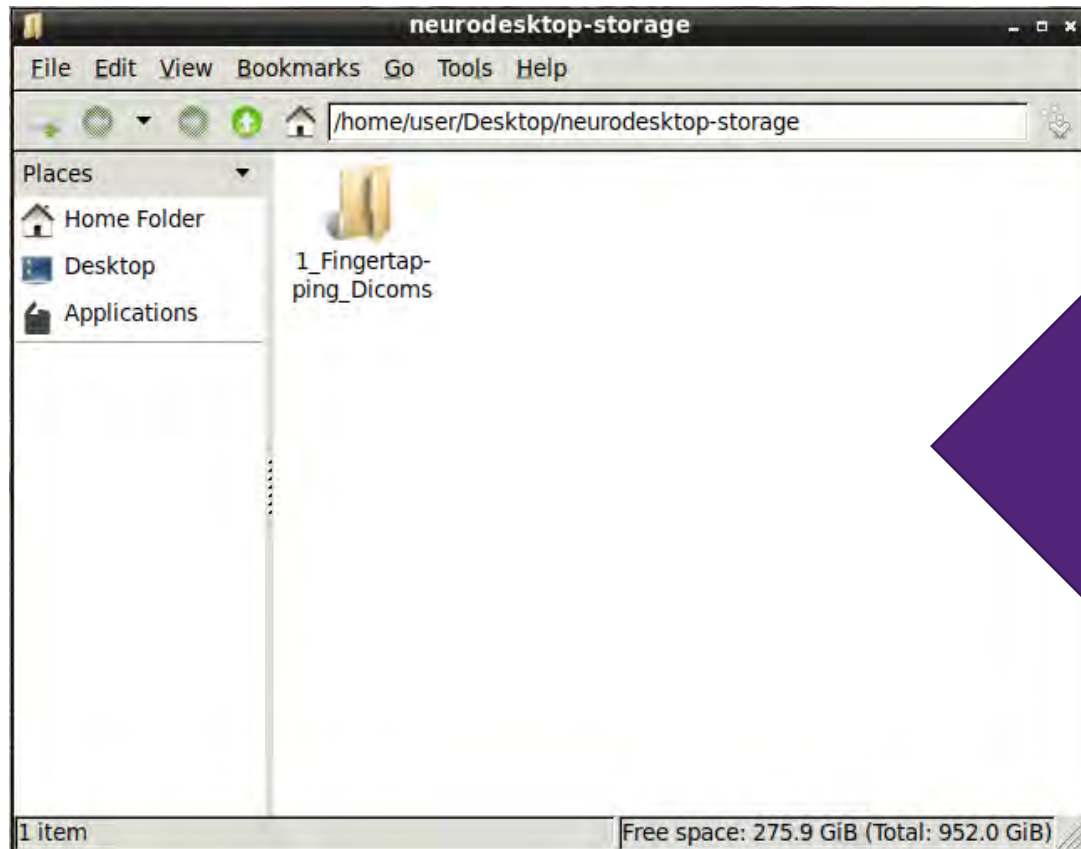
guacd[657]: INFO: Guacamole proxy daemon (guacd) version 1.3.0 started
guacd[657]: DEBUG: Successfully bound socket to host 127.0.0.1, port 4822
guacd[657]: INFO: Listening on host 127.0.0.1, port 4822
```

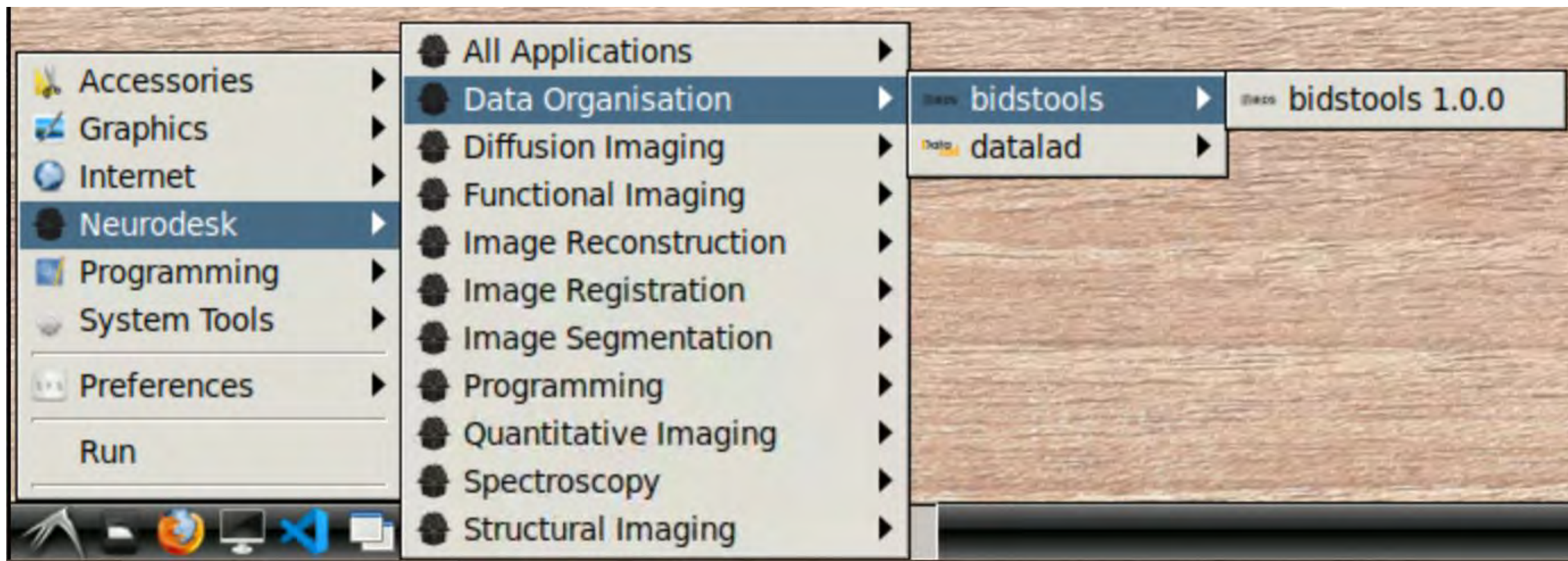
ALL CONNECTIONS

- Command Line (SSH)
- 🖥 Desktop Auto-Resolution (RDP)
- 🖥 Desktop Fixed-Resolution (VNC)



Getting access to my data:





```
bash
File Edit Tabs Help

+++++++ bidstools ++++++++
Contains a collection of tools needed for DICOM to BIDS conversion

Example:
***
dcm2niix
bidsmapper
bidscoiner
bidseditor
bidsparticipants
bidstrainer
deface
dicomsort
pydeface
rawmapper

convert dicom to bids:
dicomsort dicomfolder/sub-folder -r -e .IMA
bidsmapper dicomfolder bidsoutputfolder
bidscoiner dicomfolder bidsoutputfolder

also contains Bru2Nii: https://github.com/neurolabusc/Bru2Nii
Bru2 -o /Users/cr/dir2/out /Users/cr/dir/acqp
***

More documentation can be found here:
https://bidscoin.readthedocs.io/en/latest/installation.html
https://github.com/rordenlab/dcm2niix

To run container outside of this environment: ml bidstools/1.0.0
+++++++ bidstools ++++++++

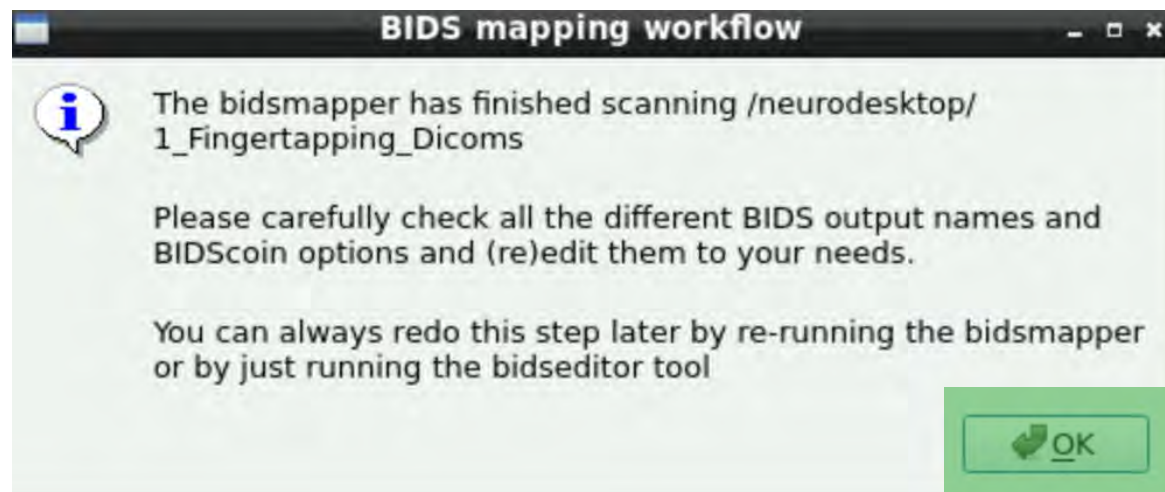
Singularity> █
```

```
user@f0db12773d42:~$ cd /neurodesktop-storage/  
user@f0db12773d42:/neurodesktop-storage$ ll  
total 4  
drwxrwxrwx 1 root root 4096 Sep 17 06:44 .  
drwxr-xr-x 1 root root 4096 Sep 17 06:41 ..  
drwxrwxr-x 1 root root 4096 Sep 17 06:44 1_Fingertapping_Dicoms  
user@f0db12773d42:/neurodesktop-storage$
```

