

1 DataLad-Dataverse integration

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The FAIR principles (Wilkinson et al., 2016) advocate to ensure and increase the Findability, Accessibility, Interoperability, and Reusability of research data in order to maximize their impact. Many open source software tools and services facilitate this aim. Among them is the Dataverse project (King, 2007). Dataverse is open source software for storing and sharing research data, providing technical means for public distribution and archival of digital research data, and their annotation with structured metadata. It is employed by dozens of private or public institutions worldwide for research data management and data publication. DataLad (Halchenko et al., 2021), similarly, is an open source tool for data management and data publication. It provides Git- and git-annex based data versioning, provenance tracking, and decentral data distribution as its core features. One of its central development drivers is to provide streamlined interoperability with popular data hosting services to both simplify and robustify data publication and data consumption in a decentralized research data management system (Hanke, Pestilli et al., 2021). Past developments include integrations with the open science framework (Hanke, Poldrack et al., 2021) or webdav-based services such as sciebo, nextcloud, or the European Open Science Cloud (Halchenko et al., n.d.).

In this hackathon project, we created a proof-of-principle integration of DataLad with Dataverse in the form of the Python package `datalad-dataverse` (github.com/datalad/datalad-dataverse). From

a technical perspective, main achievements include the implementation of a git-annex special remote protocol for communicating with Dataverse instances, a new `create-sibling-dataverse` command that is added to the DataLad command-line and Python API by the `datalad-dataverse` extension, and standard research software engineering aspects of scientific software such as unit tests, continuous integration, and documentation.

From a research data management and user perspective, this development equips DataLad users with the ability to programmatically create Dataverse datasets (containers for research data and their metadata on Dataverse) from DataLad datasets (DataLad's Git-repository-based core data structure) in different usage modes. Subsequently, DataLad dataset contents, its version history, or both can be published to the Dataverse dataset via a 'datalad push' command. Furthermore, published DataLad datasets can be consumed from Dataverse with a `datalad clone` call. A mode parameter configures whether Git version history, version controlled file content, or both are published and determines which of several representations the Dataverse dataset takes. A proof-of-principle implementation for metadata annotation allows users to supply metadata in JSON format, but does not obstruct later or additional manual metadata annotation via Dataverse's web interface.

Overall, this project delivered the groundwork for further extending and streamlining data deposition and consumption in the DataLad ecosystem. With DataLad-Dataverse interoperability, users gain easy additional means for data publication, archival, distribution, and retrieval. Post-Brainhack development aims to mature the current alpha version of the software into an initial v0.1 release and distribute it via standard Python package indices.

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2 MOSAIC for VASO fMRI

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Vascular Space Occupancy (VASO) is a functional magnetic resonance imaging (fMRI) method that is used for high-resolution cortical layer-specific imaging (Huber et al., 2021). Currently, the most popular sequence for VASO at modern SIEMENS scanners is the one by Stirnberg and Stöcker (2021) from the DZNE in Bonn, which is employed at more than 30 research labs worldwide. This sequence concomitantly acquires fMRI BOLD and blood volume signals. In the SIEMENS' reconstruction pipeline, these two complementary fMRI contrasts are mixed together within the same time series, making the outputs counter-intuitive for users. Specifically:

- The 'raw' NIfTI converted time-series are not BIDS compatible (see <https://github.com/bids-standard/bids-specification/issues/1001>).
- The order of odd and even BOLD and VASO image TRs is unprincipled, making the ordering dependent on the specific implementation of NIfTI converters.

Workarounds with 3D distortion correction, results in interpolation artifacts. Alternative workarounds without MOSAIC decorators result in unnecessarily large data sizes.

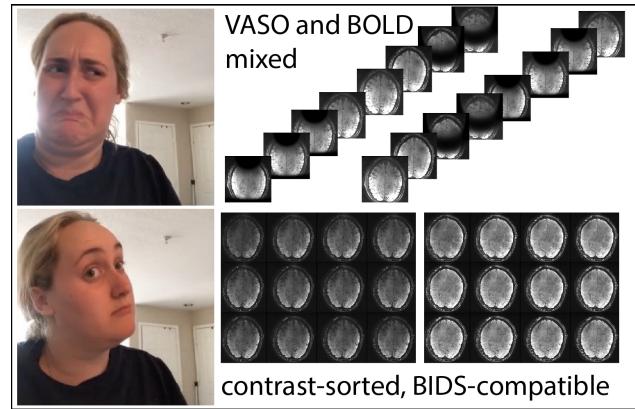


Figure 1: Previously, most VASO sequences provided unsorted image series of MRI contrasts. This was not BIDS compatible and could suffer from gradient non-linearity artifacts in the scanner's MR-reconstruction pipeline. In Brainhack 2022, we adapted the SIEMENS reconstruction and to sort volume series by fMRI contrasts. This is BIDS compatible and does not require non-linearity corrections.

