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Neurodesk: an accessible, flexible and portable data analysis environment for reproducible neuroimaging

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Neuroimaging research requires purpose-built analysis software, which is challenging to install and may produce different results across computing environments. The community-oriented, open-source Neurodesk platform (https://www.neurodesk.org/) harnesses a comprehensive and growing suite of neuroimaging software containers. Neurodesk includes a browser-accessible virtual desktop, command-line interface and computational notebook compatibility, allowing for accessible, flexible, portable and fully reproducible neuroimaging analysis on personal workstations, high-performance computers and the cloud.

Neuroimaging data analysis is challenging. Aside from the scientific background motivating the choice of analysis, advanced domain knowledge beyond the researcher's expertise is needed; for example, signal and image processing, software engineering, statistics and machine learning. Researchers faced with this task rely on specialized software packages typically developed by research teams with limited resources. The resulting analysis tools often have limited technical support, can be difficult to install, have conflicting dependencies or are inconsistently available across operating systems[1–3]. These issues not only are frustrating and time consuming, but also ultimately compromise reproducibility, a foundational scientific principle. We therefore developed Neurodesk, a community-oriented open-source solution for neuroimaging analysis with four guiding principles: accessibility, portability, flexibility and, overarchingly, reproducibility.

Ideally, scientific analysis workflows should be easily accessible, so users can deploy them from any computing environment with minimal time and effort[4], and portable, so that users can tractably shift analysis pipelines between computing environments once developed. Many researchers prototype analysis pipelines using their laptop or desktop computer, and then switch to workstations and high-performance computing clusters for processing at scale. Accessible and portable workflows allow for the optimized allocation of computing resources

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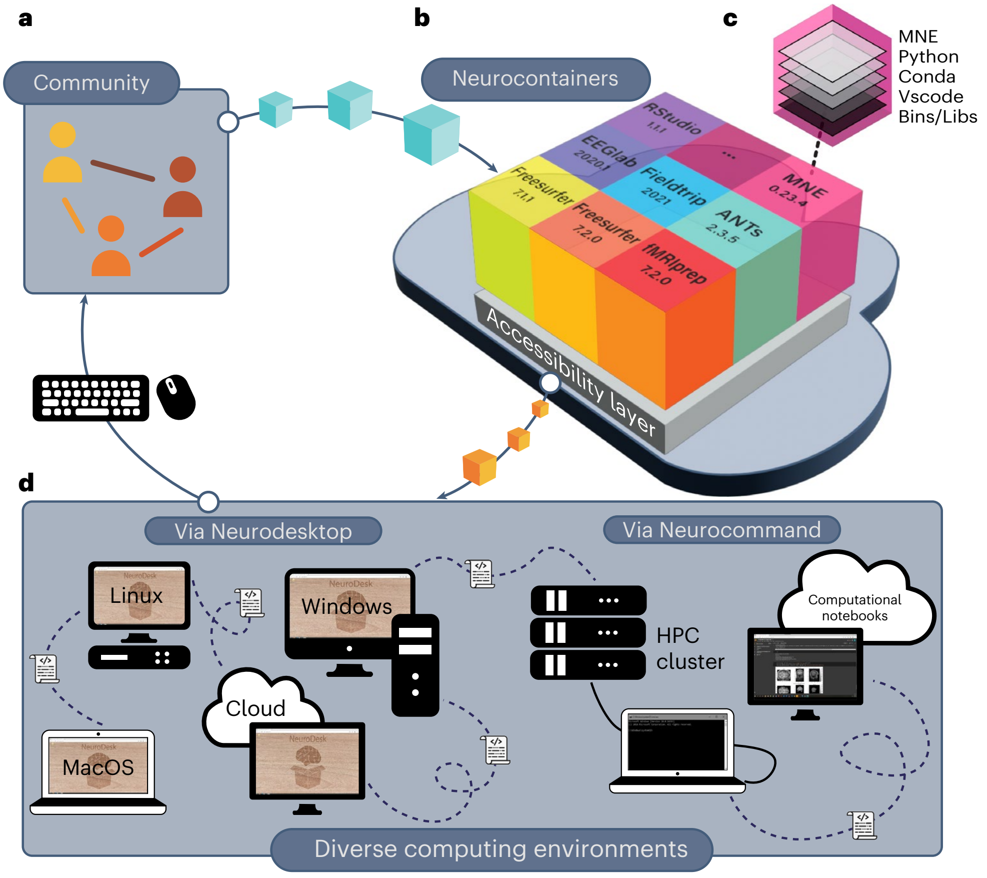