```
Singularity> dicomsort 1_Fingertapping_Dicoms/sub-01/ -r -e .IMA
2021-09-17 00:21:51 - bidscoin - INFO >> Sorting: 1_Fingertapping_Dicoms/sub-01 (469 files)
2021-09-17 00:21:51 - bidscoin - INFO Creating: 1_Fingertapping_Dicoms/sub-01/006-mp2rage_highRes_0p5iso_slab_UNI-DEN
2021-09-17 00:22:01 - bidscoin - INFO Creating: 1_Fingertapping_Dicoms/sub-01/020-fingertapping_run1_SBRef
2021-09-17 00:22:01 - bidscoin - INFO Creating: 1_Fingertapping_Dicoms/sub-01/021-fingertapping_run1
Singularity> █
```



```
Singularity> mkdir bids
Singularity> bidsmapper 1_Fingertapping_Dicoms/ bids/
2021-09-17 00:23:28 - bidscoin - ----- START BIDSmapper -----
2021-09-17 00:23:28 - bidscoin - >>> bidsmapper sourcefolder=/neurodesktop/1_Fingertapping_Dicoms bidsfolder=/neurodesktop/bids bidsmap=bidsmap.yaml template=bidsmap_template.yaml subprefix=sub-
2021-09-17 00:23:28 - bidscoin - sesprefix=ses- store=False interactive=1
2021-09-17 00:23:28 - bidscoin - No existing bidsmap file found: /opt/miniconda-latest/lib/python3.6/site-packages/heuristics/bidsmap.yaml
2021-09-17 00:23:28 - bidscoin - Reading: /opt/miniconda-latest/lib/python3.6/site-packages/heuristics/bidsmap_template.yaml
QStandardPaths: XDG_RUNTIME_DIR not set, defaulting to '/tmp/runtime-user'
2021-09-17 00:23:33 - bidscoin - Parsing: /neurodesktop/1_Fingertapping_Dicoms/sub-01 (subject 1/1)
2021-09-17 00:23:37 - bidscoin - Found 'extra_data' DICOM sample: /neurodesktop/1_Fingertapping_Dicoms/sub-01/006-mp2rage_highRes_0p5iso_slab_UNI-DEN/S16_SB_006_mp2rage_highRes_0p5iso_slab_UNI-DE
N_00001_00001.IMA
2021-09-17 00:23:41 - bidscoin - Found 'extra_data' DICOM sample: /neurodesktop/1_Fingertapping_Dicoms/sub-01/020-fingertapping_run1_SBRef/SB_020_fingertapping_run1_SBRef_00001_00001.IMA
2021-09-17 00:23:45 - bidscoin - Found 'extra_data' DICOM sample: /neurodesktop/1_Fingertapping_Dicoms/sub-01/021-fingertapping_run1/SB_021_fingertapping_run1_00001_00001.IMA
2021-09-17 00:23:45 - bidscoin - Writing bidsmap to: /neurodesktop/bids/code/bidscoin/bidsmap.yaml
```



BIDS editor

File Help

File browser Options BIDS map

Participant labels

subject <<SourceFilePath>>
session <<SourceFilePath>>

Data samples

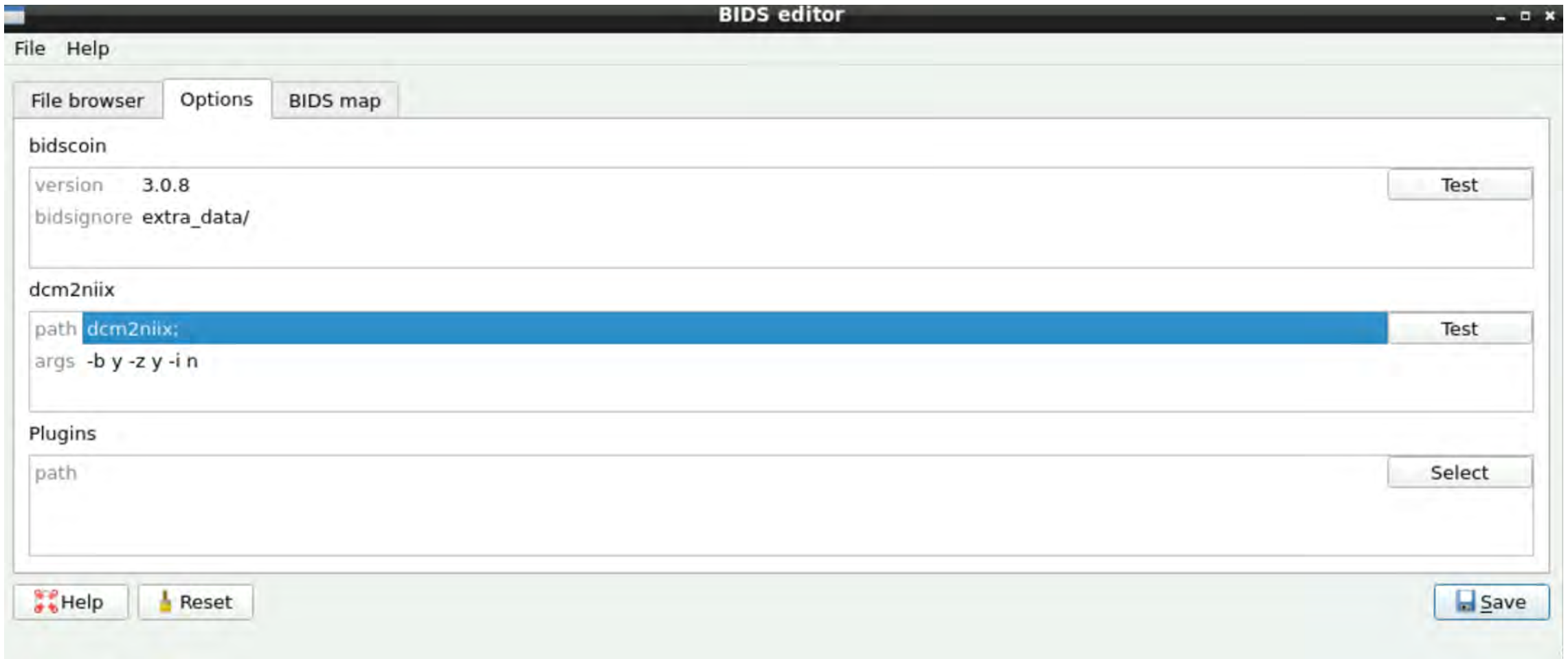
	DICOM input	BIDS output	Action
001	S16_SB_006_mp2rage_highRes_0p5iso_slab_UNI-...	extra_data/sub-01_acq-mp2ragehighRes0p5isoslabUNIDEN_dir-ROW_run-1_echo-1.*	Edit
002	SB_020_fingertapping_run1_SBRef_00001_00001.IMA	extra_data/sub-01_acq-fingertappingrun1SBRef_dir-COL_run-1_echo-1.*	Edit
003	SB_021_fingertapping_run1_00001_00001.IMA	extra_data/sub-01_acq-fingertappingrun1_dir-COL_run-1_echo-1.*	Edit

Help

Reset

Save

Change path to dcm2niix



The screenshot shows the 'BIDS editor' application window. It has a menu bar with 'File' and 'Help'. Below the menu bar are three tabs: 'File browser', 'Options', and 'BIDS map'. The 'Options' tab is selected. The main area is divided into three sections: 'bidscoin', 'dcm2niix', and 'Plugins'. The 'bidscoin' section has a 'version' field with the value '3.0.8' and a 'bidsignore' field with the value 'extra_data/'. There is a 'Test' button to the right of the 'bidsignore' field. The 'dcm2niix' section has a 'path' field with the value 'dcm2niix;' and an 'args' field with the value '-b y -z y -i n'. There is a 'Test' button to the right of the 'path' field. The 'Plugins' section has a 'path' field and a 'Select' button to its right. At the bottom of the window are three buttons: 'Help' (with a red cross icon), 'Reset' (with a yellow trash icon), and 'Save' (with a blue floppy disk icon).

BIDS editor

File Help

File browser Options **BIDS map**

