# Nordic PET-BIDS Onboarding and ezBIDS Workshop: 28-29 August 2025

## Analysis Workflows, Derivatives, and BIDS Apps

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NIH National Institute of Mental Health

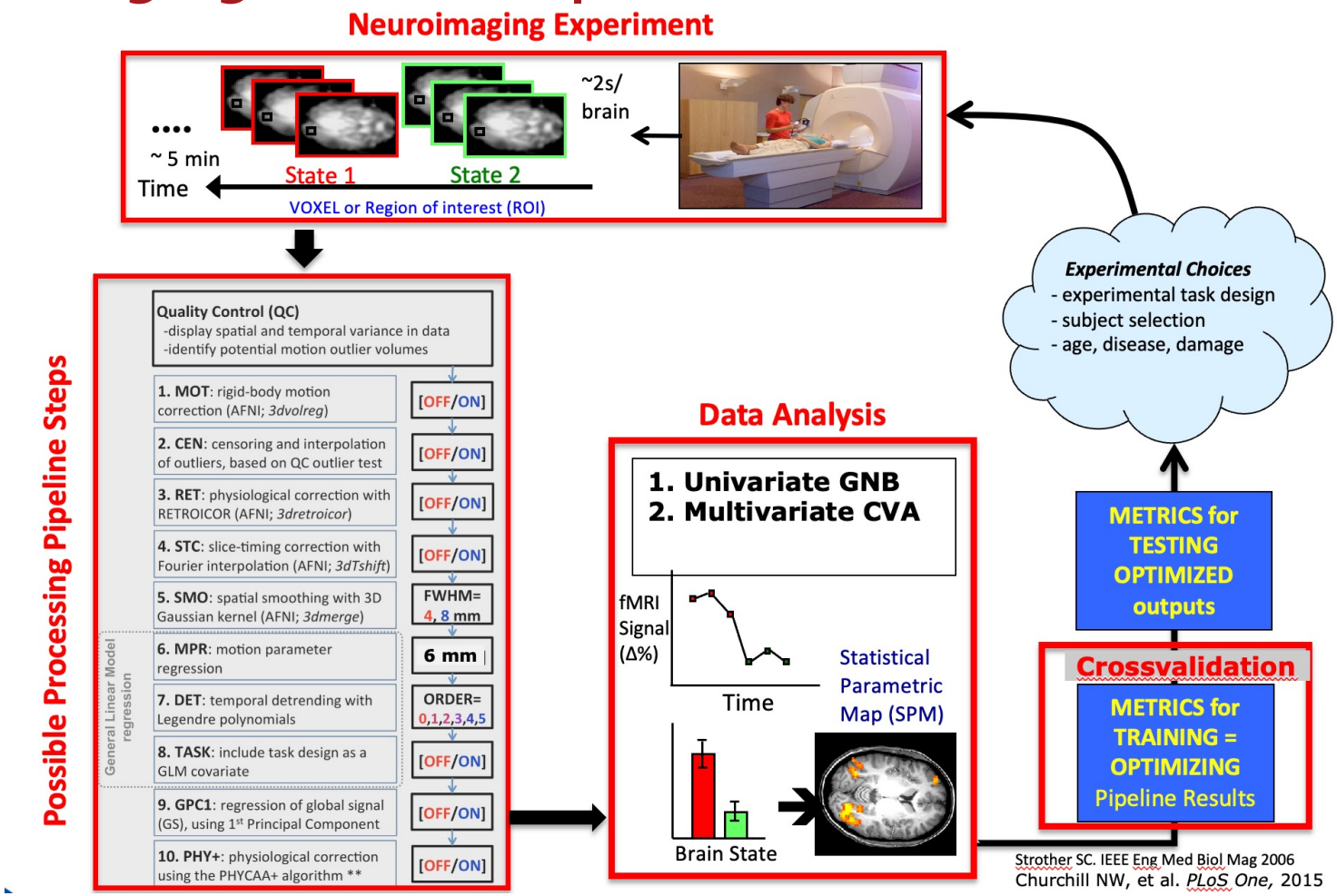
Stanford | Center for Reproducible Neuroscience

UNIVERSITY OF COPENHAGEN

# Agenda

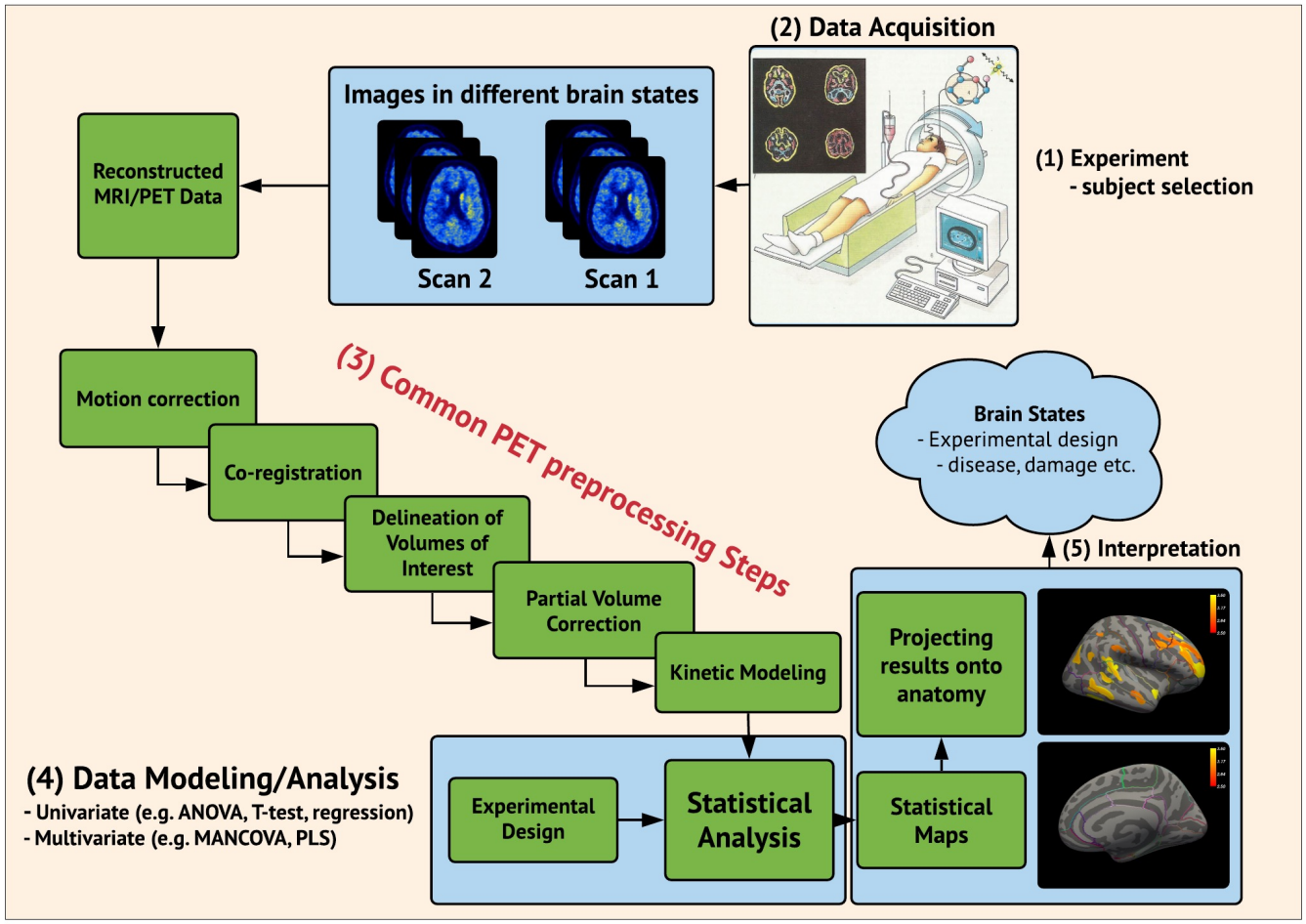
- BIDS Applications
- Derivatives
- Executing analysis workflows using containers
- Questions & wrap-up

