

CBRAIN

A Web-based Distributed
Computing Platform for Collaborative
Neuroinformatics Research



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McGill University

Outline

- The motivating challenges of neuroinformatics and big data science
- CBRAIN for Big Data Processing and Workflow Management
- The software ecosystem for reproducibility and interoperability

The Challenges in Neuroinformatics



Big Data



Big Computation



International
Collaboration



Interdisciplinary
Health Research

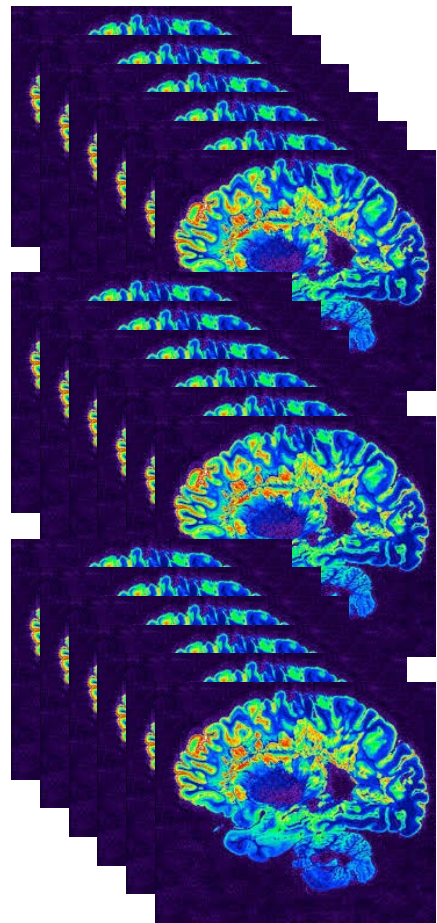
What does it take?

Infrastructure and services for accomplishing science

Longitudinal Acquisition, Storage and Curation, **Interoperability**, **Reproducibility**, Transfer, Anonymization, **Security**, Privacy, Ethics, APIs, Validation, Quality Control, Protocol Checking, **Preprocessing**, **Analysis**, **HPC**, **Cloud**, **Provenance**, Ontological Standardization, Data Harmonization, Upgrades, Maintenance, Bug Fixes, **User Interfaces**, Bootstrap, Tracking, Extensibility, **Data Management**, Summary Statistics, **Workflows**, **Development**, **Tool Integration**, **Data Sharing**, Download, Multi-Modal Linking, Querying, Image Processing, **Visualization**, Networking, System Administration, Partnerships, Funding, HR

Big Data Processing

cbrain



```
SupersetShell>ls -la
total 50884
-rw-r--r-- 1 superset users 12614 Aug 10 21:03 1_NeuroHub_Sessions_and_Files.ipynb
-rw-r--r-- 1 superset users 42957 Aug 10 21:02 2_NeuroHub_Groups_and_Data_Providers.ipynb
-rw-r--r-- 1 superset users 932508 Aug 24 17:29 3_NeuroHub_Application.ipynb
-rw-r--r-- 1 superset users 98765 Aug 24 17:18 4_NeuroHub_Tools_and_Tasks.ipynb
-rw-r--r-- 1 superset users 3 Aug 10 20:22 nilearn_cache
-rw-r--r-- 1 superset users 3 Aug 10 19:14 nilearn_cache-old
-rw-r--r-- 1 superset users 3 Aug 24 16:16 5
-rw-r--r-- 1 superset users 1444183 Aug 10 20:13 sub-1004555_ses-PREMIUM_run-01_T1w.nii.gz
-rw-r--r-- 1 superset users 6121806 Aug 10 20:16 sub-1004555_ses-PREMIUM_ses-acquiring_run-01_bold.nii.gz
SupersetShell>ls -la
total 12
-rw-r--r-- 1 superset users 10 Aug 10 20:16 sub-1004555_ses-PREMIUM_run-01_T1w.nii.gz
-rw-r--r-- 1 superset users 6121806 Aug 10 20:16 sub-1004555_ses-PREMIUM_ses-acquiring_run-01_bold.nii.gz
Type 'copyright' to see the license for more information
Type 'copyright' to see the license for more information
Python 7.26.0 -- An enhanced Interactive Python. Type '?' for help.

In [1]: import nilearn

In [2]: import nibabel as nib # loads the brain scan file

In [3]: from nilearn import plotting # for visualization
/home/superset/.local/lib/python3.7/site-packages/nilearn/datasets/_init_.py:86: FutureWarning: Fetchers from the nilearn.
datasets module will be updated in version 0.9 to return python strings instead of bytes and Pandas dataframes instead of 5
numpy arrays.
warn: Fetchers from the nilearn.datasets module will be ...

In [4]: file_to_load = nib.load('sub-1004555_ses-PREMIUM_run-01_T1w.nii.gz') # specify filename as string
In [5]: anat_file = nib.load(file_to_load) # loading an anatomical (T1 weighted) scan
In [6]: anat_file.shape # 3D shape
(178, 248, 256)

In [7]: plotting.plot_anat(anat_file, output_file='test.png') # minimal purpose plotting, no specific preset

In [8]: ! ls -la test.png
-rw-r--r-- 1 superset users 253810 Aug 25 21:22 test.png

In [9]:
```



cbrain

Filename	File Type	#	Owner	#	Created Date	Size	Tags	Physical Access	Provider	#	Description
sub-01_ses-anat_T1w.nii.gz	Nifti File	1	superset	1	2022-04-11	8.3 MB		Read Only	NeuroHubData	1	
sub-01_ses-func_T1w.nii.gz	Nifti File	1	superset	1	2022-04-11	9.3 MB		Read Only	NeuroHubData	1	
sub-02_ses-anat_T1w.nii.gz	Nifti File	1	superset	1	2022-04-11	10.7 MB		Read Only	NeuroHubData	1	
sub-02_ses-func_T1w.nii.gz	Nifti File	1	superset	1	2022-04-11	8.3 MB		Read Only	NeuroHubData	1	