bidscoin

version 3.0.8 Test

bidsignore extra_data/

dcm2niix

path dcm2niix; Test

args -b y -z y -i n

Plugins

path Select

Help Reset Save

Edit the runs and assign what they are

BIDS editor

File Help

File browser Options **BIDS map**

Participant labels

subject <<SourceFilePath>>
session <<SourceFilePath>>

Data samples

	DICOM input	BIDS output	Action
001	S16_SB_006_mp2rage_highRes_0p5iso_slab_UNI-...	extra_data/sub-01_acq-mp2ragehighRes0p5isoslabUNIDEN_dir-ROW_run-1_echo-1.*	Edit
002	SB_020_fingertapping_run1_SBRef_00001_00001.IMA	extra_data/sub-01_acq-fingertappingrun1SBRef_dir-COL_run-1_echo-1.*	Edit
003	SB_021_fingertapping_run1_00001_00001.IMA	extra_data/sub-01_acq-fingertappingrun1_dir-COL_run-1_echo-1.*	Edit

Help Reset Save

First one is anatomy

Edit BIDS mapping

DICOM input

Provenance

path /neurodesktop/1_Fingertapping_Dicoms/sub-01/006-...

filename S16_SB_006_mp2rage_highRes_0p5iso_slab_UNI-...

Attributes

Modality	MR
ProtocolName	mp2rage_highRes_0p5iso_slab
SeriesDescription	mp2rage_highRes_0p5iso_slab_UNI-DEN
ImageType	['ORIGINAL', 'PRIMARY', 'M', 'ND', 'UNI']
SequenceName	tf13d1
SequenceVariant	['SP', 'MP']
ScanningSequence	['GR', 'IR']
MRAcquisitionType	3D
SliceThickness	0.5
FlipAngle	0
EchoNumbers	1
EchoTime	2.88
RepetitionTime	4300
PhaseEncodingDirection	

BIDS output

Modality

anat

Labels

acq mp2ragehighRes0p5isoslabUNIDEN

ce

rec

run <<1>>

mod

suffix T1w

Output name

anat/sub-01_acq-mp2ragehighRes0p5isoslabUNIDEN_run-1_T1w.*

Help Reset Export Cancel OK

Second is reference scan – not needed

Edit BIDS mapping

DICOM input

Provenance

path /neurodesktop/1_Fingertapping_Dicoms/sub-01/020-...

filename SB_020_fingertapping_run1_SBRef_00001_00001.IMA

Attributes

Modality	MR
ProtocolName	fingertapping_run1
SeriesDescription	fingertapping_run1_SBRef
ImageType	['ORIGINAL', 'PRIMARY', 'M', 'ND', 'MOSAIC']
SequenceName	epfid2d1_164
SequenceVariant	['SK', 'SS']
ScanningSequence	EP
MRAcquisitionType	2D
SliceThickness	1.2999999523163
FlipAngle	70
EchoNumbers	1
EchoTime	25
RepetitionTime	1990
PhaseEncodingDirection	

BIDS output

Modality

leave_out

Labels

task

acq fingertappingrun1SBRef

ce

rec

dir COL

run <<1>>


mod


echo 1

suffix


Output name


leave_out/sub-01_acq-fingertappingrun1SBRef_dir-COL_run-1_echo-1.*

 Help

 Reset

Export

 Cancel

 OK

Change to “func” Modality

Edit BIDS mapping

DICOM input

Provenance

path /neurodesktop/1_Fingertapping_Dicoms/sub-01/021-...

filename SB_021_fingertapping_run1_00001_00001.IMA

Attributes

Modality	MR
ProtocolName	fingertapping_run1
SeriesDescription	fingertapping_run1
ImageType	['ORIGINAL', 'PRIMARY', 'M', 'MB', 'ND', 'MOSAIC']
SequenceName	epfid2d1_164
SequenceVariant	['SK', 'SS']
ScanningSequence	EP
MRAcquisitionType	2D
SliceThickness	1.2999999523163
FlipAngle	70
EchoNumbers	1
EchoTime	25
RepetitionTime	1990
PhaseEncodingDirection	

BIDS output

Modality

func

Labels

task fingertappingrun1

acq epfid2d1164

ce

rec

dir COL

run <<1>>

echo 1

suffix bold

Output name

func/sub-01_task-fingertappingrun1_acq-epfid2d1164_dir-COL_run-1_echo-1_bold.*

Help Reset Export Cancel OK

Hit Ok and Save

BIDS editor

File Help

File browser Options **BIDS map**

Participant labels

subject <<SourceFilePath>>
session <<SourceFilePath>>

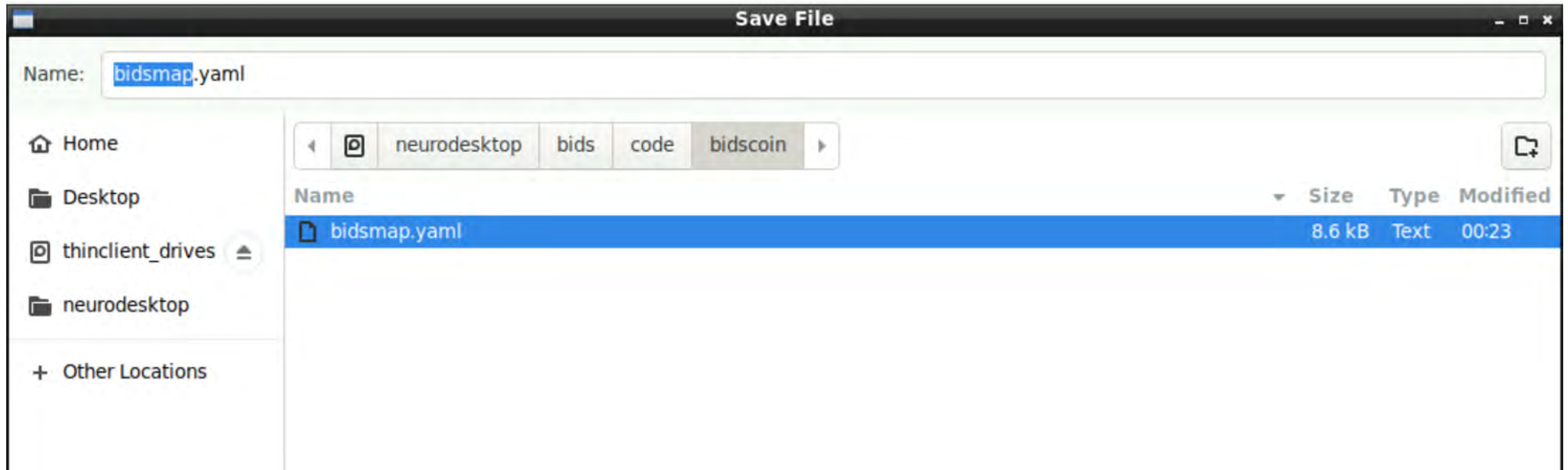
Data samples

	DICOM input	BIDS output	Action
001	S16_SB_006_mp2rage_highRes_0p5iso_slab_UNI-...	anat/sub-01_acq-mp2ragehighRes0p5isoslabUNIDEN_run-1_T1w.*	Edit
002	SB_020_fingertapping_run1_SBRef_00001_00001.IMA	leave_out/sub-01_acq-fingertappingrun1SBRef_dir-COL_run-1_echo-1.*	Edit