# Neuroimaging Workflow | fMRI



# Neuroimaging Workflow | PET

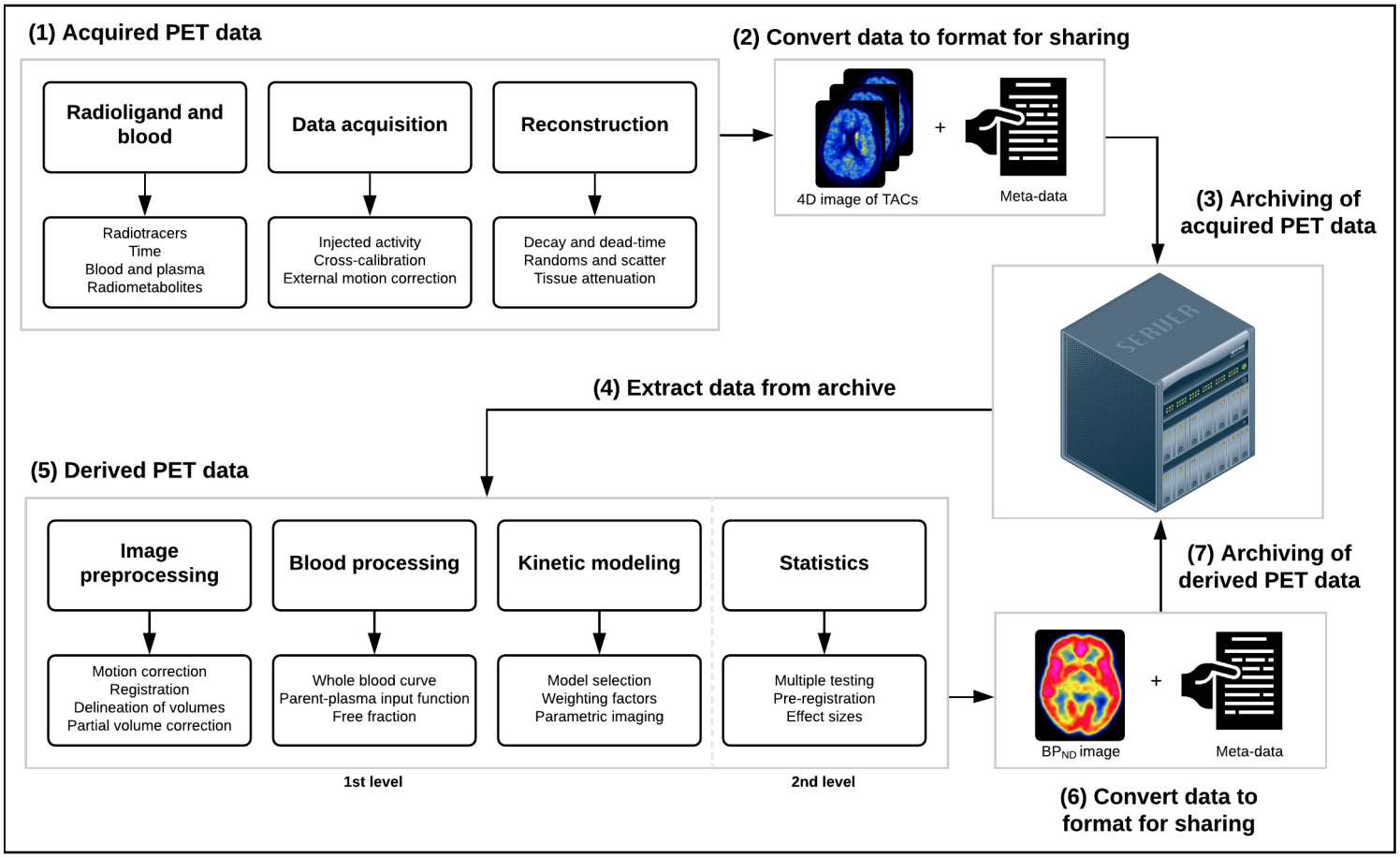
Norgaard et al. 2019, Neuroimage 199, 466-479.




## Stages

1. Subject selection
2. Data acquisition
3. Preprocessing
4. Data modeling
5. Interpretation

# Neuroimaging Workflow | Dataflow




Knudsen & Innis et al. 2020, JCBFM

# BIDS – more reproducible research

## BIDS defines a clear interface

- Standardized through a large-community agreement
- Human readable (as opposed to DICOM)
- Machine readable (enabling tooling, see below)
- Stable (e.g., backward compatibility principle), extensible, and predictable (*BIDS Schema*)

## Harnesses data-sharing and archival (sharing with self)

- Can be checked for correctness (*BIDS Validator*)
- Establishes a solid *contract* on the organization of data between authors and reusers (or your future self)
- Separates *data blobs* and metadata, facilitating agile management and understanding of the dataset, HPC operations (e.g., *datalad drop*), etc.
- Enables open-sharing (e.g., *OpenNeuro*)

## Supports tooling

- Querying the dataset, filtering data, etc. (*PyBIDS*)
- Conversion from other formats (mostly *DICOM*)
- Interpreting unprocessed data (development of *BIDS Apps* such as *MRIQC* or *fMRIPrep*)
- *BIDS Derivatives* enable concatenating *BIDS Apps* (e.g., *fMRIPrep* + *XCPD*, *brainlife.io*)
- Data-management-friendly (*DataLad*)

# BIDS Applications

A common specification of neuroimaging datasets affords queries for and adaptation to the available data.

* Note that `participant` is an analysis level. Apps may also operate at the `run`, `session` or `group` levels.

# BIDS Applications

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Queryable (meta)data allows a very simple protocol for a BIDS App:

```
bids-app /bids-directory /output-directory participant [OPTIONS]
```

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## Examples

### MRIQC

```
mriqc /data/bids/openneuro/ds000228 /data/processed/ds000228-mriqc group
```

* Note that `participant` is an analysis level. Apps may also operate at the `run`, `session` or `group` levels.

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## Examples

### MRIQC

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mriqc /data/bids/openneuro/ds000228 /data/processed/ds000228-mriqc group
```

### fMRIPrep