In the previous Brainhack (Gau et al., 2021), we extended the existing 3D-MOSAIC functor that was previously developed by Benedikt Poser and Philipp Ehses. This functor had been previously used to sort volumes of images by dimensions of echo-times, by RF-channels, and by magnitude and phase signals. In this Brainhack, we successfully extended and validated this functor to also support the dimensionality of SETs (that is representing BOLD and VASO contrast).

We are happy to share the compiled SIEMENS ICE (Image Calculation Environment) functor that does this sorting. Current VASO users, who want to upgrade their reconstruction pipeline to get the MOSAIC sorting feature too, can reach out to Renzo Huber (RenzoHuber@gmail.com) or Rüdiger Stirnberg (Ruediger.Stirnberg@dzne.de).

Furthermore, Remi Gau, generated a template dataset that exemplifies how one could to store layer-fMRI VASO data. This includes all the meta data for 'raw' and 'derivatives'. Link to this VASO fMRI BIDS demo: https://gin.g-node.org/RemiGau/ds003216/src/bids_demo.

Acknowledgements: We thank Chris Rodgers for instructions on how to overwrite existing reconstruction binaries on the SIEMENS scanner without rebooting. We thank David Feinberg, Alex

Beckett and Samantha Ma for helping in testing the new reconstruction binaries at the Feinbergat-ton scanner in Berkeley via remote scanning. We thank Maastricht University Faculty of Psychology and Neuroscience for supporting this project with 2.5 hours of 'development scan time'.

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3 Handling multiple testing problem through effect calibration: implementation using PyMC

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3.1 Introduction

Human brain imaging data is massively multidimensional, yet current approaches to modelling functional brain responses entail the application of univariate inferences to each voxel separately.

This leads to the multiple testing problem and unrealistic assumptions about the data such as artificial dichotomization (statistically significant or not) in result reporting. The traditional approach of massively univariate analysis assumes that no information is shared across the brain, effectively making a strong prior assumption of a uniform distribution of effect sizes, which is unrealistic given the connectivity of the human brain. The consequent requirement for multiple testing adjustments results in the *calibration of statistical evidence* without considering the estimation of effect, leading to substantial information loss and an unnecessarily heavy penalty.

A more efficient approach to handling multiplicity focuses on the *calibration of effect estimation* under a Bayesian multilevel modeling framework with a prior assumption of, for example, normality across space (Chen et al., 2019). The methodology has previously been implemented at the region level into the AFNI program RBA (Chen et al., 2022) using Stan through the R package brms (Bürkner, 2017). We intend to achieve two goals in this project:

- (i) To re-implement the methodology using PyMC to improve the performance and flexibility of the modeling approach.
- (ii) To explore the possibility of analyzing voxel-level data using the multilevel modeling approach

3.2 Implementation using PyMC

We used the dataset from Chen et al. (2019) to validate our PyMC implementation. The data contain the subject-level response variable y and a predictor of the behavioral measure x from $S = 124$ subjects at $R = 21$ regions. The modeling framework is formulated for the data y_{rs} of the s th subject at the r th region as below,

$$\begin{aligned} y_{rs} &\sim \mathcal{N}(\mu_{rs}, \sigma^2) \\ \mu_{rs} &= \alpha_0 + \alpha_1 x_s + \theta_{0r} + \theta_{1r} x_s + \eta_s \\ \begin{bmatrix} \theta_{0r} \\ \theta_{1r} \end{bmatrix} &\sim \mathcal{N}(\mathbf{0}_{2 \times 1}, \mathbf{S}_{2 \times 2}) \\ \eta_s &\sim \mathcal{N}(0, \tau^2) \end{aligned} \quad (1)$$

where $r = 1, 2, \dots, R$ and $s = 1, 2, \dots, S$

where μ_{rs} and σ are the mean effect and standard deviation of the s th subject at the r th region, α_0 and α_1 are the overall mean and slope effect across all regions and subjects, θ_{0r} and θ_{1r} are the mean and slope effect at the r th region, η_s is the