003	SB_021_fingertapping_run1_00001_00001.IMA	func/sub-01_task-fingertappingrun1_acq-epfid2d1164_dir-COL_run-1_echo-1_bold.*	Edit

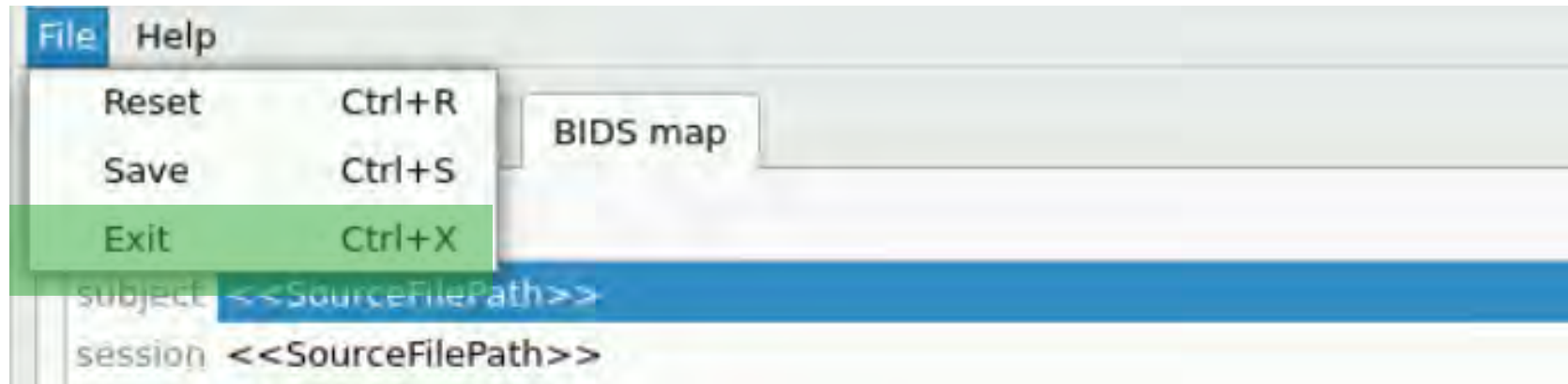
Help Reset

Save

Save bidsmap.yaml in the suggested location



Exit BIDS editor

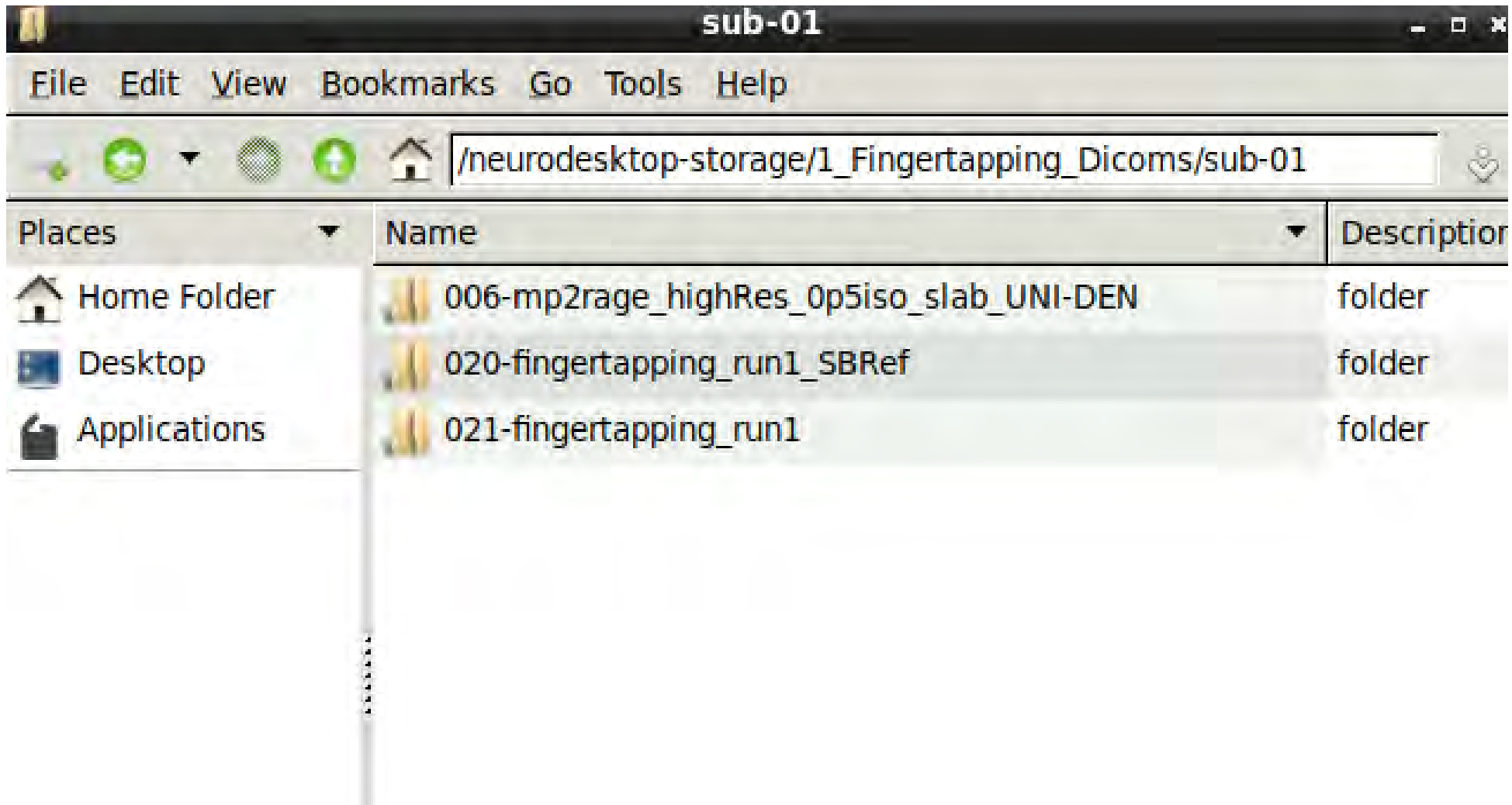


Start the conversion to bids 😊

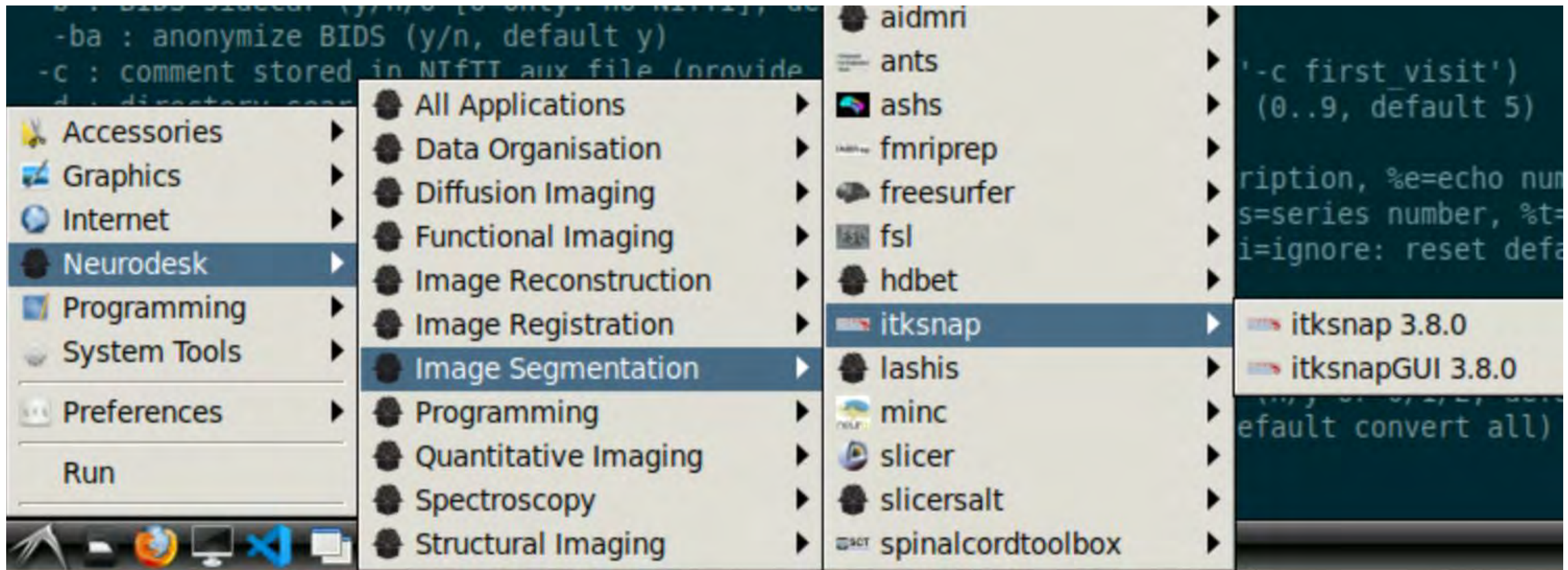
```
 bidscoiner 1_Fingertapping_Dicoms/ bids/
```

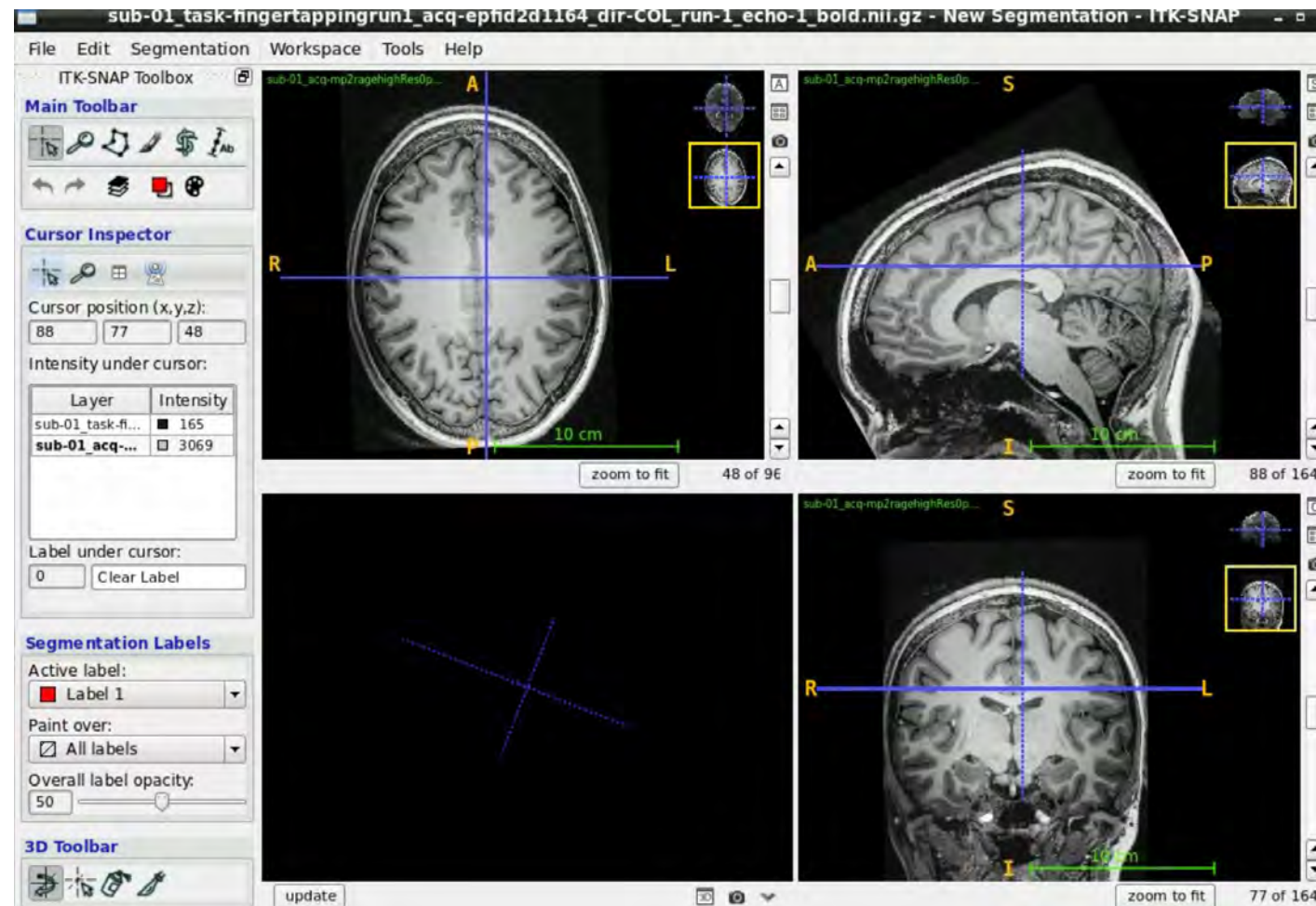
```
Singularity> bidscoiner 1_Fingertapping_Dicoms/ bids/
2021-09-17 00:33:03 - bidscoiner -
2021-09-17 00:33:03 - bidscoiner - ----- START BIDScoiner 3.0.8: BIDS 1.2.2 -----
2021-09-17 00:33:03 - bidscoiner - >>> bidscoiner sourcefolder=/neurodesktop/1_Fingertapping_Dicoms bidsfolder=/neurodesktop/bids subjects=None force=False participants=False bidsmap=bidsmap.yaml s
ubprefix=sub- sesprefix=ses-
2021-09-17 00:33:03 - bidscoiner - Creating dataset description file: /neurodesktop/bids/dataset_description.json
2021-09-17 00:33:03 - bidscoiner - Creating README file: /neurodesktop/bids/README
2021-09-17 00:33:03 - bidscoiner - Reading: /neurodesktop/bids/code/bidscoiner/bidsmap.yaml
2021-09-17 00:33:03 - bidscoiner - Writing ['extra_data/'] entries to /neurodesktop/bids.bidsignore
2021-09-17 00:33:03 - bidscoiner - ----- Subject 1/1 -----
2021-09-17 00:33:03 - bidscoiner - Coining session: /neurodesktop/1_Fingertapping_Dicoms/sub-01
2021-09-17 00:33:03 - bidscoiner - Processing: /neurodesktop/1_Fingertapping_Dicoms/sub-01/006-mp2rage_highRes_0p5iso_slab_UNI-DEN
2021-09-17 00:33:03 - bidscoiner - Running: dcm2niix;dcm2niix -b y -z y -i n -f "sub-01_acq-mp2ragehighRes0p5isoslabUNIDEN_run-1_T1w" -o "/neurodesktop/bids/sub-01/anat" "/neurodesktop/1_Fingertapp
ing_Dicoms/sub-01/006-mp2rage_highRes_0p5iso_slab_UNI-DEN"
2021-09-17 00:33:10 - bidscoiner - Output:
Chris Rorden's dcm2niix version v1.0.20201102 GCC9.3.0 x86-64 (64-bit Linux)
usage: dcm2niix [options] <in_folder>
Options :
-l..9 : gz compression level (1=fastest..9=smallest, default 6)
-a : adjacent DICOMs (images from same series always in same folder) for faster conversion (n/y, default n)
-b : BIDS sidcar (y/n/o [o=only: no NIfTI], default y)
-ba : anonymize BIDS (y/n, default y)
-c : comment stored in NIfTI aux_file (provide up to 24 characters e.g. '-c first_visit')
-d : directory search depth. Convert DICOMs in sub-folders of in_folder? (0..9, default 5)
-e : export as NRRD instead of NIfTI (y/n, default n)
-f : filename (%a=antenna (coil) name, %b=basename, %c=comments, %d=description, %e=echo number, %f=folder name, %i=ID of patient, %j=seriesInstanceUID, %k=studyInstanceUID, %m=manufacturer, %n=name
of patient, %o=mediaObjectInstanceUID, %p=protocol, %r=instance number, %s=series number, %t=time, %u=acquisition number, %v=vendor, %x=study ID; %z=sequence name; default '%f_%p_%t_%s')
-g : generate defaults file (y/n/o/i [o=only: reset and write defaults; i=ignore: reset defaults], default n)
-h : show help
-i : ignore derived, localizer and 2D images (y/n, default n)
-l : losslessly scale 16-bit integers to use dynamic range (y/n/o [yes=scale, no=no, but uint16->int16, o=original], default n)
-m : merge 2D slices from same series regardless of echo, exposure, etc. (n/y or 0/1/2, default 2) [no, yes, auto]
-n : only convert this series CRC number - can be used up to 16 times (default convert all)
-o : output directory (omit to save to input folder)
-p : Philips precise float (not display) scaling (y/n, default y)
```

Look at the output files created

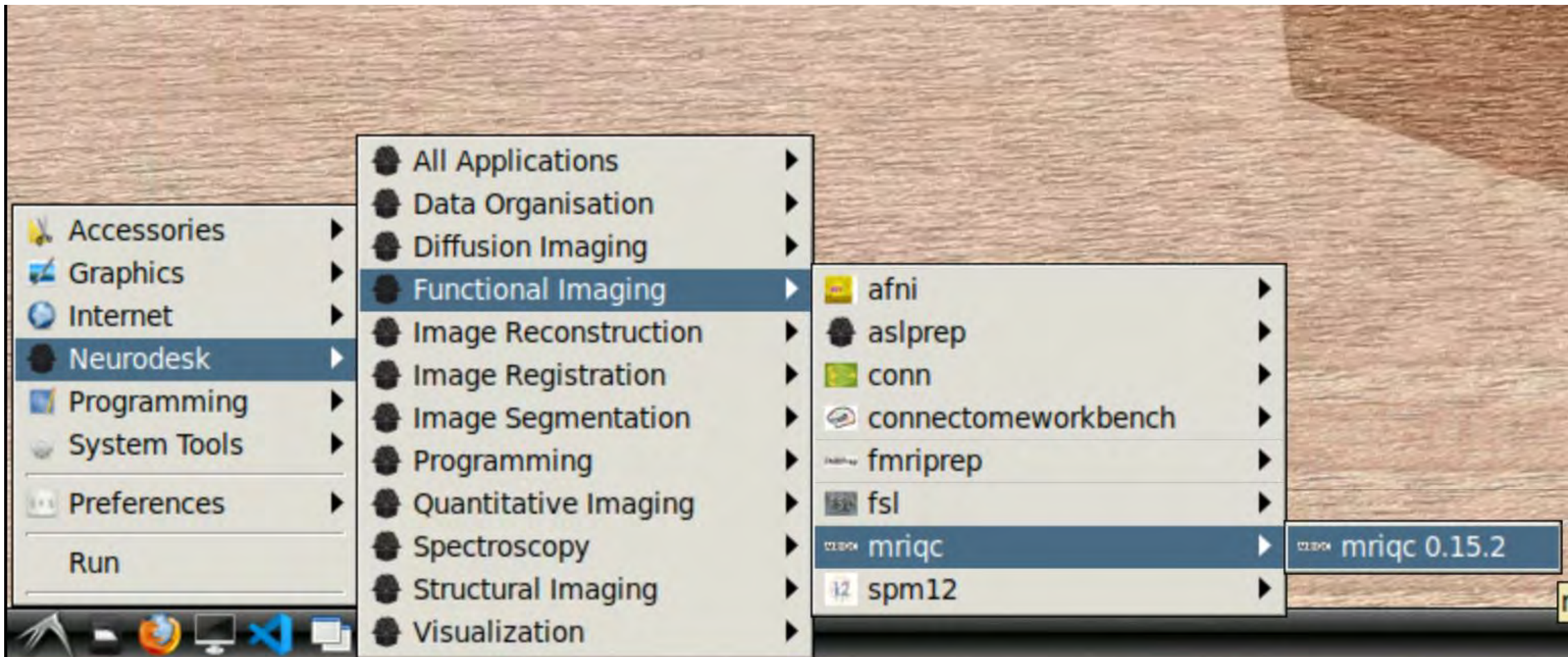


Look at data in ITKsnap





now we could use MRlqc



or fMRIPrep



BUT: computer too slow