```
fmriprep /data/bids/openneuro/ds000228 /data/processed/ds000228-fmriprep \
    participant --participant-label pixar001
```

* Note that `participant` is an analysis level. Apps may also operate at the `run`, `session` or `group` levels.

# BIDS Applications

## Many application types are possible

## Available BIDS Apps

| | | | |
|---|---|---|---|
| BIDS-Apps/example | version 0.0.7 | open bug issues 0 | build passing |
| BIDS-Apps/freesurfer | version | open bug issues 0 | build failing |
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| BIDS-Apps/BROCCOLI | version v1.0.1 | open bug issues 1 | build passing |
| BIDS-Apps/FibreDensityAndCrosssection | version v0.0.1 | open bug issues 0 | build passing |
| BIDS-Apps/SPM | version v0.0.15 | open bug issues 1 | build passing |
| poldracklab/mriqc | version 0.14.2 | open bug issues 5 | build passing |
| BIDS-Apps/QAP | Image not found | open bug issues 0 | build passing |
| BIDS-Apps/CPAC | version v1.0.1a_22 | open bug issues 0 | build passing |
| BIDS-Apps/hyperalignment | Image not found | open bug issues 0 | build passing |
| BIDS-Apps/mindboggle | version 0.0.4-1 | open bug issues 2 | build passing |
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# BIDS Applications

## Many application types are possible

- Quality control

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# BIDS Applications

## Many application types are possible

- Quality control
- Anatomical pipelines

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- Functional pipelines
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# BIDS Applications

## Many application types are possible

- Quality control
- Anatomical pipelines
- Functional pipelines
- Diffusion pipelines

## Lowered friction encourages adoption

- Researchers gain easy access to tools by formatting data in BIDS
- Accepting BIDS datasets makes your tools easy to try

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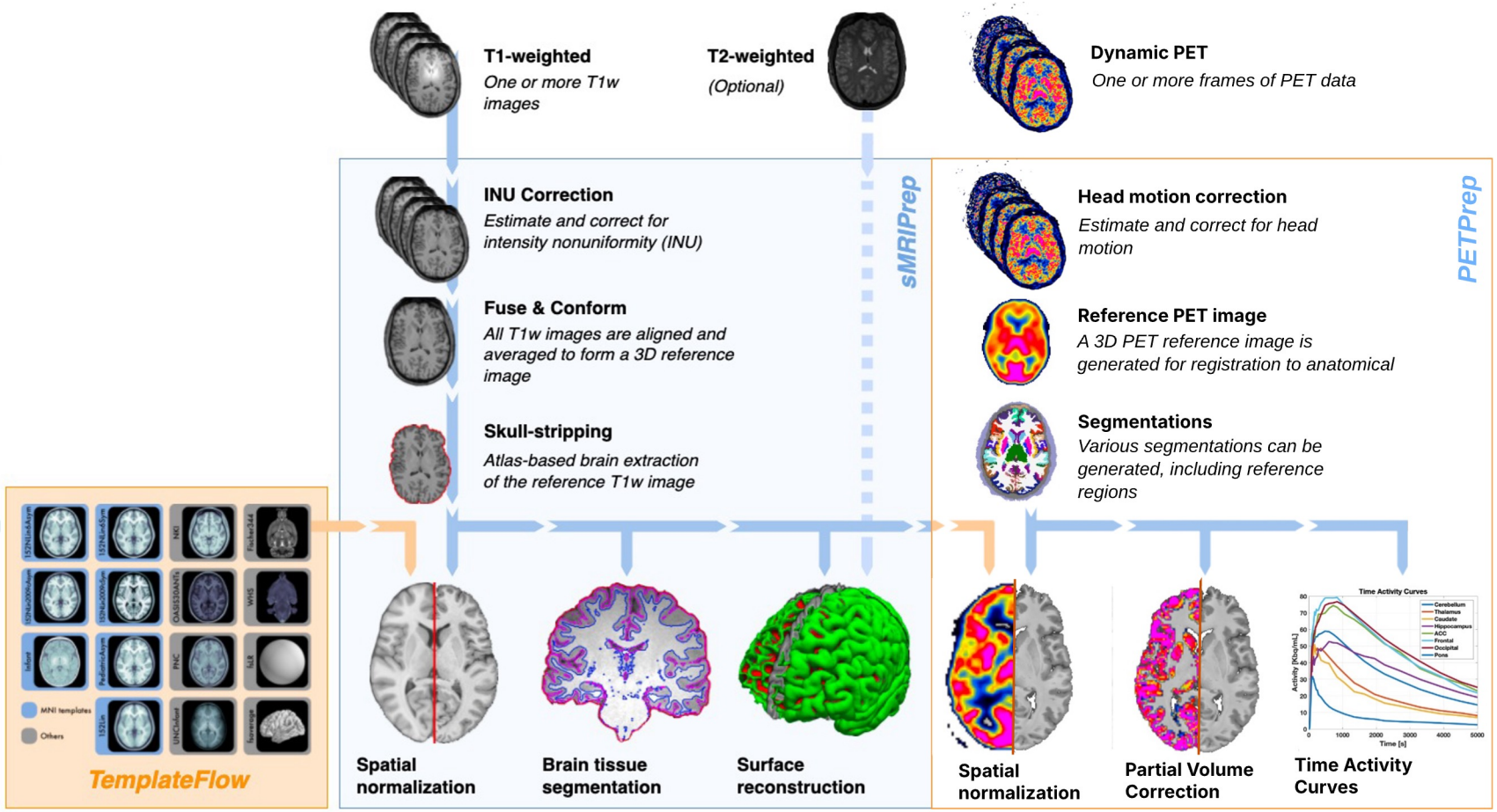
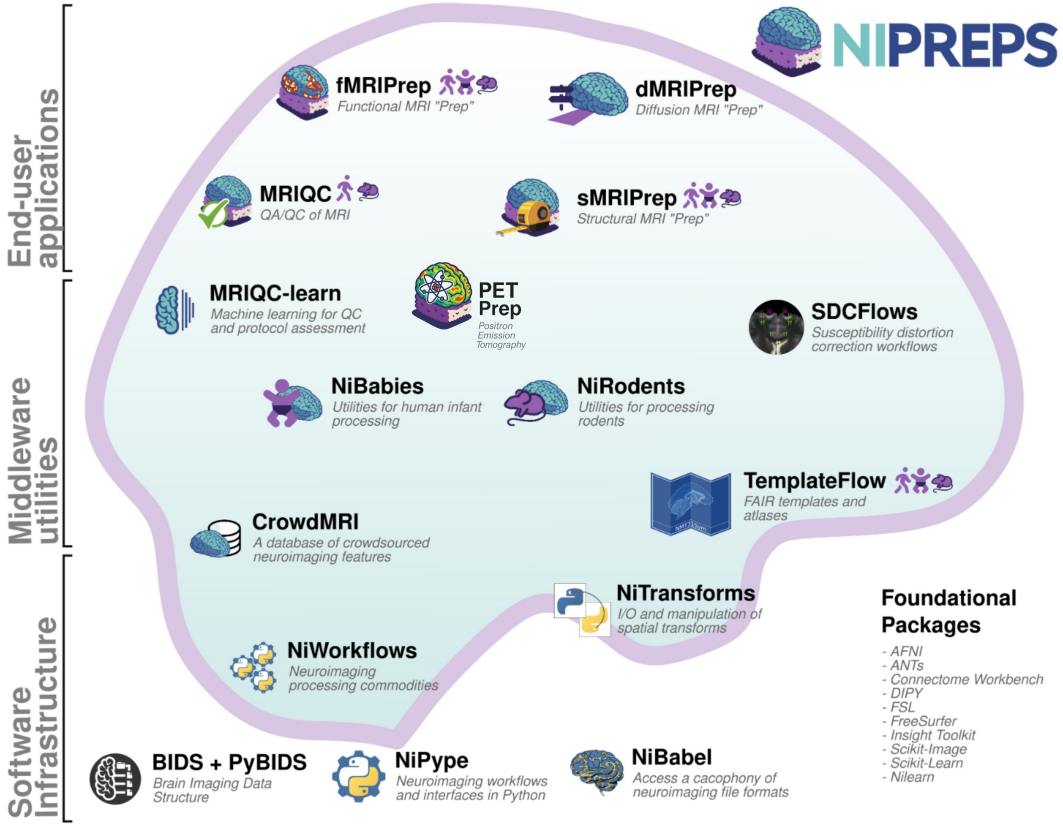
# BIDS Applications | PETPrep

https://github.com/nipreps/petprep

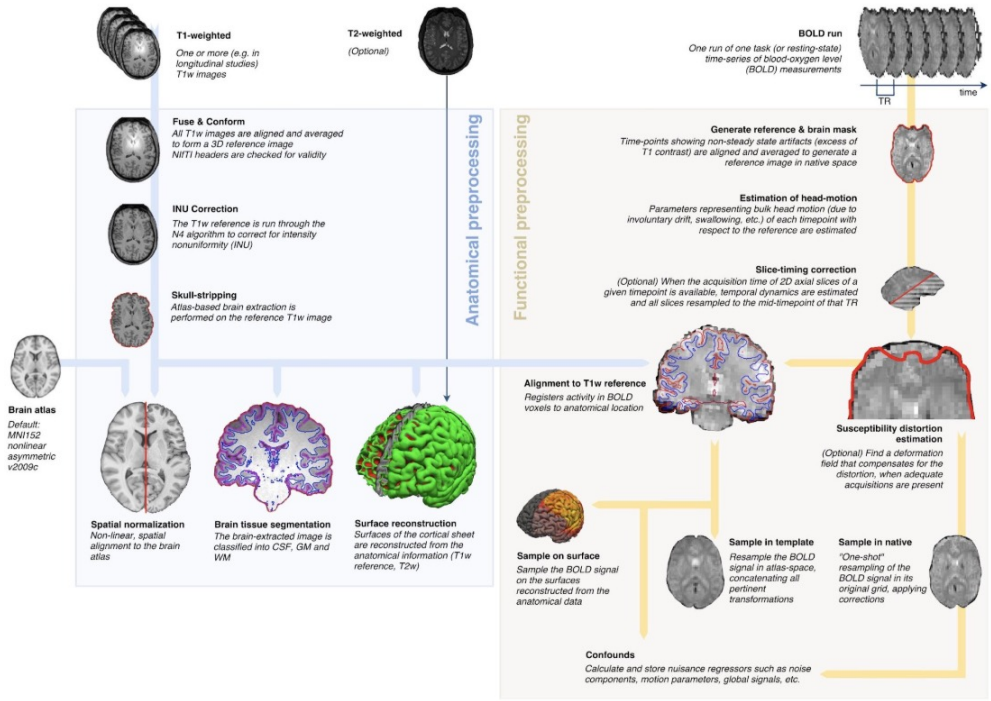


# An open source software ecosystem for neuroimaging



# fMRIPrep: a new design pattern for fMRI preprocessing

- **A robust workflow for preprocessing fMRI data**
  - Adapt to each dataset and processes it in the best way possible
  - Outputs to BIDS-Derivatives format
  - Provides powerful visualizations :
    - to help identify problems
    - allowing glass-box access to help train researchers

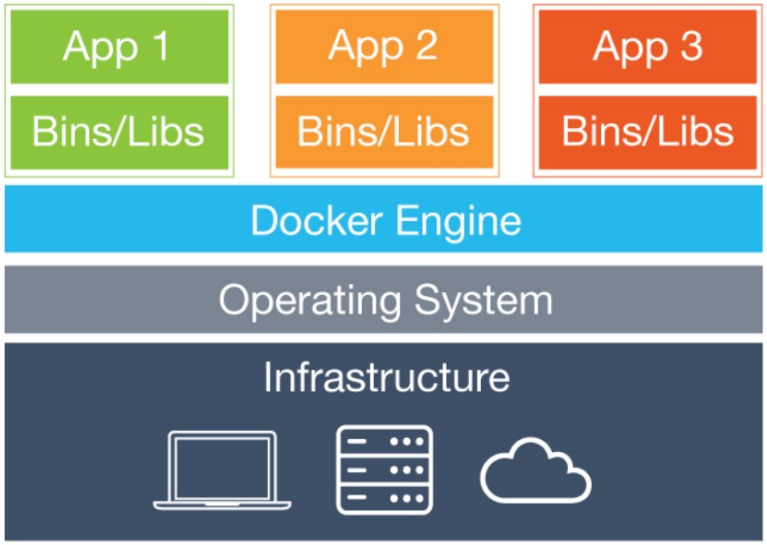



**Cited 3691 times**

Esteban et al. 2019

# BIDS apps: Improving ease of use, accessibility, and reproducibility of neuroimaging data analysis methods

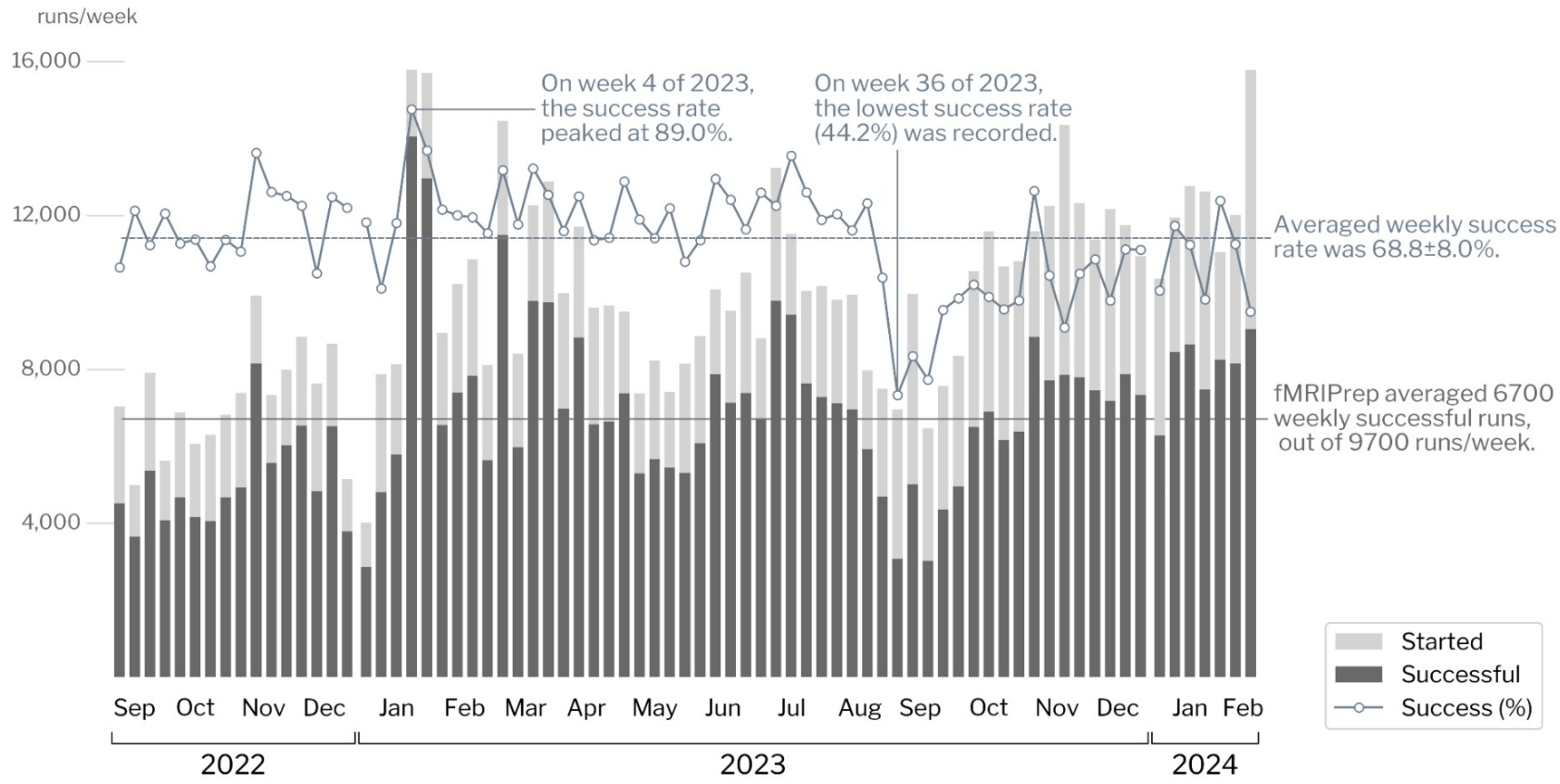