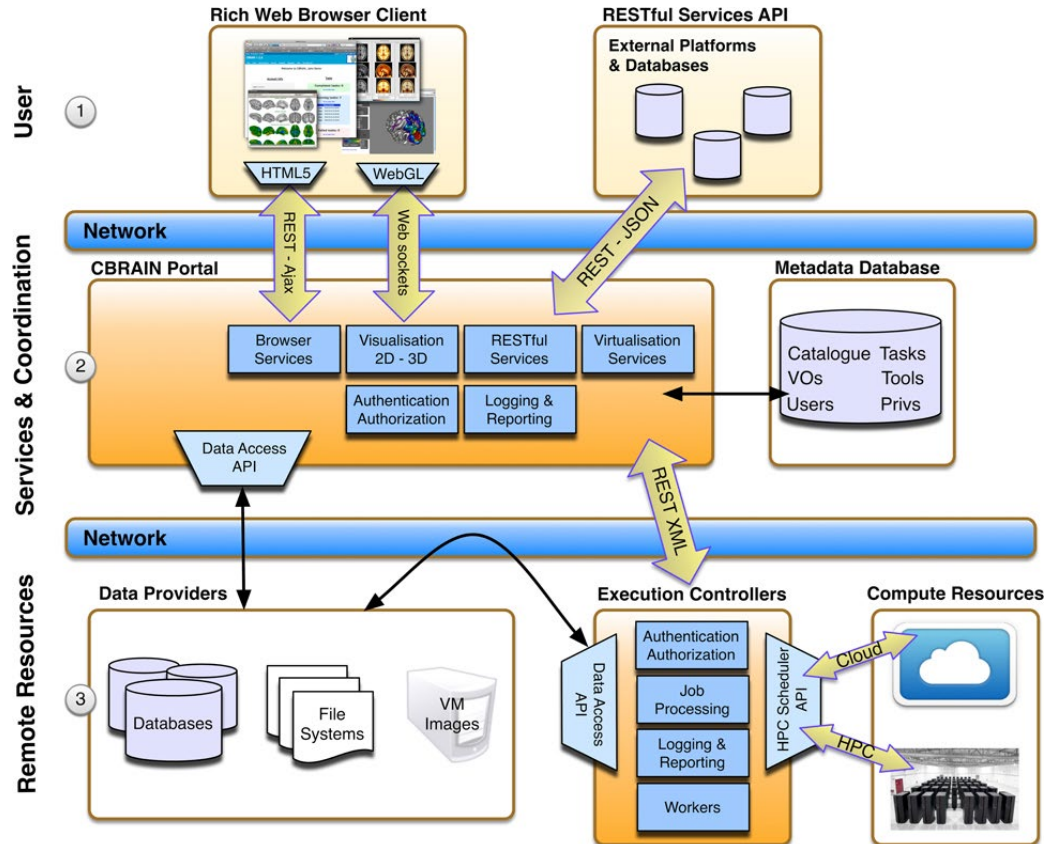


CBRAIN orchestrates large amounts of data and computation running on remote High Performance Computing and Cloud resources.

Makes big science **easier, manageable, reliable** and **reproducible**!

Big Data Processing

cbrain



Sherif T, Rioux P, Rousseau M-E, Kassis N, Beck N, Adalat R, Das S, Glatard T and Evans AC (2014)
CBRAIN: a web-based, distributed computing platform for collaborative neuroimaging research. 5

[Front. Neuroinform. 8:54. doi: 10.3389/fninf.2014.00054](https://doi.org/10.3389/fninf.2014.00054)

Features of CBRAIN



- Convenient, secure web access and API
- Lightweight core components, low requirements for deployment and operation
- Distributed storage with automated, multipoint data movement, and cataloging
- Transparent access to research tools and computing (HPC and cloud)
- Flexibility to adapt to extremely heterogeneous computing and data sites
- Full audit trail (data provenance) and logs across all user actions
- Scalability (no architectural bottlenecks)
- Full ecosystem security and monitoring

<https://github.com/aces/cbrain>

Features of CBRAIN



Enables distributed execution of software pipelines

NeuroHub Dashboard My Account Projects Messages (10) Resources Support Forum Rev: 6.2.0-197 (last updated 1m ago) Logged in as Bryan Caron Sign out

cbrain - bcaron - Tasks Search for anything

Files Tasks

Update Attributes For Failed Tasks For Completed Tasks Terminating And Cleaning Up Archiving Filters

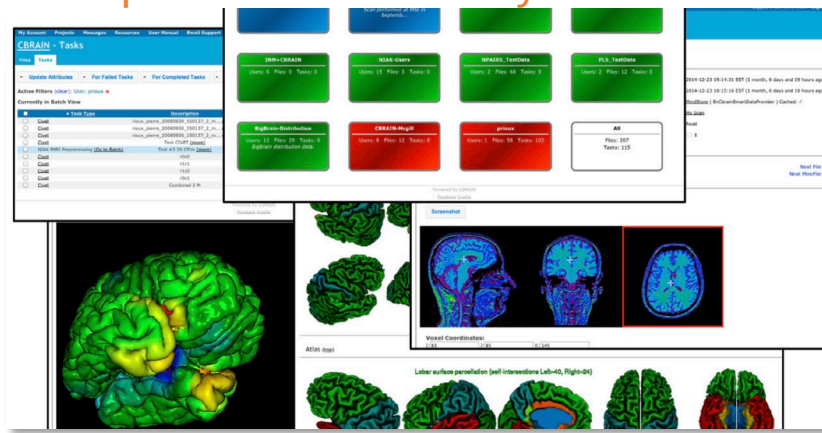
Switch to List View (128 tasks) Total task space used: 46.2 MB 25 per page.

<input type="checkbox"/>	Task Type	Version	Description	Owner	Execution Server	Current Status	Run Number	Workdir Size	Time Submitted	Last Updated
<input type="checkbox"/>	+ Civet	2.1.1	sub-01_ses-test_T1w.mnc	bcaron	Bridges2	3 x Failed		0 bytes	2021-05-20 12:45:28 EDT	2021-05-20 12:46:46 EDT ...
<input type="checkbox"/>	+ Civet	2.1.1	sub-01_ses-test_T1w.mnc	bcaron	Bridges2	3 x Failed		0 bytes	2021-05-20 12:55:37 EDT	2021-05-20 12:56:38 EDT ...
<input type="checkbox"/>	+ Civet	2.1.1	sub-01_ses-test_T1w.mnc	bcaron	Graham	3 x Completed		0 bytes	2021-05-20 13:28:30 EDT	2021-05-20 20:56:50 EDT ...
<input type="checkbox"/>	FailFirst	5.0.9	My test task!	bcaron	Converter-2	Completed	1	V (25.7 MB)	2021-08-10 17:06:47 EDT	2021-08-10 17:16:15 EDT ...
<input type="checkbox"/>	+ FMRIPrepSingleSubject	20.2.0		bcaron	Beluga	25 x Failed		0 bytes	2021-12-15 13:51:54 EST	2021-12-16 21:25:26 EST ...
<input type="checkbox"/>	FreeSurfer_Recon_all	v7.1.1		bcaron	GrahamPlatform	Completed	1	V (299.7 MB)	2022-03-16 13:17:34 EDT	2022-03-16 23:26:10 EDT ...
<input type="checkbox"/>	FMRIPrepBidsSubject	21.0.0		bcaron	Narval	46 x Terminated		0 bytes	2022-05-11 14:51:49 EDT	2022-05-11 14:52:34 EDT ...
<input type="checkbox"/>	FMRIPrepBidsSubject	21.0.0		bcaron	Narval	46 x Failed		46.2 MB	2022-05-11 15:50:07 EDT	2022-05-11 15:54:36 EDT ...