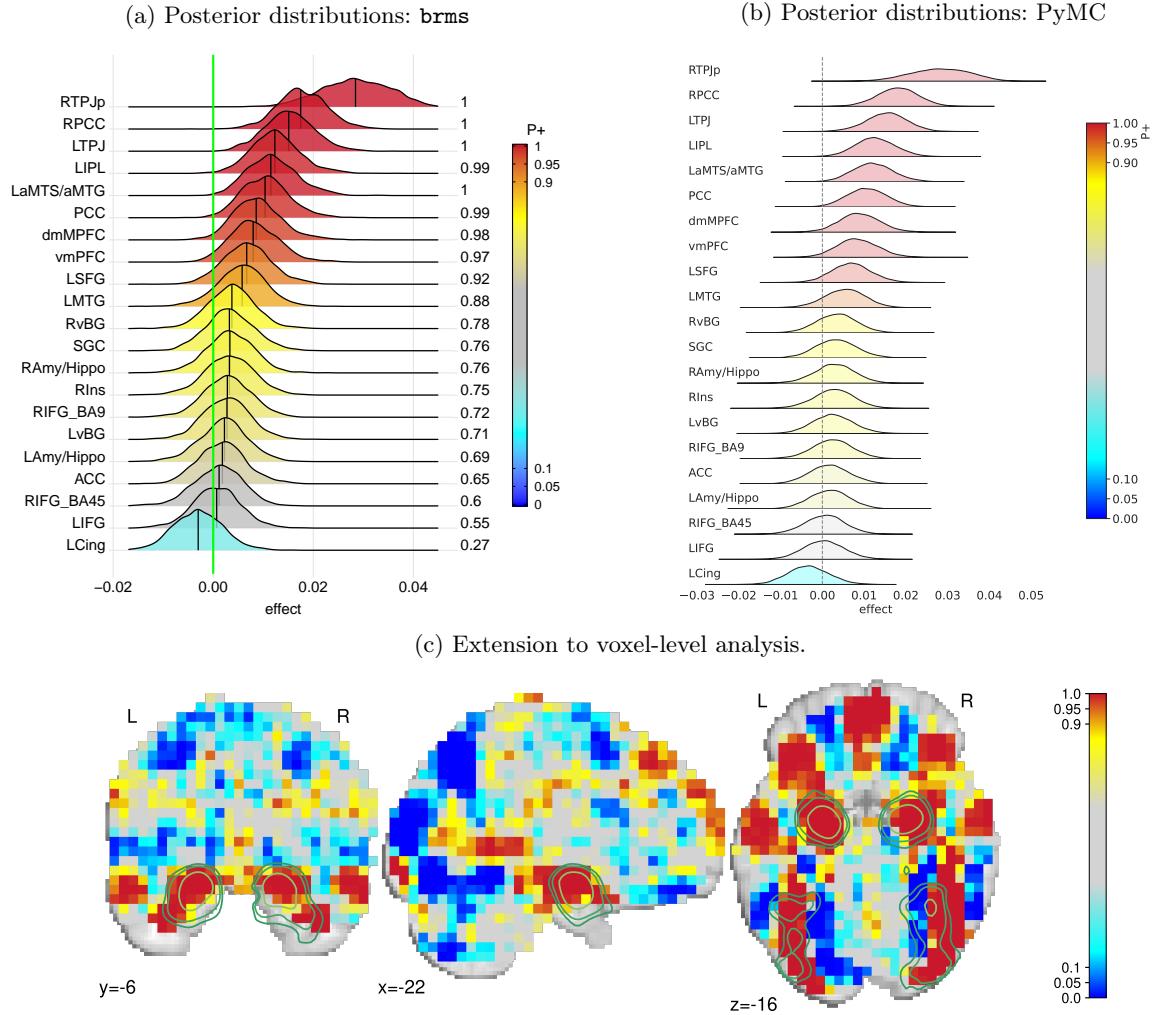


Figure 2: Validation of implementation using PyMC. (A) Posterior distributions of region-level behavior effects using `brms`. (B) Posterior distributions of region-level behavior effects using PyMC. (C) Posterior probabilities of the voxel-level effects being positive or negative, obtained using PyMC (plotted using Nilearn and overlaid in green with the NeuroQuery (Dockès et al., 2020) map for the term “emotional faces”).

mean effect of the s th subject, $\mathbf{S}_{2 \times 2}$ is the variance-covariance of the mean and slope effect at the r th region, and τ is the standard deviation of the s th subject’s effect η_s .