Krzysztof J. Gorgolewski[1]*, Fidel Alfaro-Almagro[2], Tibor Auer[3], Pierre Bellec[4,5], Mihai Capotă[6], M. Mallar Chakravarty[7,8], Nathan W. Churchill[9], Alexander Li Cohen[10], R. Cameron Craddock[11,12], Gabriel A. Devenyi[7,8], Anders Eklund[13,14,15], Oscar Esteban[1], Guillaume Flandin[16], Satrajit S. Ghosh[17,18], J. Swaroop Guntupalli[19], Mark Jenkinson[2], Anisha Keshavan[20], Gregory Kiar[21,22], Franziskus Liem[23], Pradeep Reddy Raamana[24,25], David Raffelt[26], Christopher J. Steele[7,8], Pierre-Olivier Quirion[15], Robert E. Smith[26], Stephen C. Strother[24,25], Gaël Varoquaux[27], Yida Wang[6], Tal Yarkoni[28], Russell A. Poldrack[1]




BIDS App: A containerized software application

The container encapsulates all software and dependencies
- allows better reproducibility

# Telemetry provides information about usage and user success



# fMRIPrep/MRIQC stress test

- All relevant datasets from OpenNeuro are being run through fMRIPrep and MRIQC
  - Pathways allocation on TACC Frontera (1.68M core-hours)
  - All derivatives are being shared on OpenNeuro
- To date:
  - 320 datasets run with MRIQC
  - 73 datasets run with fMRIPrep
- This test has revealed a number of issues that has driven several improvements

TACC
TEXAS ADVANCED COMPUTING CENTER

From: help@consult.tacc.utexas.edu

Hello Joe,

Your access was once again revoked, this time due to the unmanageable quantity of files and empty directories in your /scratch1 space. We're seeing activity of up to 40 million files in less than a 24-hour span, which is putting an unreasonable strain on the file system servers. You will need to bring this down to below 15 million in total as well as address this activity in your jobs to prevent putting so much stress on the system during your runs.

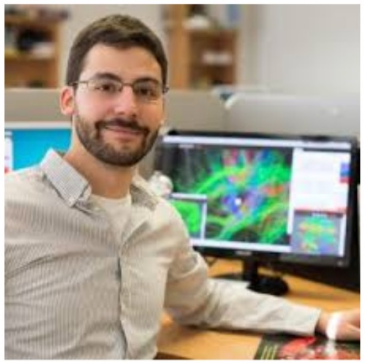
# fMRIPrep: implementing a fit/transform model

Execute the minimal flow of operations to generate the minimal set of derivative results (“fit”) that are sufficient to deterministically [re]generate (“transform”) any necessary output.

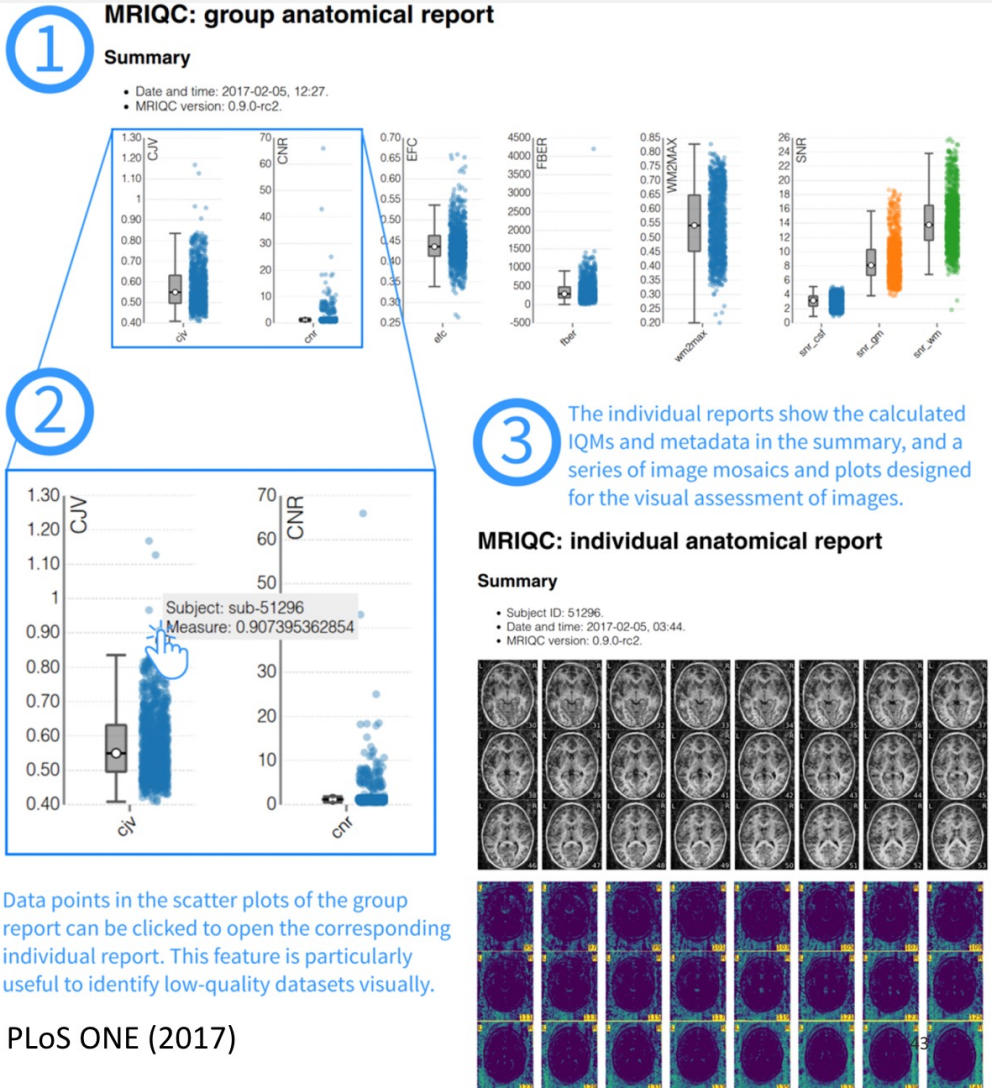
- Generating minimal derivatives shifts workflows to higher CPU and lower I/O usage, taking advantage of HPC strengths.
- Avoiding saving resampled BOLD series allows more registrations to target spaces (MNI, fsaverage, fsLR) to be calculated with little impact on storage costs.
- Enables one-shot resamplings

| | **Derivatives** | **Work dir** | **Total** |
|---|---|---|---|
| **v23.1.4 (latest)** | 2.7GB 184 files | 43GB 28K files | |
| **v23.2.0. dev (next)** | 461MB 126 files | 4.5GB 6.1K files | |
| **Δ Size** | -2.2GB | -38.5GB | -41GB (-89%) |
| **Δ Files** | -58 | -22K | -22K (-78%) |

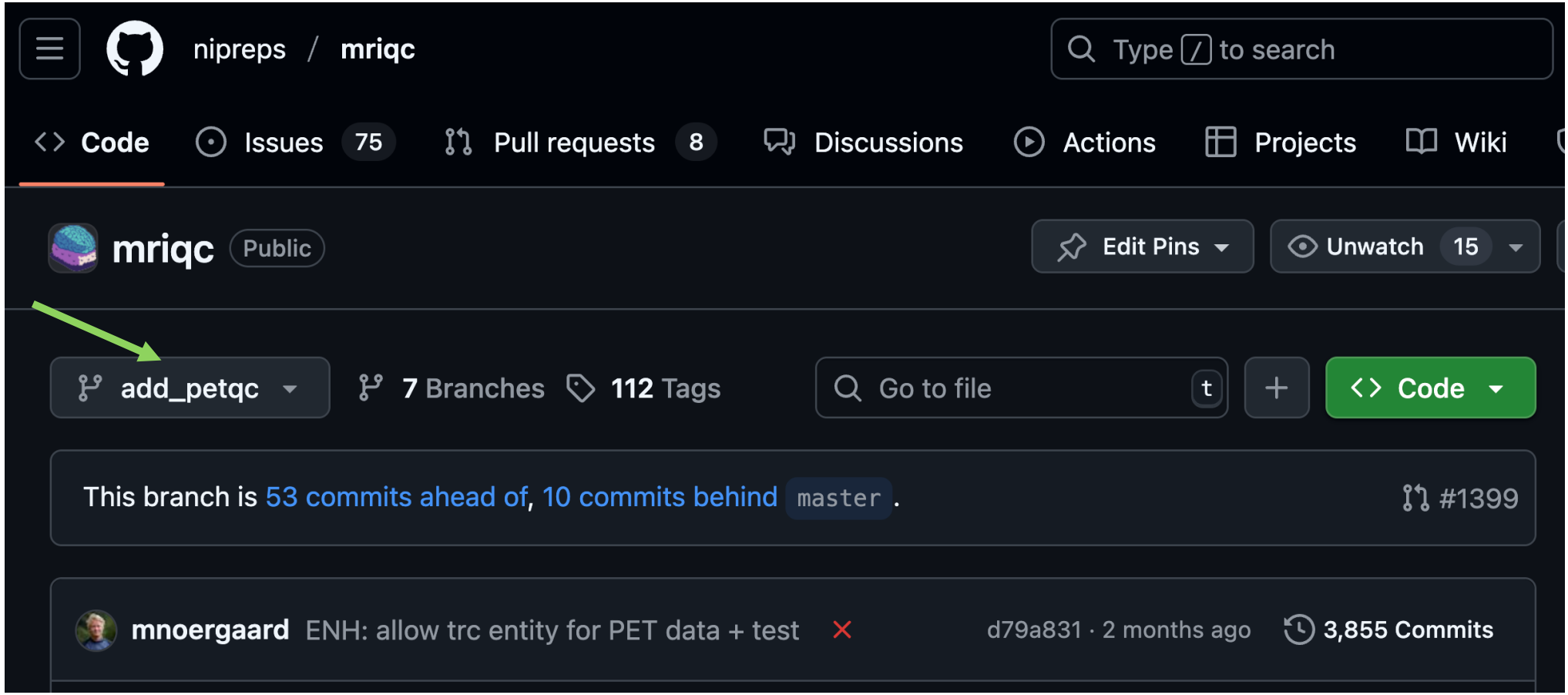
# MRIQC: Robust quality control for MRI



Oscar Esteban




Esteban et al. PLoS ONE (2017)

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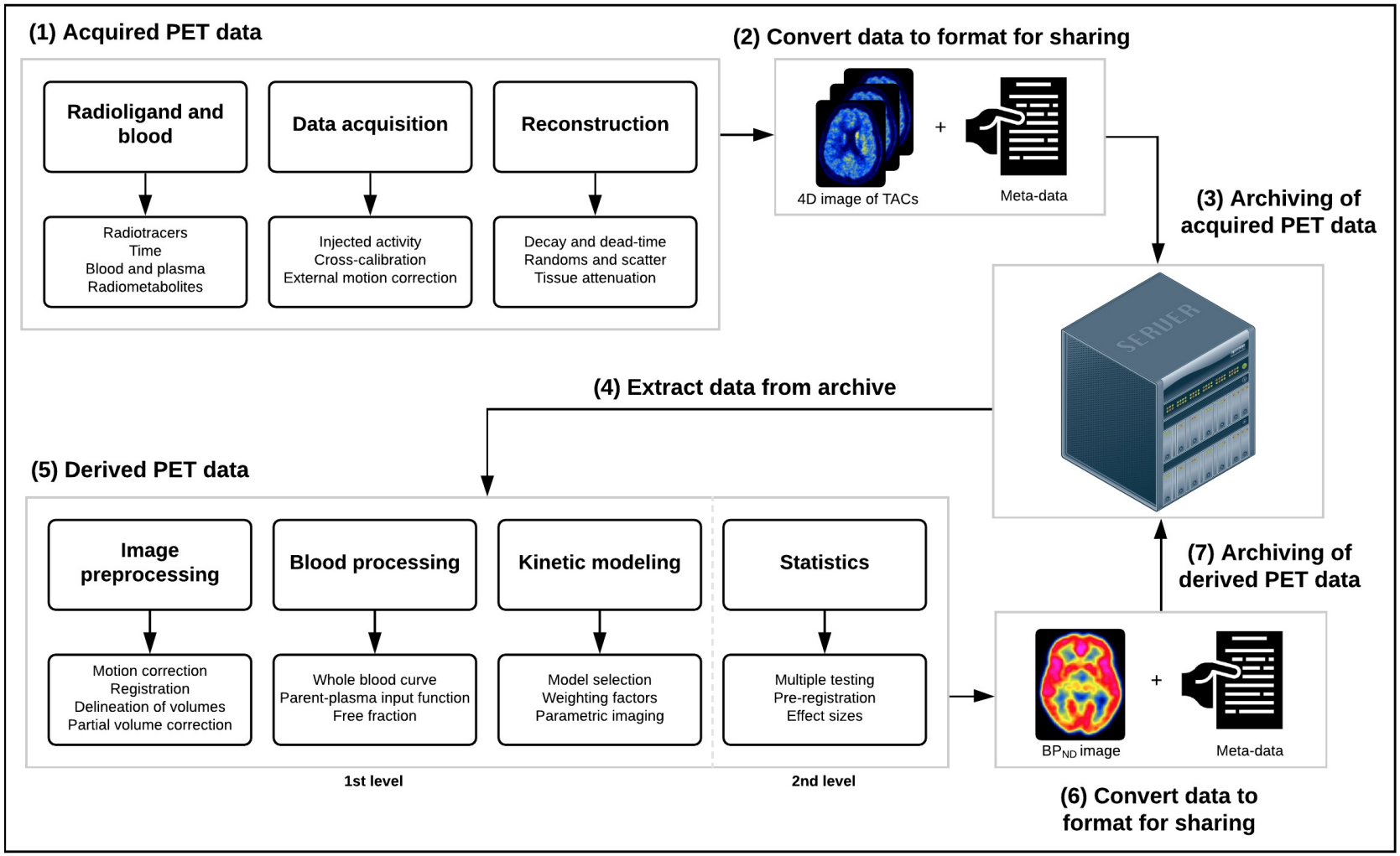


Knudsen & Innis et al. 2020, JCBFM

# BIDS Derivatives

BIDS Derivatives generally mirror the raw dataset.