```

user@3d18c112661d: ~
File Edit Tabs Help

 1 [ | ] 5 [ | ]
 2 [ | ] 6 [ | ]
 3 [ | ] 7 [ | ]
 4 [ | ] 8 [ | ]
Mem[|||||]
Swp[ ] Tasks: 39, 134 thr; 1 running
Load average: 0.10 0.11 0.14
Uptime: 04:29:52

  PID USER      PRI  NI  VIRT   RES   SHR  S  CPU% MEM%   TIME+  Command
  655 root        20   0 11.0G  497M 33756 S   2.7  2.0  0:18.84 /usr/bin/java -Dj
  709 user        20   0  498M  46332 14780 S   2.0  0.2  0:04.48 guacd -L debug -f
  714 user        20   0  498M  46332 14780 S   1.3  0.2  0:03.68 guacd -L debug -f
  726          20   0 28200  21064  6060 S   0.7  0.1  0:01.44 /usr/sbin/xrdp
  716          20   0 11.0G  497M 33756 S   0.7  2.0  0:01.15 /usr/bin/java -Dj
  693          20   0 11.0G  497M 33756 S   0.7  2.0  0:01.37 /usr/bin/java -Dj
  715 user        20   0  498M  46332 14780 S   0.7  0.2  0:00.69 guacd -L debug -f
  710 user        20   0  240M  14820  4912 S   0.7  0.1  0:00.51 guacd -L debug -f
  705          20   0 11.0G  497M 33756 S   0.7  2.0  0:00.26 /usr/bin/java -Dj
  758 user        20   0  89620  5004  4268 S   0.7  0.0  0:00.01 /usr/sbin/xrdp-ch
 1210 user        20   0  5112  3656  2704 R   0.0  0.0  0:00.07 htop
  658 user        20   0  240M  14820  4912 S   0.0  0.1  0:01.05 guacd -L debug -f
  695          20   0 11.0G  497M 33756 S   0.0  2.0  0:00.23 /usr/bin/java -Dj
F1Help F2Setup F3Search F4Filter F5Tree F6SortBy F7Nice -F8Nice +F9Kill F10Quit

```



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CREATE CHANGE

NeuroDesktop in the Cloud

Cloud setup – connect to cloud instance with tunnel

NEURODESK

DocumentationGitHubSearch this site...

Search this site...

Documentation

Overview

Neurodesktop

Getting Started

Linux

MacOS

Windows

HPC

Cloud

Demo

What's next?

What's in the box?

Storage

Troubleshooting

Cloud

Run neurodesktop using Oracle or Azure cloud computing

Minimum System Requirements

1. At least 3GB free space for neurodesktop base image
2. Docker requirements. Details found under <https://docs.docker.com/get-docker/>

Quickstart

1. Open an SSH connection to your cloud instance with port forwarding