Workdir archiving status symbols: ◇: On Cluster V: As File

Powered by CBRAIN Credits

Aggregates multiple distributed file systems into uniform view



Why use CBRAIN?

cbrain



Access to Big Data and Big Computing

- Easy access to a full range of lab-based through to large-scale ARC resources including Alliance systems
- Access to a diverse range and scale of datasets and storage for high-speed, high throughput computing



Reproducible science

- Deployed, standardized, and tested over 115+ software tools
- Software runs exactly the same, no matter where it executes



Scale up your science

- Web-based platform makes it easy to execute large computation easily
- High degree of parallelism can accelerate your science



Collaborate and Share your science

- Work in a virtual organization sharing data with your team anywhere in the world
- Make your pipelines and results available to others

What is Boutiques?



- Fully-automated integration of applications
- Deployment on heterogeneous computing resources through containers
- Comprehensive input validation through a strict JSON schema
- Flexible application description through a rich JSON schema

<https://github.com/boutiques>



(GIGA)ⁿ
SCIENCE

Giga Science, 7, 2018, 1–11

doi: 10.1093/gigascience/giy016

Advance Access Publication Date: 23 March 2018

Technical Note

TECHNICAL NOTE

Boutiques: a flexible framework to integrate command-line applications in computing platforms

Tristan Glatard^{1,*}, Gregory Kiar^{2,3}, Tristan Aumentado-Armstrong^{2,3}, Natacha Beck^{2,3}, Pierre Bellec⁴, Rémi Bernard^{2,3}, Axel Bonnet⁵, Shawn T Brown^{2,3}, Sorina Camarasu-Pop⁵, Frédéric Cervenansky⁵, Samir Das^{2,3}, Rafael Ferreira da Silva⁶, Guillaume Flandin⁷, Pascal Girard⁵, Krzysztof J. Gorgolewski⁸, Charles R.G. Guttman⁹, Valérie Hayot-Sasson¹, Pierre-Olivier Quirion⁴, Pierre Rioux^{2,3}, Marc-Étienne Rousseau¹⁰ and Alan C. Evans^{2,3}

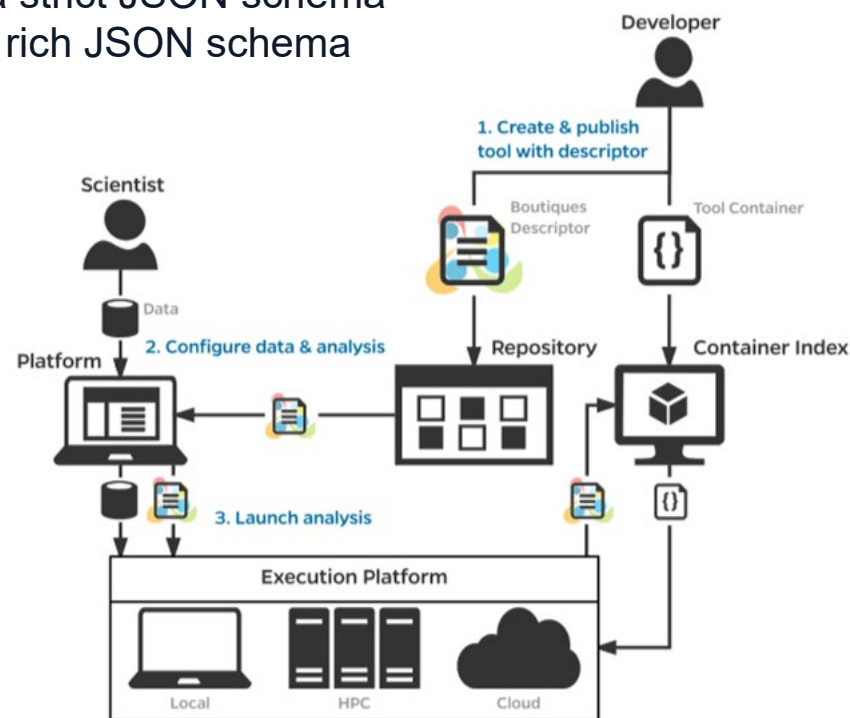


Figure 1. Publication, integration, and execution of applications with Boutiques.