```
fmriprep/
    README
    dataset_description.json
    sub-11
        anat/
            sub-11_desc-preproc_T2w.nii.gz
            sub-11_acq-denoised_desc-preproc_T1w.nii.gz
            sub-11_acq-denoised_desc-brain_mask.nii.gz
            sub-11_acq-denoised_from-T1w_to-MNI152NLin2009cAsym_mode-image_xfm.h5
            ...
        fmap/
            sub-11_fmapid-auto00000_desc-coeff_fieldmap.nii.gz
            sub-11_fmapid-auto00000_desc-magnitude_fieldmap.nii.gz
            sub-11_fmapid-auto00000_desc-preproc_fieldmap.nii.gz
        func/
            sub-11_task-mixed_desc-coreg_boldref.nii.gz
            sub-11_task-mixed_desc-hmc_boldref.nii.gz
            sub-11_task-mixed_from-boldref_to-T1w_mode-image_desc-coreg_xfm.txt
            sub-11_task-mixed_from-boldref_to-auto00000_mode-image_desc-fmapreg_xfm.txt
            sub-11_task-mixed_from-orig_to-boldref_mode-image_desc-hmc_xfm.txt
            sub-11_task-mixed_space-MNI152NLin2009cAsym_desc-preproc_bold.nii.gz
            ...
    sub-14
    sub-15
```

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            sub-11_acq-denoised_desc-brain_mask.nii.gz
            sub-11_acq-denoised_from-T1w_to-MNI152NLin2009cAsym_mode-image_xfm.h5
            ...
        fmap/
            sub-11_fmapid-auto00000_desc-coeff_fieldmap.nii.gz
            sub-11_fmapid-auto00000_desc-magnitude_fieldmap.nii.gz
            sub-11_fmapid-auto00000_desc-preproc_fieldmap.nii.gz
        func/
            sub-11_task-mixed_desc-coreg_boldref.nii.gz
            sub-11_task-mixed_desc-hmc_boldref.nii.gz
            sub-11_task-mixed_from-boldref_to-T1w_mode-image_desc-coreg_xfm.txt
            sub-11_task-mixed_from-boldref_to-auto00000_mode-image_desc-fmapreg_xfm.txt
            sub-11_task-mixed_from-orig_to-boldref_mode-image_desc-hmc_xfm.txt
            sub-11_task-mixed_space-MNI152NLin2009cAsym_desc-preproc_bold.nii.gz
            ...
    sub-14
    sub-15
```