We implemented this model using the PyMC probabilistic programming framework (Salvatier, Wiecki & Fonnesbeck, 2016), and the BAyesian Model-Building Interface (BAMBI) (Capretto et al., 2020). The latter is a high-level interface that allows for specification of multilevel models using the formula notation that is also adopted by `brms`. A notebook describing the implementation is available here. Our PyMC implementation was successfully validated: as shown in Figure 2a and Figure 2b, the posterior distributions from the PyMC implementa-

tion matched very well with their counterparts from the `brms` output.

3.3 Extension of Bayesian multilevel modeling to voxel-level analysis

After exploring the model on the region level, we wanted to see if recent computational and algorithmic advances allow us to employ the multilevel modeling framework on the voxel level as well. We obtained the OpenNeuro dataset `ds000117` (Wakeman & Henson, 2015) from an experiment based on a face processing paradigm. Using `HALFpipe` (Waller et al., 2022), which is based on `fMRIprep` (Esteban et al., 2019), the func-

tional images were preprocessed with default settings and z -statistic images were calculated for the contrast “famous faces + unfamiliar faces versus 2 · scrambled faces”.

We applied the same modeling framework and PyMC code as for region-based analysis, but without the explanatory variable x in the model (Equation (1)). To reduce computational and memory complexity, the z -statistic images were downsampled to an isotropic resolution of 5mm. Using the GPU-based `nuts_numpyro` sampler (Phan, Pradhan & Jankowiak, 2019) with default settings, we were able to sample 2,000 posterior samples of the mean effect parameter for each of the 14,752 voxels. Sampling four chains took 23 minutes on four Nvidia Tesla V100 GPUs.

The resulting posterior probabilities are shown in Figure Figure 2c overlaid with the meta-analytic map for the term “emotional faces” obtained from NeuroQuery (Dockès et al., 2020). The posterior probability map is consistent with meta-analytic results, showing strong statistical evidence in visual cortex and amygdala voxels. The posterior probability maps also reveal numerous other clusters of strong statistical evidence for both positive and negative effects.

This implementation extension shows that large multilevel models are approaching feasibility, suggesting an exciting new avenue for statistical analysis of neuroimaging data. Next steps will be to investigate how to interpret and report these posterior maps, and to try more complex models that include additional model terms.

Acknowledgements

Computation has been performed on the HPC for Research cluster of the Berlin Institute of Health.

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4 Exploding brains in Julia

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Particle simulations are used to generate visual effects (in movies, games etc...). In this project, we explore how we can use magnetic resonance imaging (MRI) data to generate interesting visual effects by using (2D) particle simulations. We highlight that, historically, we were first inspired by a detailed blog post (https://nialltl.neocities.org/articles/mpm_guide.html) on the material point method (Jiang, Selle & Teran, 1965; Love & Sulsky, 2006; Stomakhin, Schroeder, Chai, Teran & Selle, 2013). Our aim in Brainhack 2022 is to convert our previous progress in Python programming language to Julia. The reason why we have moved to Julia language is because it has convenient parallelization methods that are easy to implement while giving immediately speeding-up the particle simu-

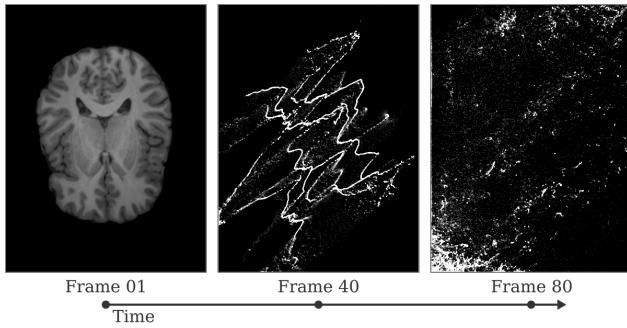


Figure 3: A video compilation of brain explosions can be seen at https://youtu.be/_5ZDctWv5X4.

lations.