```
ssh -L 8080:127.0.0.1:8080 opc@133.71.33.71
```

2. Install Docker from here: <https://docs.docker.com/get-docker/>

[Edit this page](#)

[Create child page](#)

[Create documentation issue](#)

[Create project issue](#)

[Print entire section](#)

Minimum System Requirements

Quickstart

Stopping neurodesktop:

Cloud-provider specific Tutorials

```
ssh -L 8080:127.0.0.1:8080 opc@152.67.98.39
```


Start Neurodesktop in the cloud

```
[opc@neurodesk ~]$ sudo docker run --shm-size=1gb -it --privileged --name neurodesktop -v ~/neurodesktop:/neurodesktop -e HOST_UID="$(id -u)" -e HOST_GID="$(id -g)" -p 8080:8080 vnmd/neurodesktop:20210917
Unable to find image 'vnmd/neurodesktop:20210917' locally
Trying to pull repository docker.io/vnmd/neurodesktop ...
20210917: Pulling from docker.io/vnmd/neurodesktop
35807b77a593: Already exists
c437049e42e2: Pull complete
4f2c86384465: Pull complete
a48fd7885107: Pull complete
2f6bfd9717ed: Pull complete
a214dad4d0d5: Pull complete
76e8846454c6: Pull complete
ea49baeab7f7: Pull complete
fa07df76b394: Pull complete
d2dbf549b363: Pull complete
0e3b6f679c40: Pull complete
7f33d04c8695: Pull complete
f1f13f2d6905: Pull complete
13c01807ec10: Pull complete
6d12a01dfa41: Extracting [=====>] 1.559kB/1.559kB
e3ceb6309db5: Download complete
f46a4d16b597: Download complete
4c9c971bf06c: Download complete
80f27ec6015f: Download complete
7e34cf62418f: Download complete
1388325df2f9: Download complete
537491dc8667: Download complete
732a930002ee: Download complete
aa36700b2e1e: Download complete
63ee34713a09: Download complete
3fb276372cc1: Download complete
82052eeb7161: Download complete
df71ea59471d: Download complete
fb5f580fbca3: Download complete
050f481e3aa2: Download complete
48595544fb94: Download complete
```

Starting Guacamole Daemon

Use this link for direct Neurodesktop:

!!! <http://localhost:8080/#/?username=user&password=password> !!!

Once connected to the session, your user info is:

Username: "user"

Password: "password"

```
guacd[656]: INFO:      Guacamole proxy daemon (guacd) version 1.3.0 started
guacd[656]: DEBUG:    Successfully bound socket to host 127.0.0.1, port 4822
guacd[656]: INFO:      Listening on host 127.0.0.1, port 4822
```

Connect to cloud storage



Storage

Add storage to Neurodesktop

Cloud-storage

The easiest way to get your data into Neurodesktop is to use a cloud storage provider like CloudStor, Dropbox, OneDrive and their sync tools like OwnCloud, Nextcloud or very flexible tools like rclone or davfs2. Another good option could be to utilize Globus for large amounts of data.

Nextcloud and Owncloud desktop clients

Under the menu item "Accessories" you can find "Nextcloud" and "ownCloud" desktop sync clients that you can configure with your cloud service accounts.

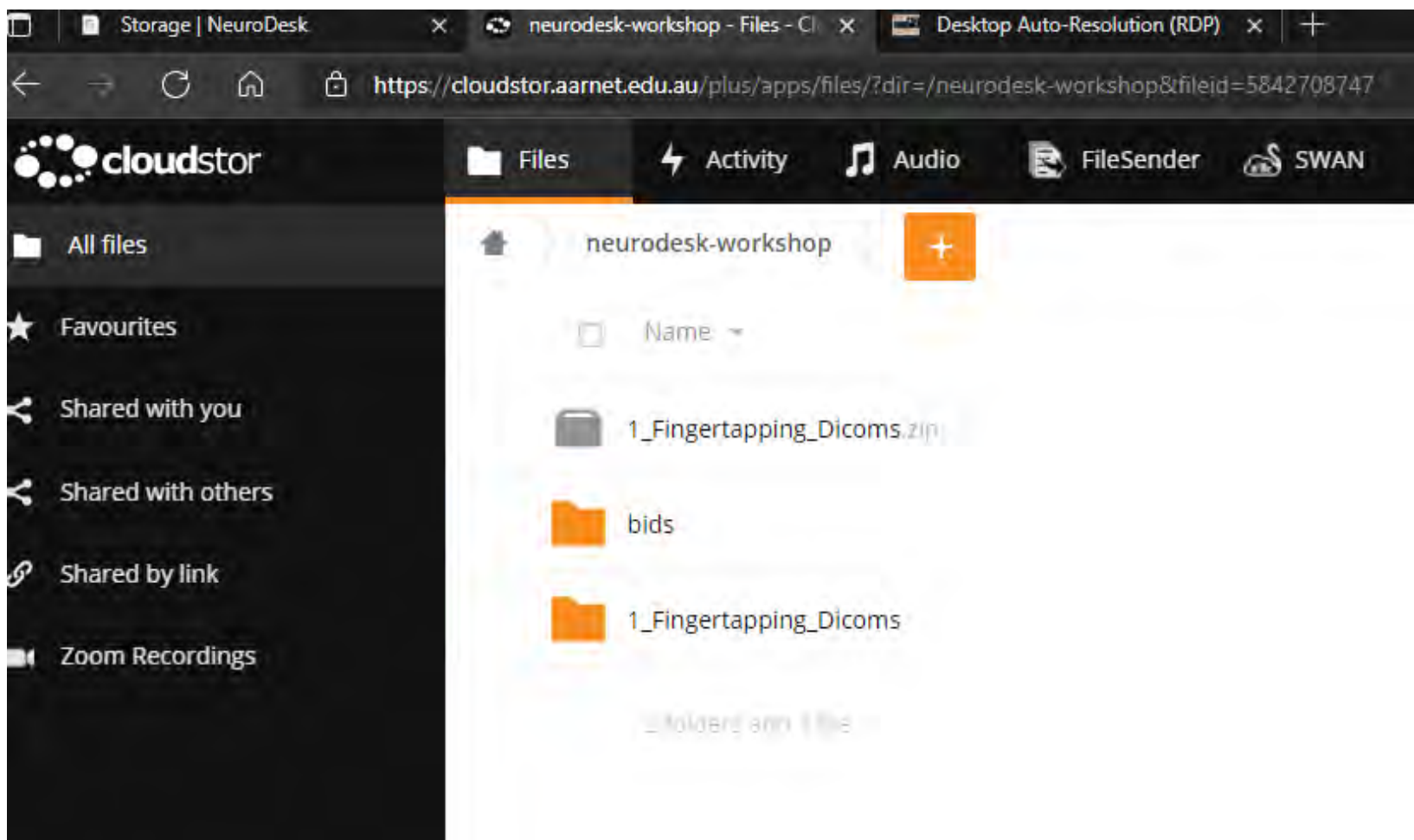
Mounting webdav storage using davfs2

Another option is to directly mount webdav storage. Here is an example how to mount CloudStor into Neurodesktop:

```
sudo mount -t davfs https://cloudstor.aarnet.edu.au/plus/remote.php/webdav/ /data/
```

It then asks you for a username and password, which you can generate here:
<https://cloudstor.aarnet.edu.au/plus/settings/personal?sectionid=security>

<https://cloudstor.aarnet.edu.au/plus/apps/files>



CloudStor storage mounted 😊