**New file suffixes, extensions and entities are possible.**

# PyBIDS

```
pip install pybids
```

A common specification of neuroimaging datasets affords queries for and adaptation to the available data.

PyBIDS is a Python library for querying and manipulating BIDS datasets.

```
>>> from bids import BIDSLayout
>>> layout = BIDSLayout('/my_dataset')
>>> bold = layout.get(subject='11', task='rest', suffix='bold', extension='.nii.gz')
>>> bold
[<BIDSImageFile filename='/my_dataset/sub-11/func/sub-11_task-rest_bold.nii.gz'>]
>>> md = bold[0].get_metadata()
>>> md['RepetitionTime']
1.5
>>> bold[0].get_entities()
{'datatype': 'func',
 'extension': '.nii.gz',
 'subject': '11',
 'suffix': 'bold',
 'task': 'rest'}
```

# PyBIDS | Derivatives

```
pip install pybids
```

PyBIDS layouts support BIDS derivatives:

```
>>> fmri_derivs = BIDSLayout(
...     '/my_dataset-fmriprep',
...     config=['bids', 'derivatives'],
...     validate=False,
... )
>>> spaces = fmri_derivs.get_spaces(desc='preproc', suffix='bold')
>>> spaces
['MNI152NLin2009cAsym']
```

# PyBIDS | Derivatives

```
pip install pybids
```

PyBIDS layouts support BIDS derivatives:

```
>>> fmri_derivs = BIDSLayout(
...     '/my_dataset-fmriprep',
...     config=['bids', 'derivatives'],
...     validate=False,
... )
>>> spaces = fmri_derivs.get_spaces(desc='preproc', suffix='bold')
>>> spaces
['MNI152NLin2009cAsym']
```

It is also possible to provide your own config:

```
>>> import niworkflows
>>> nipreps_config = niworkflows.data.load('nipreps.json')
>>> fmri_derivs = BIDSLayout('/my_dataset-fmriprep', config=[nipreps_config], validate=False)
```

# PyBIDS | Large datasets

```
pip install pybids
```

*BIDS Apps* can spend long time indexing if they rely on *PyBIDS*

**create a cache**:

```
$ pybids layout --reset-db --no-validate --index-metadata . /my_dataset/.bids-index/
```

And then inform your *BIDS App*.

In the case of *MRIQC* and *fMRIPrep*, point the `--bids-database-dir` argument to the newly created cache:

```
$ mriqc /data/input /derivatives/output participant [OPTIONS] \
    --bids-database-dir /my_dataset/.bids-index/
```

```
$ fmriprep /data/input /derivatives/output participant [OPTIONS] \
    --bids-database-dir /my_dataset/.bids-index/
```

# Containerizing preprocessing tools to improve reproducibility

- What are containers and why researchers care?
- Docker

# What are containers?

Why do we care?

*A container is a unit of software that packages code with its required dependencies in order to run in an isolated, controlled environment. This allows you to run an application in a way that is predictable, repeatable, and without the uncertainty of inconsistent code execution across diverse development and production environments. A container will always start up and run code the same way, regardless of what machine it exists on.*

https://www.digitalocean.com/community/conceptual-articles/introduction-to-containers

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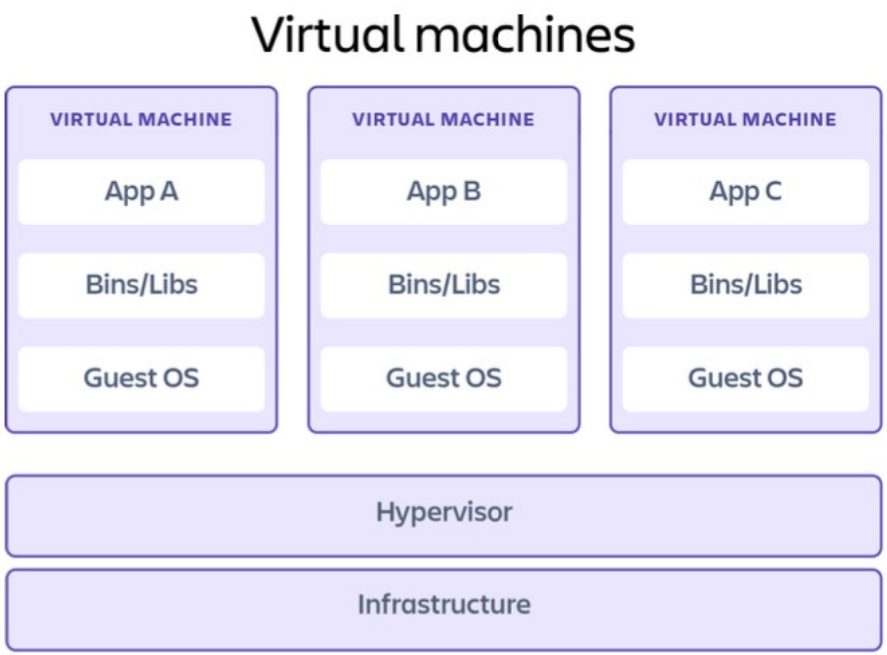
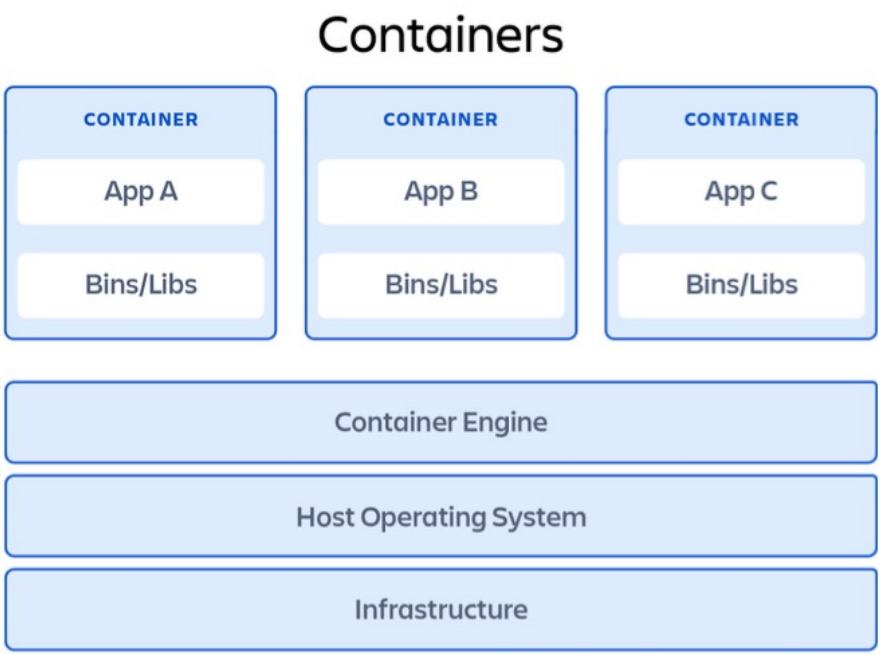
https://www.digitalocean.com/community/conceptual-articles/introduction-to-containers

# Isn't this the same as virtual machines?




From the Atlassian documentation

# First contact with docker

# Container Images

Images are software bundles

- when executed become containers

Images are made of layers

- each layer encapsulates a set of filesystem changes
- layers are akin to software deployment steps

Layers are **unmutable**

- except for a R/W layer that is added on top by the container runtime

Layers are described in the `Dockerfile`

- The `Dockerfile` establishes the instructions to create an image
- The `Dockerfile` is some sort of recipe

# Building an image: docker/whalesay

## 1 The `Dockerfile`

```
# Containers are generally bootstrapped from an existing OS image
# Alpine Linux is a Linux distribution very small and simple
# It's special in that it is not based on the GNU Core Utilities
FROM alpine

# Our container will need perl
RUN apk add --no-cache perl

# Copy the original 'cowsay' program into one layer
COPY cowsay /usr/local/bin/cowsay

# Ensure permissions
RUN chmod a+rx /usr/local/bin/cowsay

# Copy the replacement of the cow asciiart with a whale
COPY docker.cow /usr/local/share/cows/default.cow

# Instruct the runtime to execute the new program
ENTRYPOINT ["/usr/local/bin/cowsay"]
```

# Building an image: docker/whalesay

## 2 The `cowsay` script

Because it is a very long perl script, we just download it:

```
$ curl https://raw.githubusercontent.com/docker/whalesay/master/cowsay -o cowsay
```

# Building an image: docker/whalesay

## 3 The replacement for the cow (`docker.cow`)

```
##
## Docker Cow
##
$the_cow = <<EOC;
    $thoughts
     $thoughts
      $thoughts
EOC
$the_cow .= <<'EOC';
                    ##         .
              ## ## ##        ==
           ## ## ## ## ##    ===
       /""""""""""""""""\___/ ===
      {                       /  ===-
       \______ O           __/
         \    \         __/
          \____\_______/

EOC
```

# Building an image: docker/whalesay

## 4 Build it

```
$ docker build -t oesteban/whalesay .
```

# Docker images and the *Docker Hub*

Images can be distributed through **registries**.