Our previous efforts are documented at:

1. 2020 OpenMR Benelux: <https://github.com/OpenMRBenelux/openmrb2020-hackathon/issues/7>
2. 2020 OHBM Brainhack: <https://github.com/ohbm/hackathon2020/issues/124>
3. Available within the following github repository: <https://github.com/ofgulban/slowest-particle-simulator-on-earth>

As a result of this hackathon project, a compilation of our progress (Figure 3) can be seen at https://youtu.be/_5ZDctWv5X4 as a video. Our future efforts will involve sophisticating the particle simulations, the initial simulation parameters to generate further variations of the visual effects, and potentially synchronizing the simulation effects with musical beats.

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5 Exploring the AHEAD brains together

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5.1 Introduction

One of the long-standing goals of neuroanatomy is to compare the cyto- and myeloarchitecture of the human brain. The recently made available 3D whole-brain post-mortem data set provided by Alkemade et al. (2022) includes multiple microscopy contrasts and 7-T quantitative multi-parameter MRI reconstructed at 200µm from two human brains. Through the co-registration across MRI and microscopy modalities, this data set provides a unique direct comparison between histological markers and quantitative MRI parameters for the same human brain. In this BrainHack project, we explored this dataset, focusing on: (i) data visualization in online open science platforms, (ii) data integration of quantitative MRI with microscopy, (iii) data analysis of cortical profiles from a selected region of interest.

5.2 Results

Visualization and annotation of large neuroimaging data sets can be challenging, in particular for collaborative data exploration. Here we tested two different infrastructures: BrainBox <https://brainbox.pasteur.fr/>, a web-based visualization and annotation tool for collaborative manual delineation of brain MRI data, see e.g. (Heuer et al., 2019), and Dandi Archive <https://dandiacrchive.org/>, an online repository of microscopy data with links to Neuroglancer <https://github.com/google/neuroglancer>. While Brainbox could not handle the high resolution data well, Neuroglancer visualization was successful after conversion to the Zarr microscopy format (Figure 4A).

To help users explore the original high-resolution microscopy sections, we also built a python notebook to automatically query the stains around a given MNI coordinate using the Nighres tool-

box (Huntenburg, Steele & Bazin, 2018) (Figure 4B).

For the cortical profile analysis we restricted our analysis on S1 (BA3b) as a part of the somato-motor area from one hemisphere of an individual human brain. S1 is rather thin ($\sim 2\text{mm}$) and it has a highly myelinated layer 4 (see arrow Figure 4C). In a future step, we are aiming to characterize differences between S1 (BA3b) and M1 (BA4). For now, we used the MRI-quantitative-R1 contrast to define, segment the region of interest and compute cortical depth measurement. In ITK-SNAP (Yushkevich et al., 2006) we defined the somato-motor area by creating a spherical mask (radius 16.35mm) around the ‘hand knob’ in M1. To improve the intensity homogeneity of the qMRI-R1 images, we ran a bias field correction (N4BiasFieldCorrection, (Cox, 1996)). Tissue segmentation was restricted to S1 and was obtained by combining four approaches: (i) fsl-fast (Smith et al., 2004) for initial tissues probability map, (ii) semi-automatic histogram fitting in ITK-SNAP, (iii) Segmentator (Gulban, Schneider, Marquardt, Haast & De Martino, 2018), and (iv) manual editing. We used the LN2_LAYERS program from LAYNII open source software (Huber et al., 2021) to compute the equi-volume cortical depth measurements for the gray matter. Finally, we evaluated cortical depth profiles for three quantitative MRI contrasts (R1, R2, proton density) and three microscopy contrasts (thionin, bieloschowsky, parvalbumin) by computing a voxel-wise 2D histogram of image intensity (Figure 4C). Some challenges are indicated by arrows 2 and 3 in the lower part of Figure 4C.

From this Brainhack project, we conclude that the richness of the data set must be exploited from multiple points of view, from enhancing the integration of MRI with microscopy data in visualization software to providing optimized multi-contrast and multi-modality data analysis pipeline for high-resolution brain regions.