```
user@976519ac6124:~$ sudo mount -t davfs https://cloudstor.aarnet.edu.au/plus/remote.php/webdav/ /data/
Please enter the username to authenticate with server
https://cloudstor.aarnet.edu.au/plus/remote.php/webdav/ or hit enter for none.
Username: s.bollmann@uq.edu.au
Please enter the password to authenticate user s.bollmann@uq.edu.au with server
https://cloudstor.aarnet.edu.au/plus/remote.php/webdav/ or hit enter for none.
Password:
user@976519ac6124:~$ cd /data/
user@976519ac6124:/data$ ls
Notebooks      Shared      lost+found    projects
SWAN_SESSIONS backups    neurodesk-workshop  zotero
```

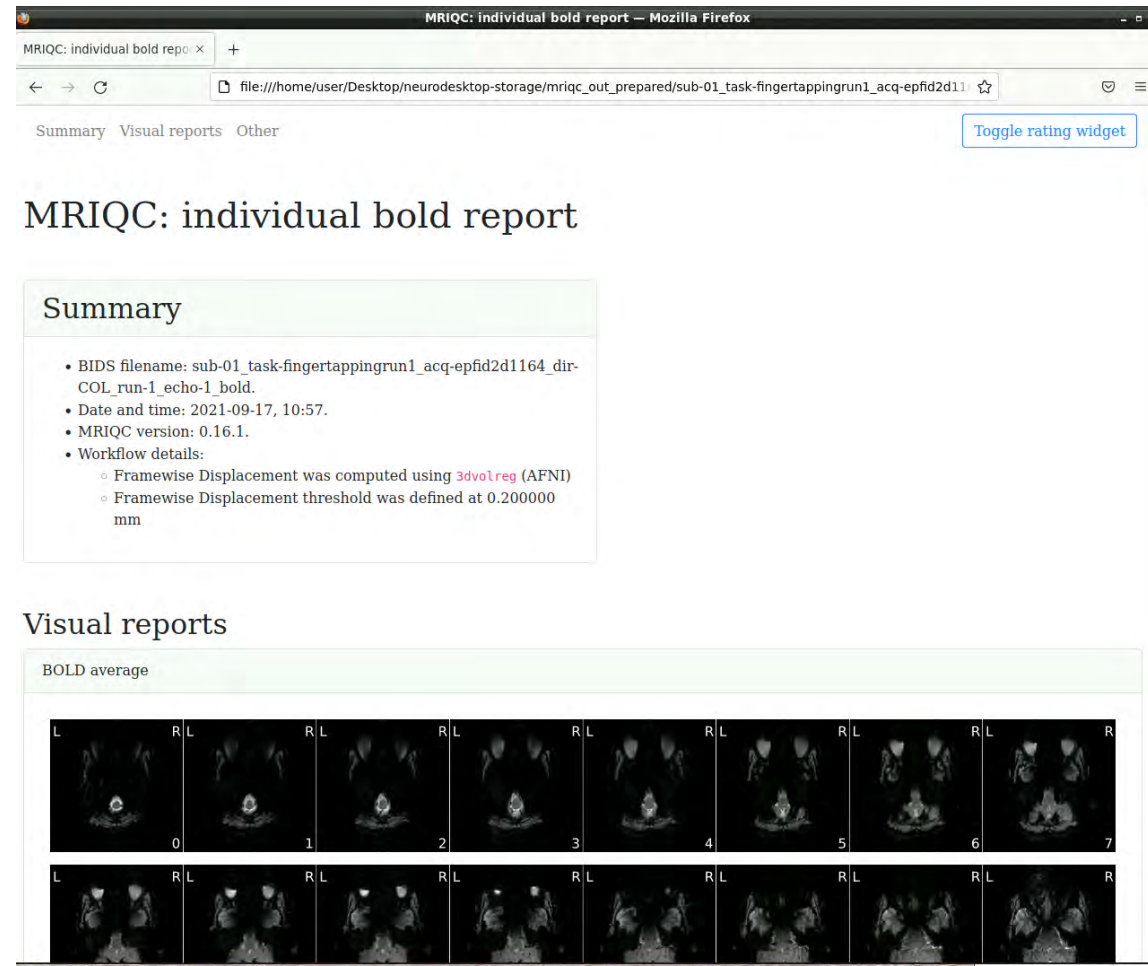
Start MRIQC in cloud

```
bash
File Edit Tabs Help
usage: mriqc [-h] [--version]
            [--participant_label [PARTICIPANT_LABEL [PARTICIPANT_LABEL ...]]]
            [--session-id [SESSION_ID [SESSION_ID ...]]]
            [--run-id [RUN_ID [RUN_ID ...]]]
            [--task-id [TASK_ID [TASK_ID ...]]]
            [-m [MODALITIES [MODALITIES ...]]] [--dsname DSNAME]
            [-w WORK_DIR] [--verbose-reports] [--write-graph] [--dry-run]
            [--profile] [--use-plugin USE_PLUGIN] [--no-sub] [--email EMAIL]
            [-v] [--webapi-url WEBAPI_URL] [--webapi-port WEBAPI_PORT]
            [--upload-strict] [--n_procs N_PROCS] [--mem_gb MEM_GB]
            [--testing] [-f] [--ica] [--hmc-afni] [--hmc-fsl]
            [--fft-spikes-detector] [--fd_thres FD_THRES]
            [--ants-nthreads ANTS_NTHREADS] [--ants-float]
            [--ants-settings ANTS_SETTINGS] [--deoblique] [--despike]
            [--start-idx START_IDX] [--stop-idx STOP_IDX]
            [--correct-slice-timing]
            bids_dir output_dir {participant,group} [{participant,group} ...]
...

More documentation can be found here: https://mriqc.readthedocs.io/en/stable/running.html

Singularity> mriqc /data/bids/ /data/qc_output participant
```


Open Firefox and inspect MRIQC outputs



MRIQC: individual bold report — Mozilla Firefox

MRIQC: individual bold report x +

file:///home/user/Desktop/neurodesk-storage/mriqc_out_prepared/sub-01_task-fingertappingrun1_acq-epfd2d11

Summary Visual reports Other [Toggle rating widget](#)

MRIQC: individual bold report

Summary

- BIDS filename: sub-01_task-fingertappingrun1_acq-epfd2d1164_dir-COL_run-1_echo-1_bold.
- Date and time: 2021-09-17, 10:57.
- MRIQC version: 0.16.1.
- Workflow details:
 - Framewise Displacement was computed using **3dvolreg** (AFNI)
 - Framewise Displacement threshold was defined at 0.200000 mm

Visual reports

BOLD average

L R L R L R L R L R L R L R L R

0 1 2 3 4 5 6 7



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Neurocommand on CVL

<https://desktop.cvl.org.au/strudel-web/#/system-selector>

NEURODESK

Documentation

 Search this site...

Documentation

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MacOS

Windows

HPC

Cloud

Demo

What's next?

What's in the box?

Storage

Troubleshooting

Release History

Neurocommand

Getting Started

Linux

Windows

Neurocontainers

For Developers

Add tools

Linux

Install neurocommand on Linux

Requirements:

Required

- python 3.6+ <https://docs.conda.io/en/latest/miniconda.html#linux-installers>
- singularity https://sylabs.io/guides/3.5/user-guide/quick_start.html
- git

Optional

- lmod <https://lmod.readthedocs.io/en/latest/>

command line mode - For non-desktop experience (e.g. running on an HPC)

If running on cli only ...

- Load singularity and for best performance it should be 3.x e.g. `module load singularity/3.5.0`
- Load or install aria2 to optimize the download performance of our containers e.g. `module load aria2c`
- make sure the current directory is not a symlink (singularity bug): `pwd -P` and then `cd` there
- Run `git clone https://github.com/NeuroDesk/neurocommand.git` to clone the repository - make sure to clone this to a directory with enough storage, write permissions and NOT a symbolic link (to be sure run `cd `pwd -P``)!
- Run `cd neurocommand` to change into the directory
- Run `pip3 install -r neurodesk/requirements.txt --user` to install pre-requisite python packages
- Run `bash build.sh --cli` to install in cli mode
- Run `bash containers.sh` for installing individual containers or `bash containers.sh --all` for installing all containers
- Run `module use $PWD/local/containers/modules/` to add the containers to your module search path. Add this to your `.bashrc` if working.
- Run `m1 avail` to see the installed containers at the top of the list (neurodesk containers will take preference over system modules with the same name). If a container is not yet there run `m1 --ignore_cache avail`

Select a remote system

Remote system

M3 and CVL@MASSIVE



LOGIN

fMRIPrep










- Automatically pre-process fMRI data
- Reads in BIDS and outputs BIDSderivative

nature | **methods**

ARTICLES

<https://doi.org/10.1038/s41592-018-0235-4>

fMRIPrep: a robust preprocessing pipeline for functional MRI

Oscar Esteban ^{1*}, Christopher J. Markiewicz ¹, Ross W. Blair¹, Craig A. Moodie ¹, A. Ilkay Isik ², Asier Erramuzpe ³, James D. Kent⁴, Mathias Goncalves⁵, Elizabeth DuPre ⁶, Madeleine Snyder⁷, Hiroyuki Oya⁸, Satrajit S. Ghosh ^{5,9}, Jesse Wright¹, Joke Durnez ¹, Russell A. Poldrack^{1,10} and Krzysztof J. Gorgolewski ^{1,10*}


```
[uqsbollm@m3p008 neurocommand]$ module use local/containers/modules/  
[uqsbollm@m3p008 neurocommand]$ module avail fmriprep  
  