- *Docker*'s official registry is called *Docker Hub*
- Thanks to *Docker Hub* we could fetch and execute the `hello-world` image
- Website: hub.docker.com

- PETPrep_hmc

```
docker pull martinnoergaard/petprep_hmc:latest
```

# Example of Dockerfile (part 1)

Dockerfile

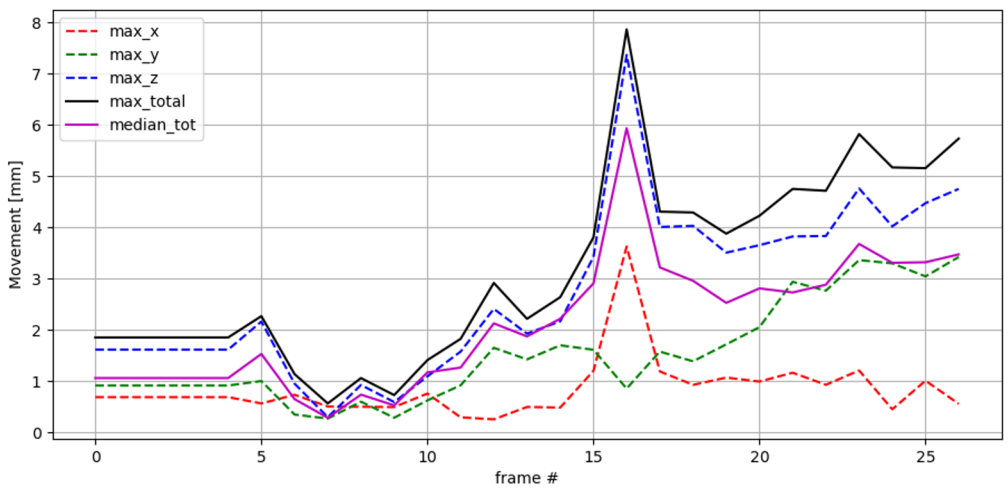
```
# Use the official Python base image for x86_64
FROM --platform=linux/x86_64 python:3.9

# Download QEMU for cross-compilation
ADD https://github.com/multiarch/qemu-user-static/releases/download/v6.1.0-8/qemu-x86_64-static /usr/bin/qemu-x86_64-static
RUN chmod +x /usr/bin/qemu-x86_64-static

# Install required dependencies for FSL and Freesurfer
RUN apt-get update && apt-get install -y --no-install-recommends \
    build-essential \
    curl \
    ca-certificates \
    git \
    tcsh \
    xfonts-base \
    gfortran \
    libjpeg62 \
    libtiff5-dev \
    libpng-dev \
    unzip \
    libxext6 \
    libx11-6 \
    libxmu6 \
    libglib2.0-0 \
    libxft2 \
    libxrender1 \
    libxt6

# Install FSL
ENV FSLDIR="/opt/fsl" \
    FSLOUTPUTTYPE=NIFTI_GZ \
    PATH="/opt/fsl/bin:$PATH"
```

# Example of Dockerfile (part 2)

```
RUN curl -sL https://fsl.fmrib.ox.ac.uk/fsldownloads/fslinstaller.py -o fslinstaller.py && python3 fslinstaller.py -d /opt/fsl -o && echo ". /opt/fsl/etc/fslconf/fsl.sh"
>> ~/.bashrc

# Install Freesurfer
ENV FREESURFER_HOME="/opt/freesurfer" \
    PATH="/opt/freesurfer/bin:$PATH" \
    SUBJECTS_DIR="/data/output"

RUN curl -sL https://surfer.nmr.mgh.harvard.edu/pub/dist/freesurfer/7.4.1/freesurfer-linux-centos7_x86_64-7.4.1.tar.gz | tar xzC /opt && \
    echo ". /opt/freesurfer/SetUpFreeSurfer.sh" >> ~/.bashrc

ENV PATH="/usr/local/bin:$PATH"

# Install BIDS application and its dependencies
RUN pip3 install numpy nibabel pybids bids-validator

# Clone and install petprep_hmc from GitHub
RUN rm -rf /opt/petprep_hmc && git clone https://github.com/mnoergaard/petprep_hmc.git /opt/petprep_hmc
RUN pip3 install --no-cache-dir -e /opt/petprep_hmc

# BIDS App entry point
ENTRYPOINT ["python3", "/opt/petprep_hmc/run.py"]
CMD ["--help"]
```

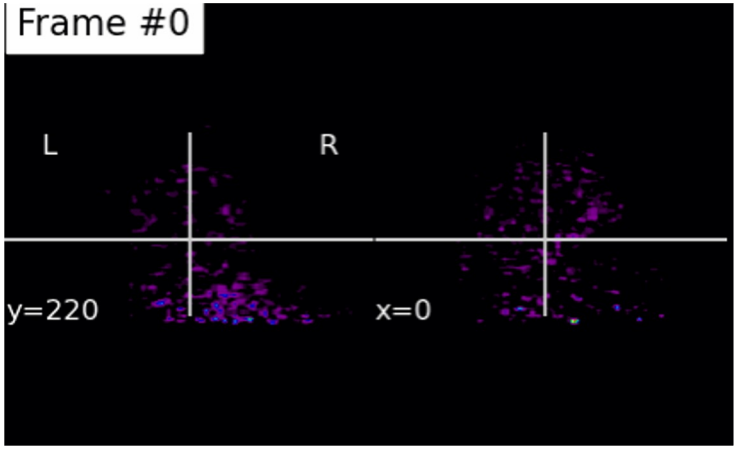
# PETPrep Robust Head Motion Correction

```
docker run -it --rm \
      -v /path/to/bids_input:/data/input \
      -v /path/to/bids_output:/data/output \
      -v /path/to/freesurfer_license:/opt/freesurfer/license.txt \
      martinnoergaard/petprep_hmc:latest \
      --bids_dir /data/input \
      --output_dir /data/output \
```