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6 Evaluating discrepancies in hippocampal segmentation protocols using automatic prediction of MRI quality (MRIQC)

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6.1 Introduction

Neuroimaging study results can vary significantly depending on the processing pipelines utilized by researchers to run their analyses, contributing to reproducibility issues. Researchers in the field are often faced with multiple choices of pipelines featuring similar capabilities, which may yield different results when applied to the same data (Carp, 2012; Kennedy et al., 2019). While these reproducibility issues are increasingly well-documented in

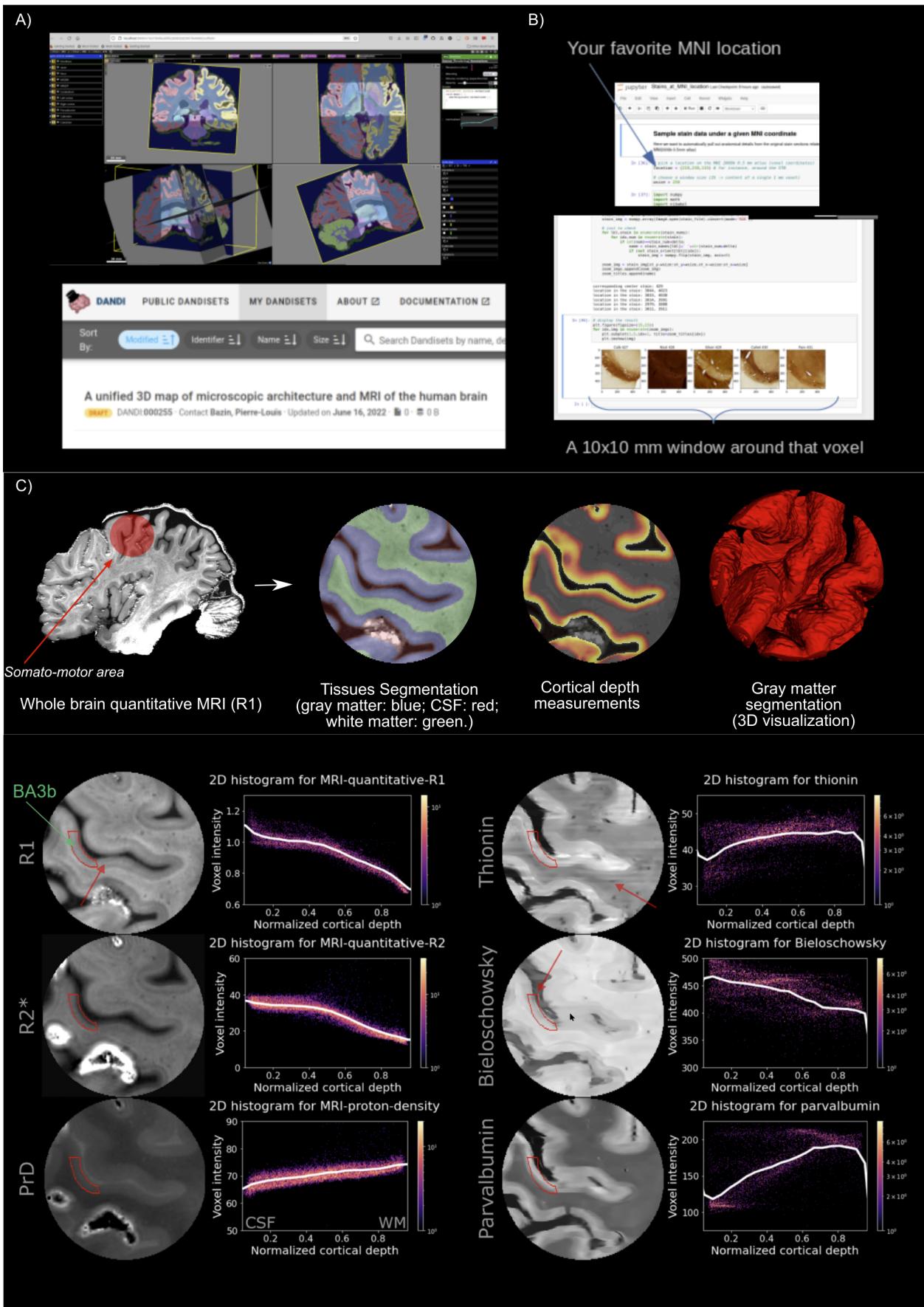


Figure 4: A) Neuroglancer visualization, B) section query notebook, C) Cortical ROI and corresponding depth histograms extracted from the different contrasts available.

the literature, there is little existing research explaining why this inter-pipeline variability occurs or the factors contributing to it. In this project, we set out to understand what data-related factors impact the discrepancy between popular neuroimaging processing pipelines.