Software Tools



cbrain 115+ Tools

fMRI Analysis

fMRI Preprocessing

Structural MRI

Genetics

Tractography

PET

Arterial Spin Labeling

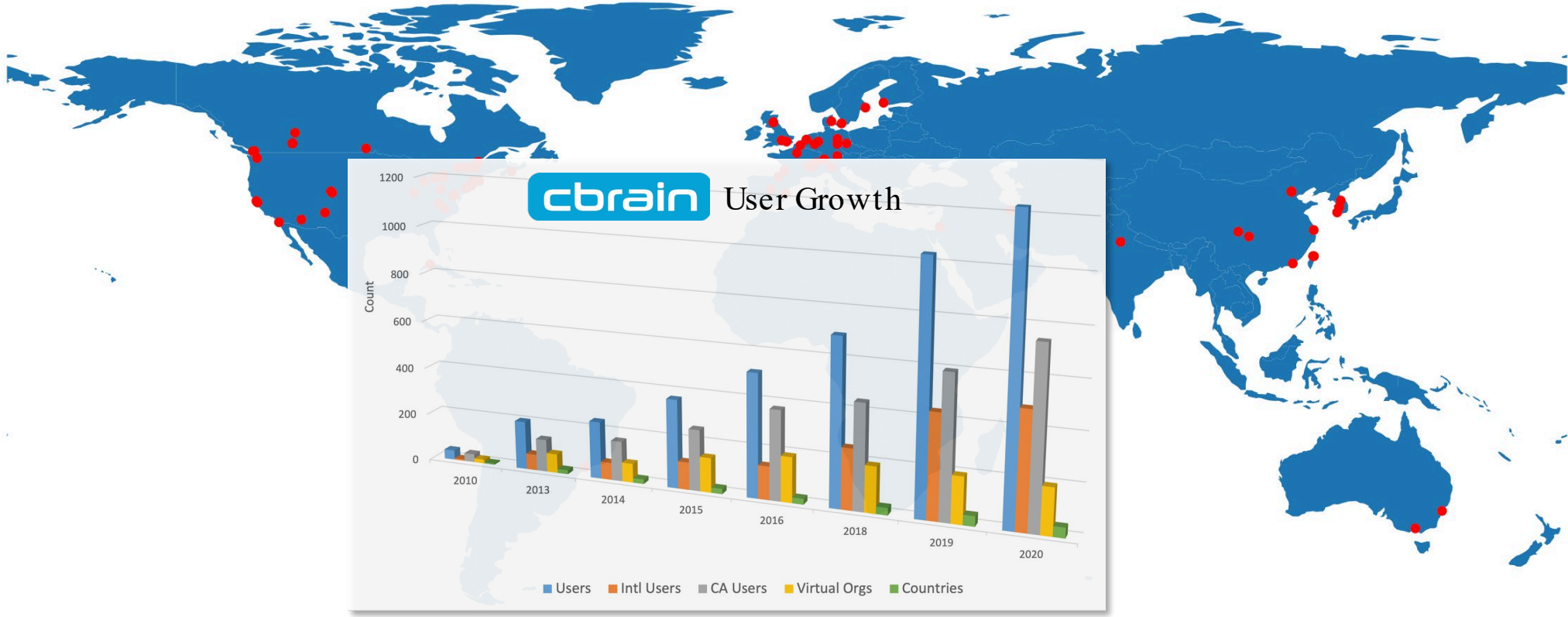
EEG

Data Conversion Tools

Statistics



Global User Community



1400+ users, 193 sites in 32 countries

Connected Resources

cbrain



Digital Research
Alliance of Canada

Alliance de recherche
numérique du Canada



200k+ tasks launched for >5M+ CPU hours processed since 2020
44M+ files, 415 TB registered files currently in CBRAIN

Share the project and the derived data

[illegible]

[Newstream](#)
[Dashboard](#)
[My Account](#)
[Projects](#)
[Messages](#)
[Resources](#)
[Help Site](#)
[Email Support](#)
[Rev: 6.0.0-6](#)
(last updated 6m ago)
[Logged in as Verena Sch](#)

cbRAIN

- Test for documentation - Files

Search for:

Files

Tasks

Launch

Upload

Download

Copy

Move

Compress

Uncompress

Details

More...

1 files currently selected (select all, clear)

(1 entry, 23.1 MB)

Search by name:

25 per page

	Filename	File Type	Owner	Creation Date	Size	Tags	Project Access	Provider	Description
<input checked="" type="checkbox"/>	11TEST_DOCUMENTATION	NIFTI file	yohuster	2020-08-28	23.1 MB		Read Only	MainStore	...

Synchronization symbols:
: InSync
: ProvNewer
: CacheNewer
: Corrupted
: ToCache
: ToProvider

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Go back

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Data Processing and Visualization

Content

Change view: CIVET Output

Show Displayable Contents

CIVET Directories Explained

	File	Size
<input type="checkbox"/>	CBRAIN_GrahamPlatform-1477704-1.params.yml	1.0 kB
<input type="checkbox"/>	References.txt	6.0 kB
<input type="checkbox"/>	classify Expand	
<input type="checkbox"/>	final Expand	
<input type="checkbox"/>	logs Expand	
<input type="checkbox"/>	mask Expand	
<input type="checkbox"/>	native Expand	
<input type="checkbox"/>	surfaces Expand	
<input type="checkbox"/>	temp Expand	
<input type="checkbox"/>	thickness Expand	
<input type="checkbox"/>	transforms Expand	
<input type="checkbox"/>	verify Expand	

Extract Files from Collection

File Log

```
[2020-11-16 09:18:10 UTC] CivetOutput revision c395894c Pierre Rioux 2017-04-19  
[2020-11-16 09:18:10 UTC] post_process() CbrainTask::Civet rev. bf5e3df3 Created/updated by task Civet@GrahamPlatform/1477704 from file sub-01_ses-test_T1w.mnc.
```

Disk Space History

Date	Space Delta
2020-11-16 04:18:10 EST (4 hours, 59 minutes and 35 seconds ago)	+ 671.0 MB

Content

Change view: Surface Viewer

Files:

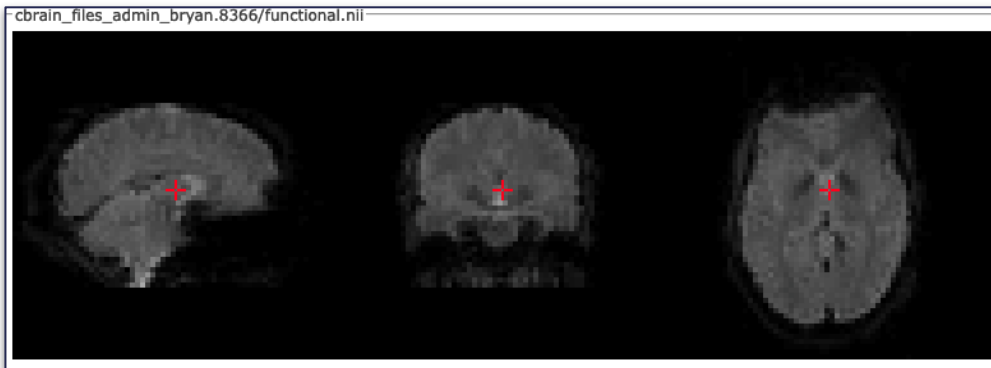
Surface File: CIVET Output

Surface Overlay: Surface Viewer

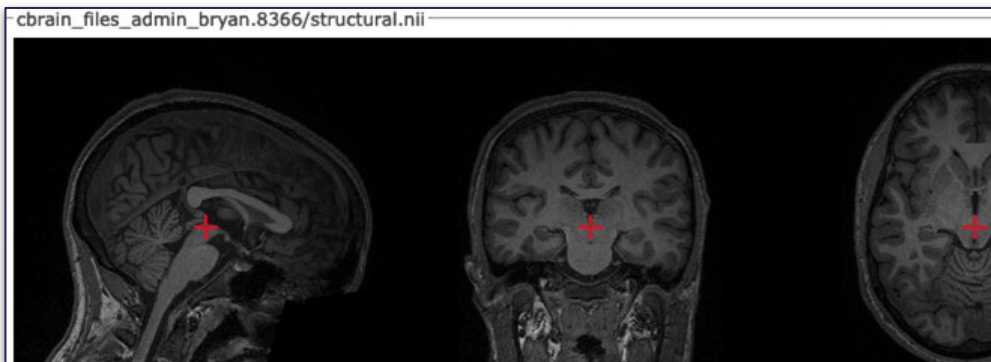
Color Map: Choose File, no file selected