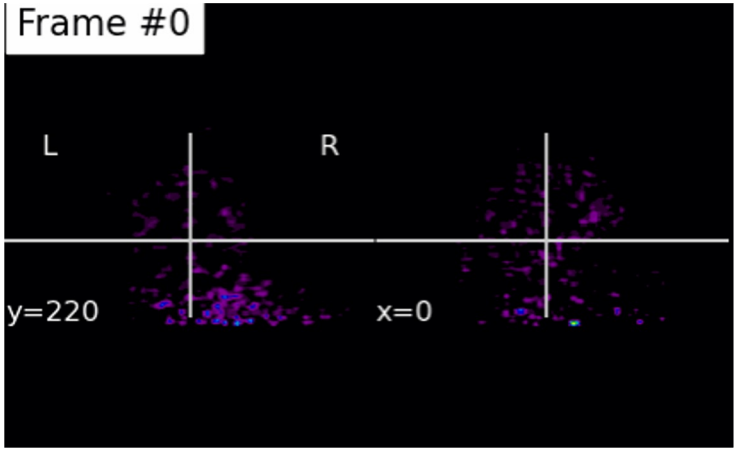



https://github.com/mnoergaard/petprep_hmc

Without motion correction

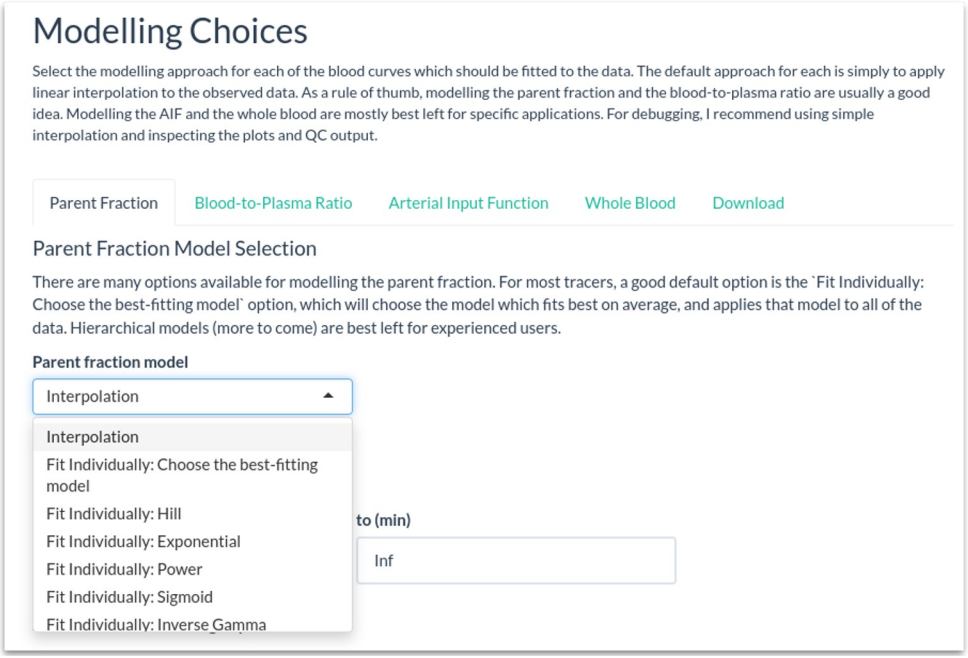


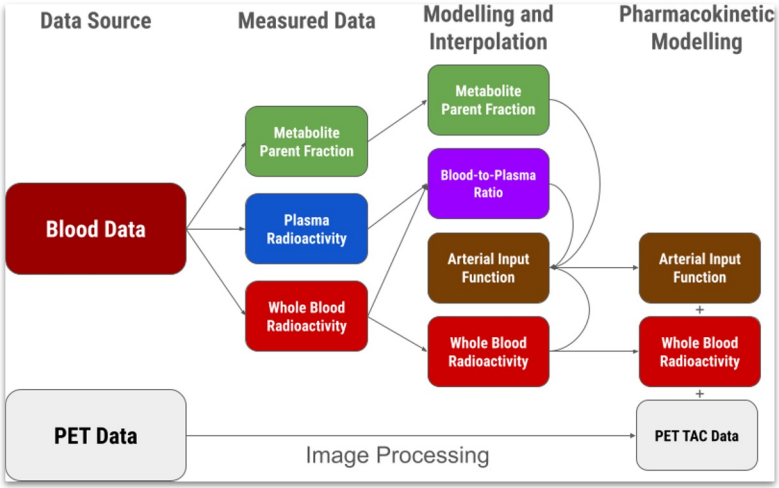

With motion correction

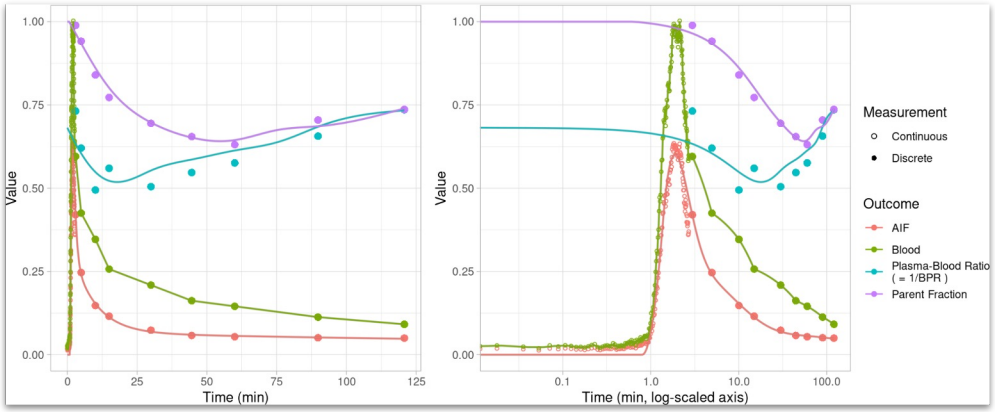


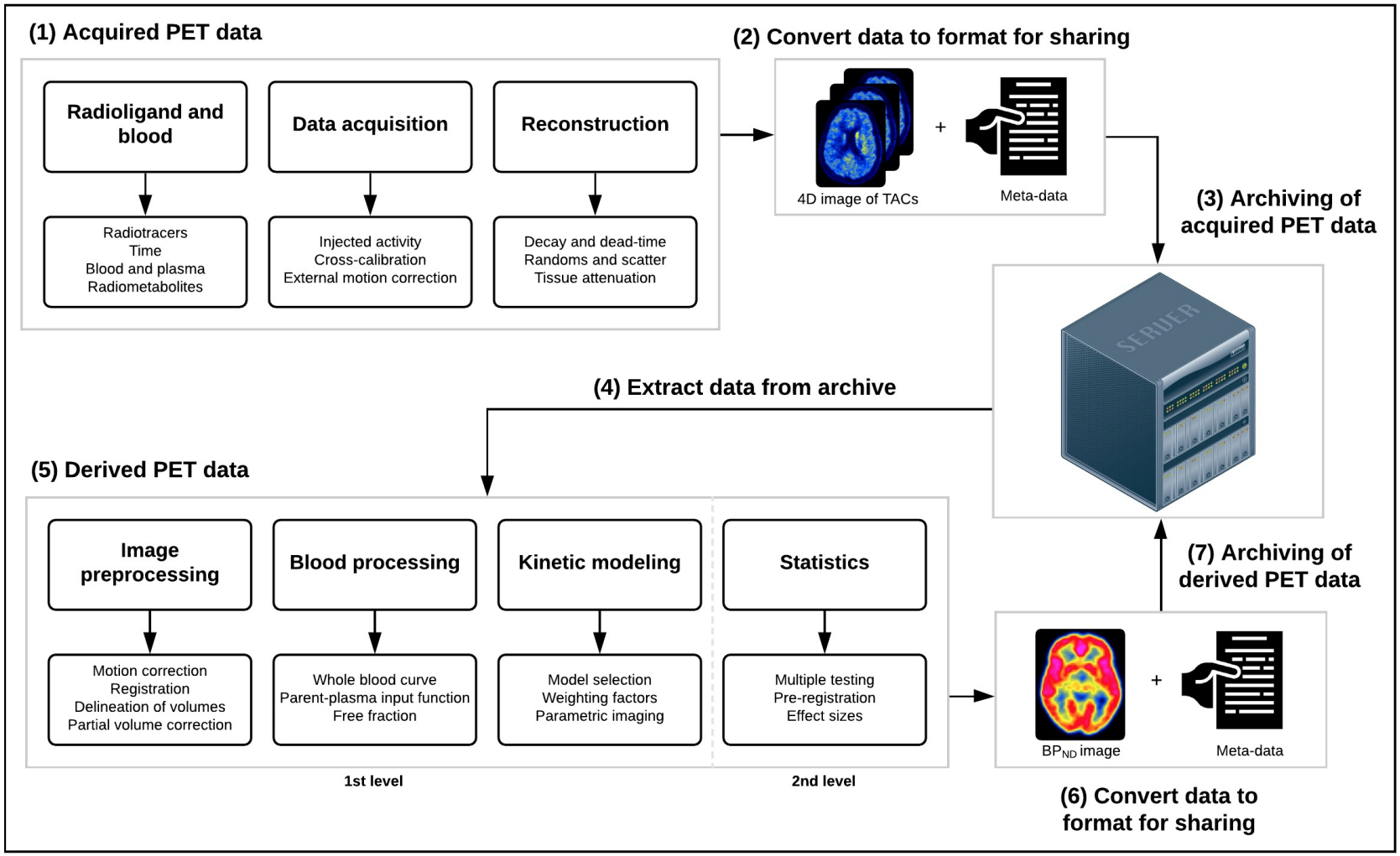
# *bloodstream* for Blood Modelling

```
docker run -v /path/:/data/ bloodstream

docker run -v /path/:/data/ bloodstream config.json
```






Knudsen & Innis et al. 2020, JCBFM

# Data sharing

**Tools for conversion**
https://bids.neuroimaging.io/tools/converters.html

**Tools for validation**
https://bids.neuroimaging.io/tools/validator.html

**Databases**
https://openneuro.org/

# Preprocessing

**BIDS applications**
https://bids.neuroimaging.io/tools/bids-apps.html

**Tools for handling data**
https://bids.neuroimaging.io/tools/others.html

# Visualization & analysis

**Visualization**
https://nilearn.github.io/dev/index.html

**Analysis**
https://nipype.readthedocs.io/en/latest/

# Discussion & wrap-up

## Key messages

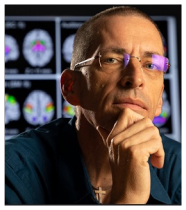
- Standardize your workflows if possible.
- Use open-source tools & formats.
- Document everything (metadata, pipelines, decisions).

# Publish your computer code: it is good enough

*Freely provided working code — whatever its quality — improves programming and enables others to engage with your research, says* **Nick Barnes**.

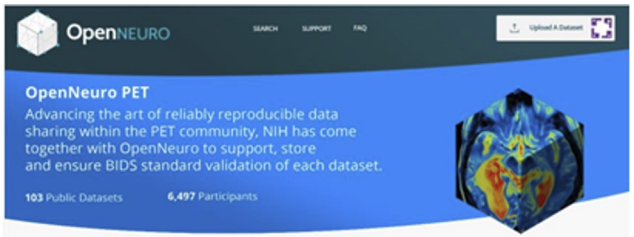
14 OCTOBER 2010 | VOL 467 | NATURE | 753

If your code is not good enough to share, then why is it good enough to publish the results that rely upon it?



Georgia State University

# Thank you for your attention



novo nordisk fonden

NIH National Institute of Mental Health

Athinoula A. Martinos Center For Biomedical Imaging

Harvard–MIT Health Sciences & Technology

MASSACHUSETTS GENERAL HOSPITAL

Stanford University

University of Copenhagen

REGION H

Rigshospitalet