----- local/containers/modules/ -----  
fmriprep/20.1.3
```



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CREATE CHANGE

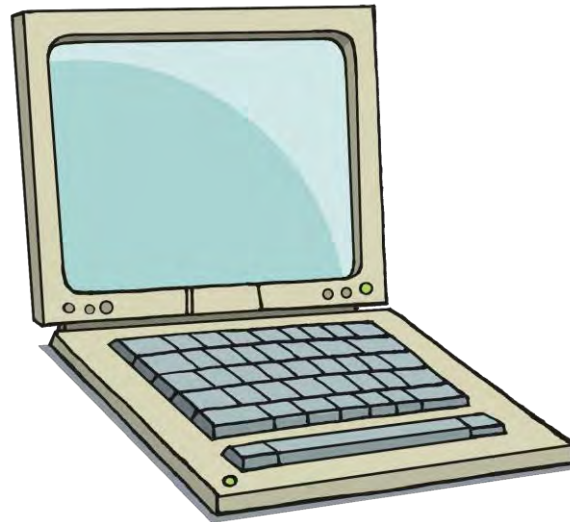
Outlook

The organic solution ...

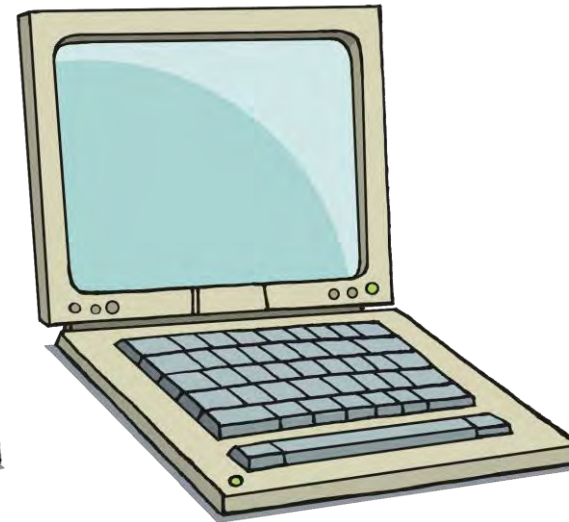
Use this one when
you do the
'normal' analysis



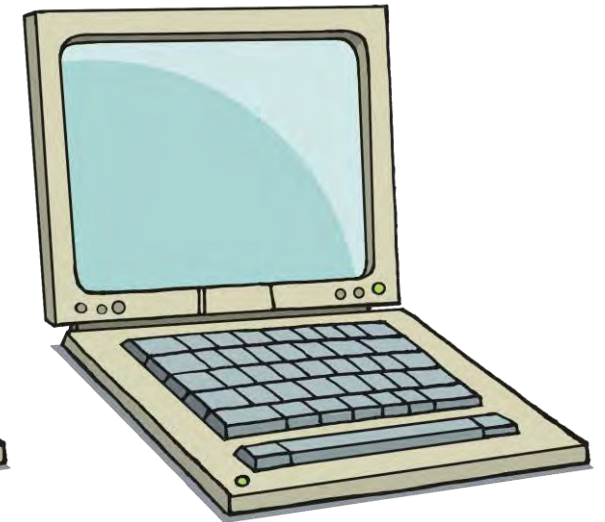
This has the 'high-
resolution' version
installed



This one is for the
study running since
1999
DO NOT TOUCH



This is the only one
where we managed
to get minc
compiled



The neurodesk solution ...

Use this one when
you do the
'normal' analysis



This has the 'high-
resolution' version
installed



This one is for the
study running since
1999
DO NOT TOUCH



This is the only one
where we managed
to get minc
compiled

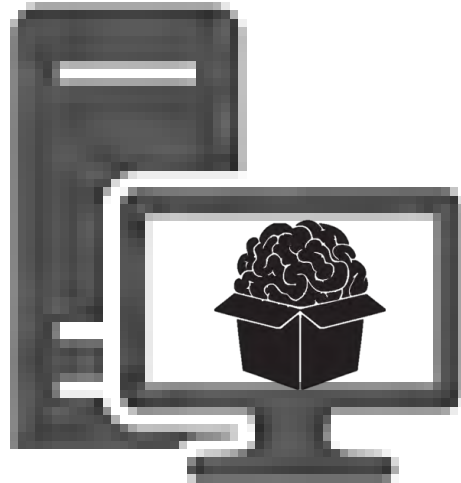


... reproducibility anywhere at anytime

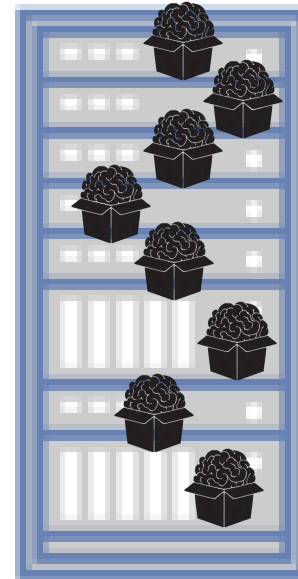
... on your notebook



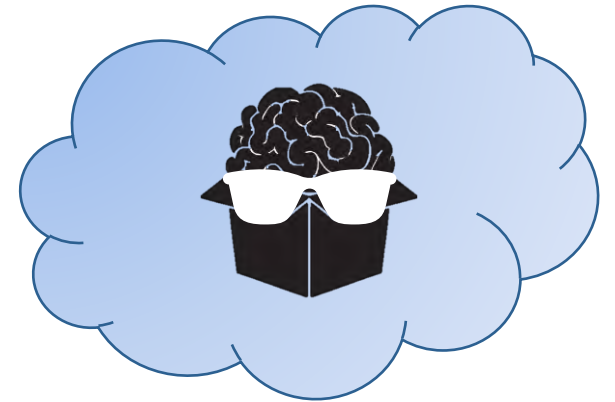
... on your lab
workstation



... on the university's high
performance cluster

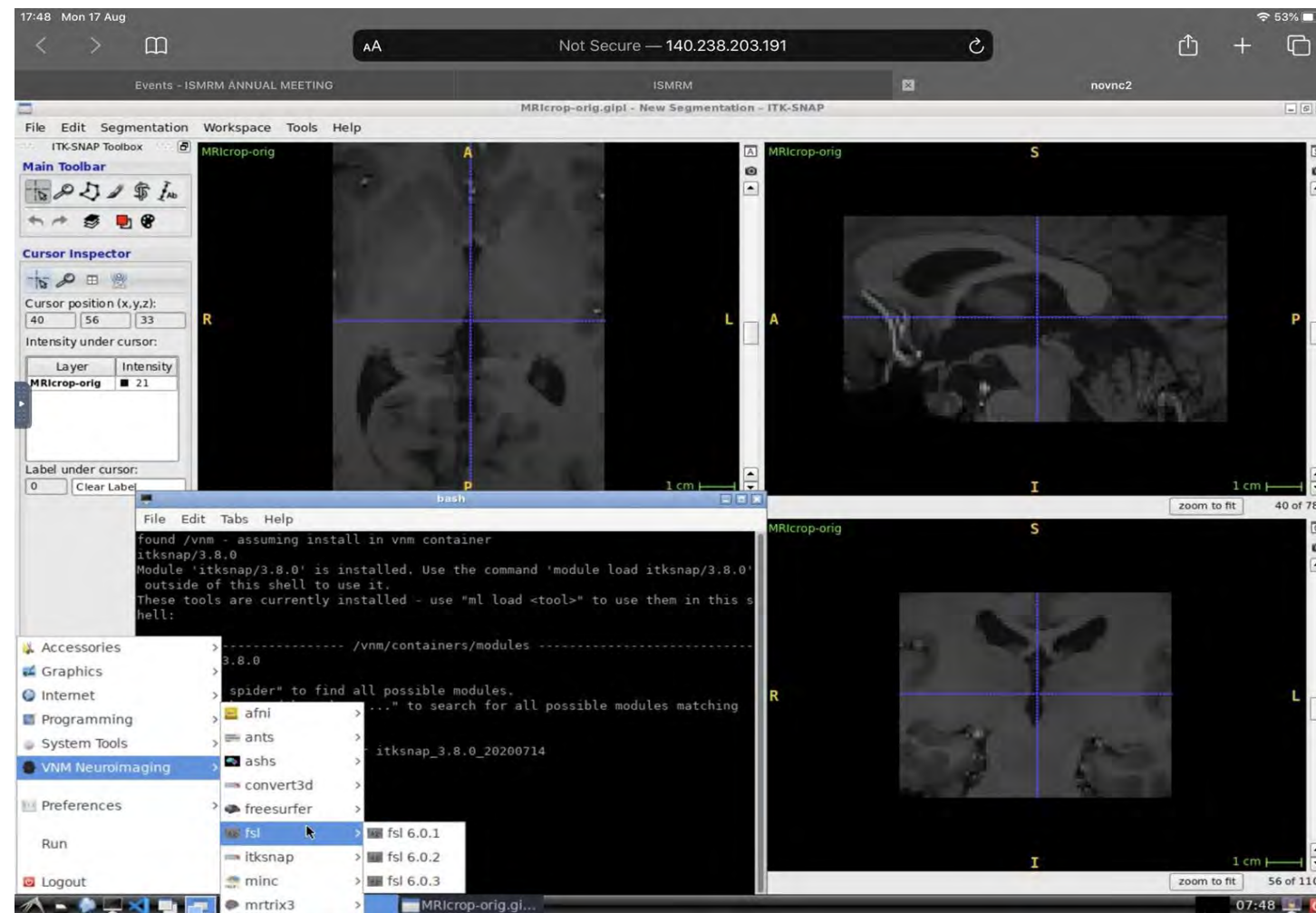


... on any cloud provider
– the sky is the limit



Outlook - github.com/NeuroDesk

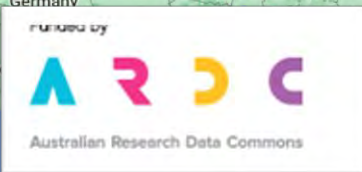
- Make start even easier
(currently requires command lines -> develop GUI)
- Integrate GPUs for DL applications
- Integrate more applications



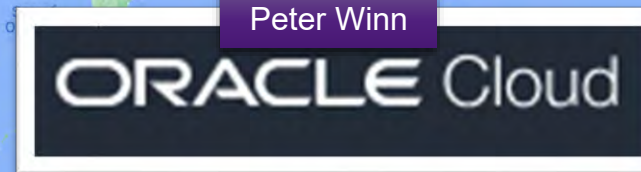
**Australian Research Container
Orchestration Service (ARCOS)**



Martin Grignard



Peter Winn



Jakub Kaczmarzyk

Niruhan Viswarupan

Dao Thanh Thuy



Yorguin Jose Mantilla

Will Woods

Aswin Narayanan

Steffen Bollmann

Tom Johnstone

Angela Renton

David White

Thomas Shaw

Oren Civier

Megan Campbell

Paris Lyons

Ryan Sullivan