Data Processing and Visualization

Functional

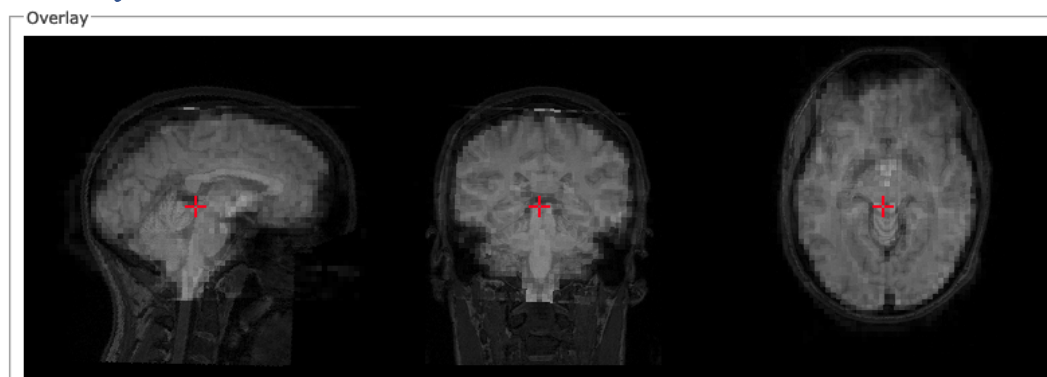


Structural



<input type="checkbox"/>	File	DL	Size
<input type="checkbox"/>	 functional.nii	±	40.4 MB
<input type="checkbox"/>	 structural.nii	±	46.1 MB

Overlay



Interactive Data Exploration

- CBRAIN API - users can interact programmatically with data and tools



cbrain API

Session Management

Authentication
Authorization
Access Control

Tools

Tool selection
Libraries and packages loading
and import

Tasks

Task submission
Task status querying
Task management

Data Handling

File upload / download
File search / selection
File read / write

```
In [24]: file_to_load = 'sub-1004359_ses-PREBL00_run-001_T1w.nii.gz' #specify filename as string
anat_file = nib.load(file_to_load) #loading an anatomical (T1 weighted) scan
print(anat_file.shape) #3D shape

file_to_load2 = 'sub-1004359_ses-PREBL00_task-encoding_run-001_bold.nii.gz'
bold_file = nib.load(file_to_load2) #loading an fMRI (BOLD) scan
print(bold_file.shape) #4D shape

plotting.plot_img(anat_file) #General purpose plotting, no specific preset
plotting.plot_anat(anat_file) #Anatomical image plotting

(176, 240, 256)
(64, 64, 32, 183)
```

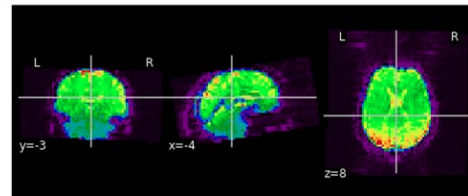
Out[24]: <nilearn.plotting.displays.OrthoSlicer at 0x7f352eae9b70>



5. fMRI visualization

```
In [26]: from nilearn.image.image import mean_img
mean_fmri = mean_img(bold_file) #Compute the mean of the images over time or the 4th dimension
from nilearn.plotting import plot_epi, show
plot_epi(mean_fmri) #plot cuts of the image (by default 3 cuts: Frontal, Axial, and Lateral)
```

Out[26]: <nilearn.plotting.displays.OrthoSlicer at 0x7f352ecce908>



Access to Large Datasets



- Centralized and efficient handling and processing
- 40000 participants with imaging data + tools to load into PyTorch
- 200000+ participants with genetics and phenotypic data



+ tools for genetics

More than 3000 patients including those with Parkinson's and ALS, with genetic data accessible via NeuroHub



HBGD (HEALTHY Brain and Child Development) Study

- 7500 participants study on the effects of opiate addiction



(50+ datasets)

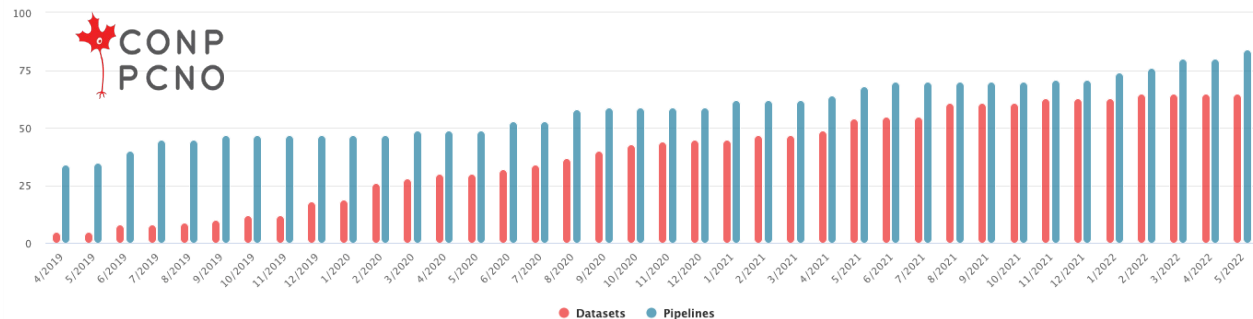


Adolescent Brain Cognitive Development®
Teen Brains. Today's Science. Brighter Future.

- 12000 participants
- NIH wants major NeuroHub components within its data curation, dissemination plan

Canadian Open Neuroscience Platform (CONP)