6.2 Method

The hippocampus is a structure commonly associated with memory function and dementia, and the left hippocampus is proposed to have higher discriminative power for identifying the progression of Alzheimer's disease than the right hippocampus in multiple studies (Schuff et al., 2009). We obtained left hippocampal volumes using three widely-used neuroimaging pipelines: FSL 5.0.9 (Patenaude, Smith, Kennedy & Jenkinson, 2011), FreeSurfer 6.0.0 (Fischl, 2012), and ASHS 2.0.0 PMC-T1 atlases (Xie et al., 2019). We ran the three pipelines on T1 images from 15 subjects from the Prevent-AD Alzheimer's dataset (Tremblay-Mercier et al., 2021), composed of cognitively healthy participants between the ages of 55-88 years old that are at risk of developing Alzheimer's Disease. We ran MRIQC (Esteban et al., 2017) - a tool for performing automatic quality control and extracting quality measures from MRI scans - on the 15 T1 scans and obtained Image Quality Metrics (IQMs) from them. We then found the correlations between the IQMs and the pairwise inter-pipeline discrepancy of the left hippocampal volumes for each T1 scan.

6.3 Results

We found that for The FSL-FreeSurfer and FSL-ASHs discrepancies, MRIQC's EFC measure produced the highest correlation, of 0.69 and 0.64, respectively. The EFC "uses the Shannon entropy of voxel intensities as an indication of ghosting and blurring induced by head motion" ("MRIQC Documentation", 2020). No such correlations were found for the ASHS-FreeSurfer discrepancies. Figure 5 shows a scatter plot of the discrepancies in left hippocampal volume and EFC IQM for each pipeline pairing. The preliminary results suggest that FSL's hippocampal segmentation may be sensitive to head motion in T1 scans, leading to larger result discrepancies, but we require larger sample sizes to make meaningful conclusions. The code for our project can be found on GitHub at this link.

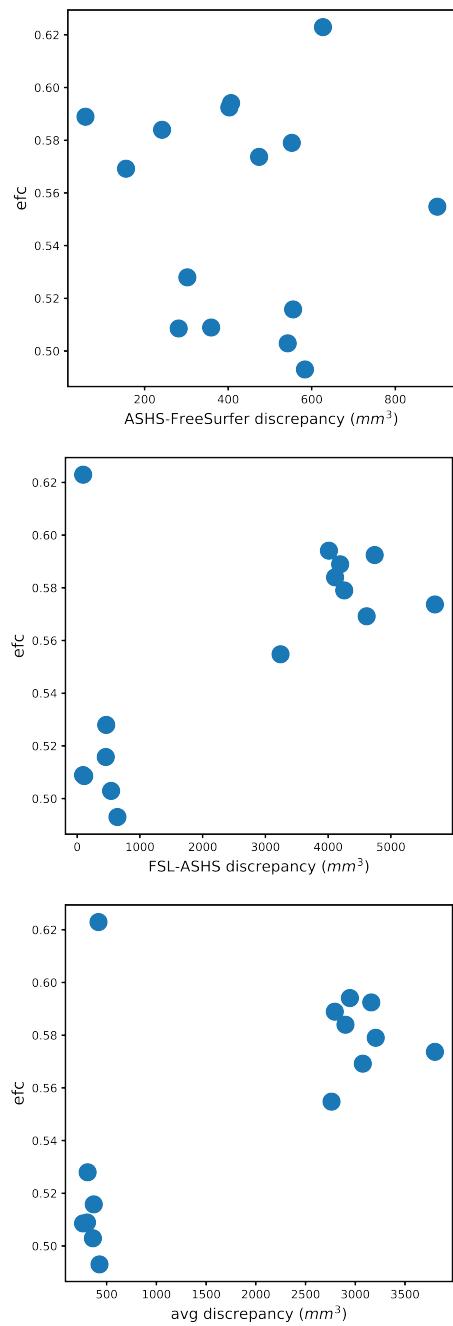


Figure 5: Plots showing the association between left hippocampal volume discrepancies and MRIQC's EFC quality measure for each of the pipeline pairings.