Cumulative Number of Datasets and Pipelines



NeuroHub



Public Project Shared Project All Project

CONP-1000-Genomes Files: 37 Tasks: 0 1000 Genomes Project	CONP-AlzheimerMouse Files: 18 Tasks: 0 Access control project for CONP...	CONP-BigBrain Files: 317 Tasks: 0 Access to files in the BigBrain...	CONP-BigBrain-3D-ROIs Files: 11 Tasks: 0 BigBrain dataset - 3D ROIs (deri...	CONP-BigBrain-3DClass... Files: 25 Tasks: 0 Access to files in the BigBrain...
CONP-BigBrain-3DSurfaces Files: 49 Tasks: 0 Access to files in the BigBrain...	CONP-BigBrain-ASD Files: 5 Tasks: 0 BigBrain dataset - ASD (derived...	CONP-BigBrain-Hippocampus Files: 9 Tasks: 0 BigBrain dataset - Hippocampus...	CONP-BigBrain-LayerSeg Files: 7 Tasks: 0 BigBrain dataset - Layer Segment...	CONP-BigBrain-MRISIM Files: 6 Tasks: 0 BigBrain dataset - MRISIM (deri...
CONP-BigBrain-RawData Files: 4 Tasks: 0 BigBrain dataset - Raw Data	CONP-BigBrain-SurfParcels Files: 6 Tasks: 0 BigBrain dataset - Surface Parcell...	CONP-BigBrain-MR2Coreg Files: 13 Tasks: 0 Accurate registration of the Big...	CONP-BrainSpan Files: 24 Tasks: 0 BrainSpan: Atlas of the Develop...	CONP-Calgary-Corpus Files: 3 Tasks: 0 Access control project for CONP...
CONP-Calgary-Preschool Files: 410 Tasks: 0 Calgary Preschool MRI Dataset	CONP-CFHH-T1 Files: 36 Tasks: 0 Files in CONP public dataset CFH...	CONP-Chol-Del-Mouse Files: 4 Tasks: 0 Brainstem cholinegic-deficient ...	CONP-Chol-Striatum Files: 4 Tasks: 0 Mouse models that differ in neur...	CONP-HCPUB100 Files: 8 Tasks: 0 HCPUB100: Healthy Adult human B...
CONP-Hippocampus Files: 14 Tasks: 0 Hippocampus reference genome and cyto...	CONP-Human-Bal-Genome Files: 3 Tasks: 0 Human genome reference genome B...	CONP-LearnNet Files: 422 Tasks: 0 CONP Learning NeuroImage Struc...	CONP-mica-mica Files: 65 Tasks: 0 CONP Mica-Mica	CONP-MiceImmune Files: 388 Tasks: 0 Longitudinal structural MRI and ...
CONP-Multimodal-GScMP Files: 12 Tasks: 0 Multimodal data with wide field ...	CONP-Nutrineocortical... Files: 95 Tasks: 0 Intracellular recordings of Nutri...	CONP-Muskrat-Squirrels Files: 4 Tasks: 0 MRI and behavioral envelopes of w...	CONP-Neural-Cog Files: 95 Tasks: 0 Quantifying Neural Cognitive Ab...	CONP-Neurocon Files: 48 Tasks: 0 Parkinson's Disease Database - R...
CONP-NeuroRehab-HS Files: 8 Tasks: 0 The Effect of Neurorehabilitati...	CONP-NEH-NIP-Atlas Files: 381 Tasks: 0 NIP Blueprint Non-human Primate ...	CONP-OpenPreventAD Files: 627 Tasks: 2 This project restricts access to...	CONP-SINON Files: 5 Tasks: 0 Access control project for CONP...	CONP-SPINS-Phantoms Files: 11 Tasks: 0 SPINS Traveling Human Phantoms
CONP-Tasou Files: 43 Tasks: 0 Parkinson's Disease Datasets - T...	CONP-VFA-T1-Mapping Files: 7 Tasks: 0 VFA T1 mapping 1.7Traw (open) ...	CONP-VisualWorkingMemory Files: 25 Tasks: 0 CONP Dataset	CONP_Integration_Testing Files: 0 Tasks: 0 This is a project to test the in...	All Files: 57859 Tasks: 25895

Filter By: Modality: File Format: Third-party account required: Search

☒ Available in CBRAIN

Advanced Search Page (NEXUS)

Results 1 - 10 displayed of 45. (Maximum results per page 10)

Sort By: Origin

SIMON
Creators: Laboratoire MEDICS
Version: 1.0 Date Added: 2019-04-26 Date Updated: 2021-11-12
Modalities: MRI, MRI License: CC BY-SA
Files: 1829 Size: 84.0 GB Subjects: 1 Formats: NIFTI
ARK ID: <https://n2t.net/ark:/99999/d7mp70228p8c8hxd>

Direct Download (Not Available)

Download With DataLad

Process On **cbrain**

BigBrain dataset
Creators: BigBrain project
Version: 1.0 Date Added: 2020-01-12 Date Updated: 2022-05-02
Modalities: histology License: Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International Public License
Files: 316 Size: 112.5 GB Subjects: 1 Formats: MINC, NIFTI
ARK ID: <https://n2t.net/ark:/99999/d7r3hp47g3419234m3>

Direct Download (Not Available)

Download With DataLad

Process On **cbrain**

Learning Naturalistic Structure: Processed fMRI dataset
Creators: DuPre, Elizabeth
Version: 0.1.0 Date Added: 2020-02-07 Date Updated: 2021-06-02
License: other-pd
Files: 240 Size: 13.9 GB Formats: TSV, NIFTI, TXT
ARK ID: <https://n2t.net/ark:/99999/d7pk8f5v7mm6p17r>

Direct Download (13.9 GB)

Download With DataLad

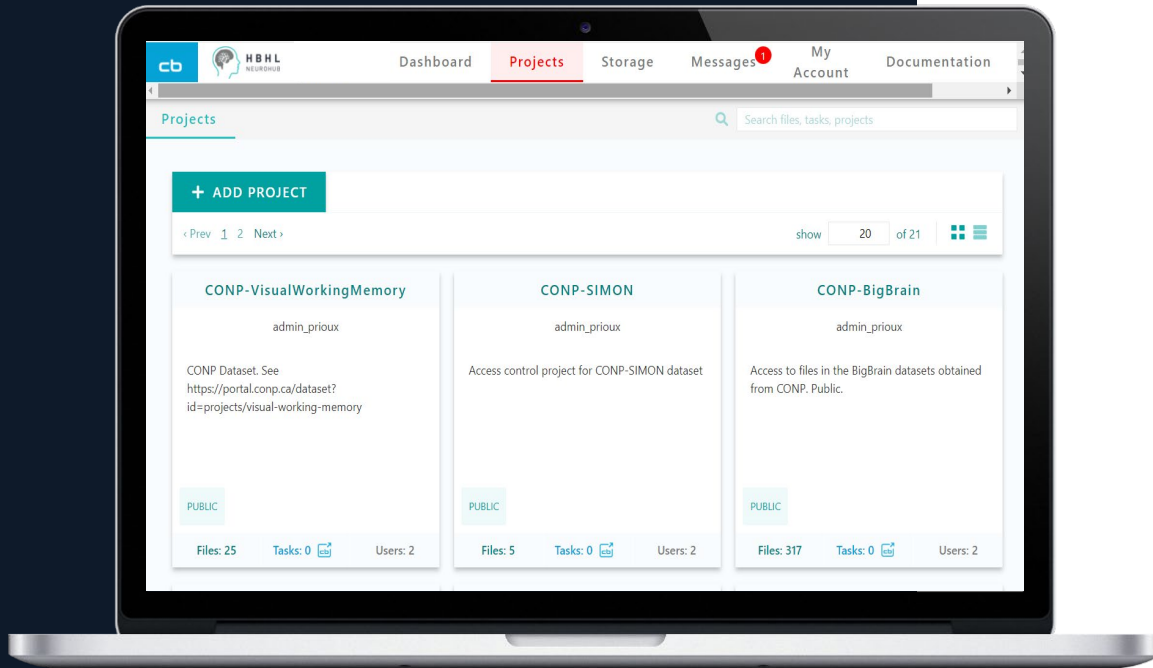
Process On **cbrain**

Recent Developments

- Some recent highlight features:
 - [New Boutiques integrator](#) - more modular, easier maintenance and tool integration
 - Users can link their account using [Globus Auth](#) for [Federated Identity Management](#)
 - Data Providers access files in [SquashFS / ext3 overlays](#) with singularity bindmount
 - large datasets are then friendly to HPC file systems
 - Fully supported [S3 Data Provider](#) configurable with distinct regions and endpoints
 - User can create [API tokens](#) for connections from external applications
 - [User definable](#) networked storage resources managed through SSH keys
 - [User storage resource quotas](#) on storage provided centrally by CBRAIN

Platform interoperability is key to building researcher communities and their success

What is NeuroHub?



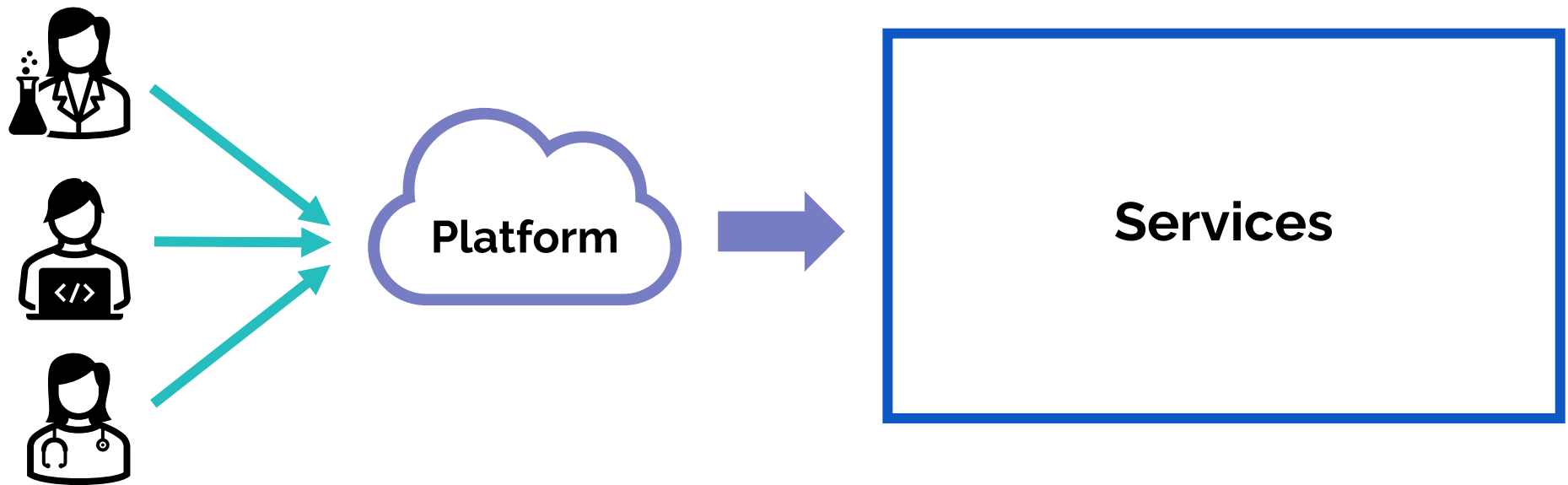
Multi-modal
data management



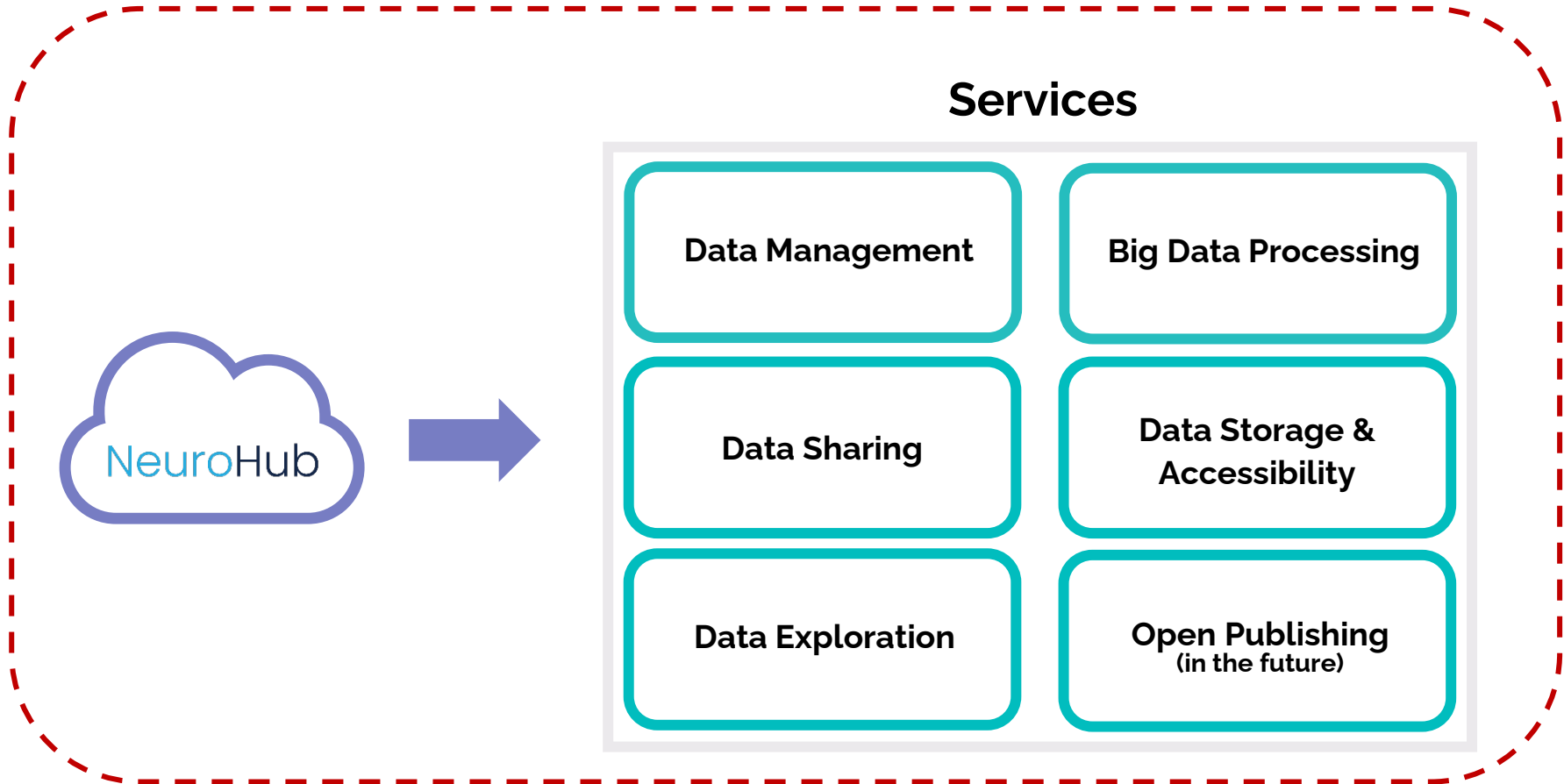
Data analysis



Data Storage & Sharing

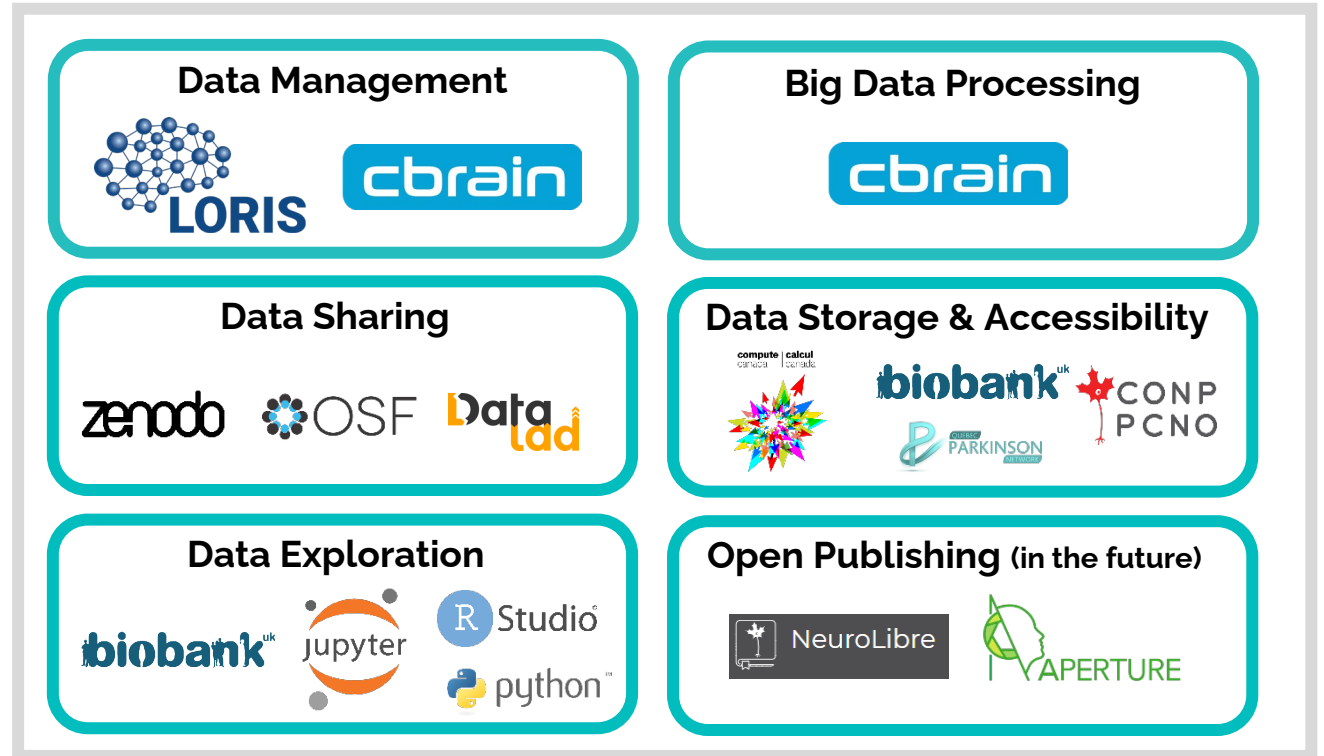


NeuroHub Ecosystem



NeuroHub Ecosystem

Services



NeuroHub Ecosystem Features



Easy-to-use interface and rich API



Securely store and share data



Access to high performance computing



Access large international datasets



Capture and curate multi-modal data



Datasets suitable for machine learning

NeuroHub for Reproducibility and Interoperability



Which dataset version you worked on



Know which software version you have used



Be able to relaunch on new datasets : Replicability



Cost and maintenance aspects

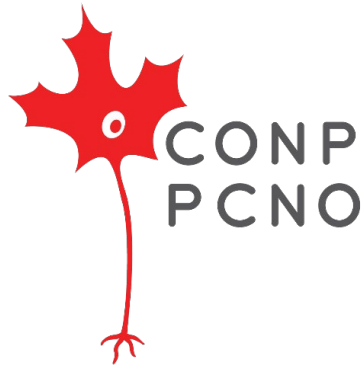
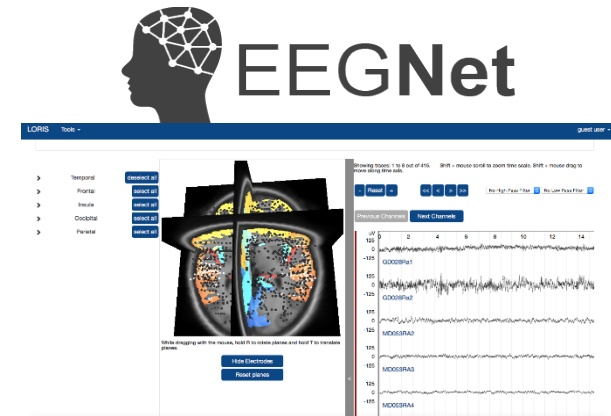


Leverage expertise that cannot be built locally



Build the bridges across communities and across platforms

Large Scale Projects



Future Directions



- Additional CBRAIN Data Provider types to support cloud-based storage
 - (e.g., Google Drive / Cloud, Microsoft SharePoint, ...)
- Update the CBRAIN Portal web interface to improve and simplify the user experience
 - Cleaner and more intuitive workflows
 - Enhanced self-help functionality
 - Updated look and feel based upon modern UI design
- Adapt CBRAIN for generalized use for scientific workflows across HPC and Cloud infrastructures



- Update the NeuroHub Portal web interface to be a clean entry point into the ecosystem

Conclusion



Big Data



Big Computation



International
Collaboration



Interdisciplinary
Health Research

Infrastructure and services for accomplishing science



CBRAIN and NeuroHub are core components for reproducibility and interoperability

- Interoperate or integrate – not reimplement



Standards are game changers



Community and use-case based development and governance

Acknowledgements



Alan Evans
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Najmeh Kalili-Manhani
Darius Valevicius
Safa Sanami
Reza Adalat
Tristan Glatard



Bryan Caron
J-B Poline
Diana Le
Pierre Rioux
Natacha Beck
Serge Boroday
James Mehta
Samir Das
Xavier Lecours-Boucher
Rida Abou-Haidar
Darcy Quesnel
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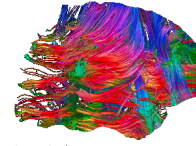
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