6.4 Conclusion and Next Steps

In this project, we investigated the correlation between MRIQC's IQMs and discrepancies in left hippocampal volume derived from three common neuroimaging pipelines on 15 subjects from the Prevent-AD study dataset. While our preliminary results indicate image ghosting and blurring induced by head motion may play a role in inter-pipeline result discrepancies, the next steps of the project will consist of computing the correlations on the full 308 subjects of the Prevent-AD dataset to investigate whether they persist with the full sample.

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7 Brainhack Cloud

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Today's neuroscientific research deals with vast amounts of electrophysiological, neuroimaging and behavioural data. The progress in the field is enabled by the widespread availability of powerful computing and storage resources. Cloud computing in particular offers the opportunity to flexibly scale resources and it enables global collaboration across institutions. However, cloud computing is currently not widely used in the neuroscience field, although it could provide important scientific, economical, and environmental gains considering its effect in collaboration and sustainability (Apon, Ngo, Payne & Wilson, 2014; "Oracle cloud sustainability", n.d.). One problem is the availability of cloud resources for researchers, because Universities commonly only provide on-premise high performance computing resources. The second problem is that many researchers lack the knowledge on how to efficiently use cloud resources. This project aims to address both problems by providing free access to cloud resources for the brain imaging community and by providing targeted training and support.

A team of brainhack volunteers (https://brainhack.org/brainhack_cloud/admins/team/) applied for Oracle Cloud Credits to support open-source projects in and around brainhack with cloud resources. The project was generously funded by Oracle Cloud for Research ("Oracle for Research", n.d.) with \$230,000.00 AUD from the 29th of January 2022 until the 28th of January 2024. To facilitate the uptake of cloud computing in the field, the team built several resources (https://brainhack.org/brainhack_cloud/tutorials/) to lower the entry barriers for members of the Brainhack community.

During the 2022 Brainhack, the team gave a presentation to share the capabilities that cloud computing offers to the Brainhack community, how they can place their resource requests and where they can get help. In total 11 projects were onboarded to the cloud and supported in their specific use cases: One team utilised the latest GPU architecture to take part in the Anatomical

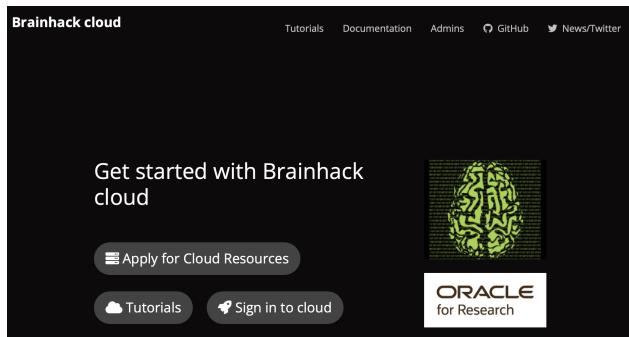


Figure 6: A team of brainhack volunteers, applied for Oracle Cloud Credits to support open source projects in and around brainhack with powerful cloud resources on the Oracle Cloud: https://brainhack.org/brainhack_cloud/

Tracings of Lesions After Stroke Grand Challenge. Others developed continuous integration tests for their tools using for example a full Slurm HPC cluster in the cloud to test how their tool behaves in such an environment. Another group deployed the Neurodesk.org (“NeuroDesk”, n.d.) project on a Kubernetes cluster to make it available for a student cohort to learn about neuroimage processing and to get access to all neuroimaging tools via the browser. All projects will have access to these cloud resources until 2024 and we are continuously onboarding new projects onto the cloud (https://brainhack.org/brainhack_cloud/docs/request/).

The Brainhack Cloud team plans to run a series of training modules in various Brainhack events throughout the year to reach researchers from various backgrounds and increase their familiarity with the resources provided for the community while providing free and fair access to the computational resources. The training modules will cover how to use and access computing and storage resources (e.g., generating SSH keys), to more advanced levels covering the use of cloud native technology like software containers (e.g., Docker/Singularity), container orchestration (e.g., Kubernetes), object storage (e.g., S3), and infrastructure as code (e.g., Terraform).

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