Fig. 1 | The Neurodesk platform. a, Neurodesk is built by and for the scientific community, enabling anyone to contribute containers. **b**, Community-contributed software recipes are automatically used to build software containers stored in the Neurocontainers repository. **c**, Each container packages a tool together with all its dependencies. **d**, Neurodesk provides two layers of accessibility: (1) Neurodesktop: a browser-accessible virtual desktop environment; (2) Neurocommand: a command-line interface that runs the same software containers programmatically. These interfaces allow users to reproduce analyses across computing environments (HPC: high-performance computing).

while supporting shared development workloads[5]. Unfortunately, many analysis workflows are neither readily accessible nor portable[6,7], and many existing solutions to these issues lack flexibility[8]. For example, single-install preprogrammed analysis pipelines are popular with clinicians, but researchers typically customize analysis pipelines for specific projects[9–11]. Virtual machines or dual-boot computers partially address these barriers, but they are resource intensive and still do not reconcile conflicts between software packages or their dependencies. Beyond productivity costs, inaccessible and unstable neuroimaging tools also pose a wider threat to reproducibility[12,13], that is, running the same software on the same input data and obtaining the same result[14]. The transparency and openness promotion guidelines, which have over 5,000 journals, publishers and other related organizations as signatories, state that all reported results should be independently reproduced before publication[15]. But realistically, results verification is usually too impractical to implement at review[6].

These issues are not unique to neuroimaging or scientific research, and similar issues in the software space led to the development of software containers; lightweight and portable solutions that package applications and their dependencies. Container engines such as Docker, Podman and Apptainer/Singularity allow containerized software to seamlessly shift between computing environments without relying on, or conflicting with, software outside the container[16]. Containers are thus well suited to address the issues facing neuroimaging analysis and form the core of the Neurodesk project[17] (Fig. 1). Neurodesk makes containerized neuroimaging software easier to both access and create through the Neurocontainers repository, a comprehensive and growing collection of versioned neuroimaging software containers (Fig. 1a,b). Neurocontainers contributed by the community are automatically made available to access through Neurodesk (Fig. 1a). Each Neurocontainer includes the packaged tool and all dependencies required to execute a specific version of that tool (Fig. 1c). Because containers isolate dependencies, different Neurocontainers can provide different versions of the same tool, allowing researchers to seamlessly switch software versions.

Neurodesk enables researchers to use Neurocontainers directly through the cloud or download containers for offline use through two possible interfaces, without the need to install neuroimaging software locally. First, Neurodesktop is a browser-accessible virtual desktop environment with all containerized tools accessible from the application menu (Fig. 1d). Neurodesktop has the look and feel of working on one's local computer, and can be executed using local or cloud resources. Second, Neurocommand can be used to launch and interact with Neurocontainers through the command line. Neurocommand is suitable for use in high-performance computing environments, and can be used to interact with neuroimaging software through computational notebooks such as Google Colab or Jupyter Notebooks[18] (Fig. 1d). These Neurodesk interfaces can be launched from most common operating systems by installing the Neurodesk App, or by launching remote instances online. Extensive documentation, tutorials and examples are available at the Neurodesk website (https://www.neurodesk.org/). By harnessing these easy-to-use interfaces, researchers can flexibly take advantage of large open datasets, reproduce reported analyses, and switch between neuroimaging modalities and computational platforms

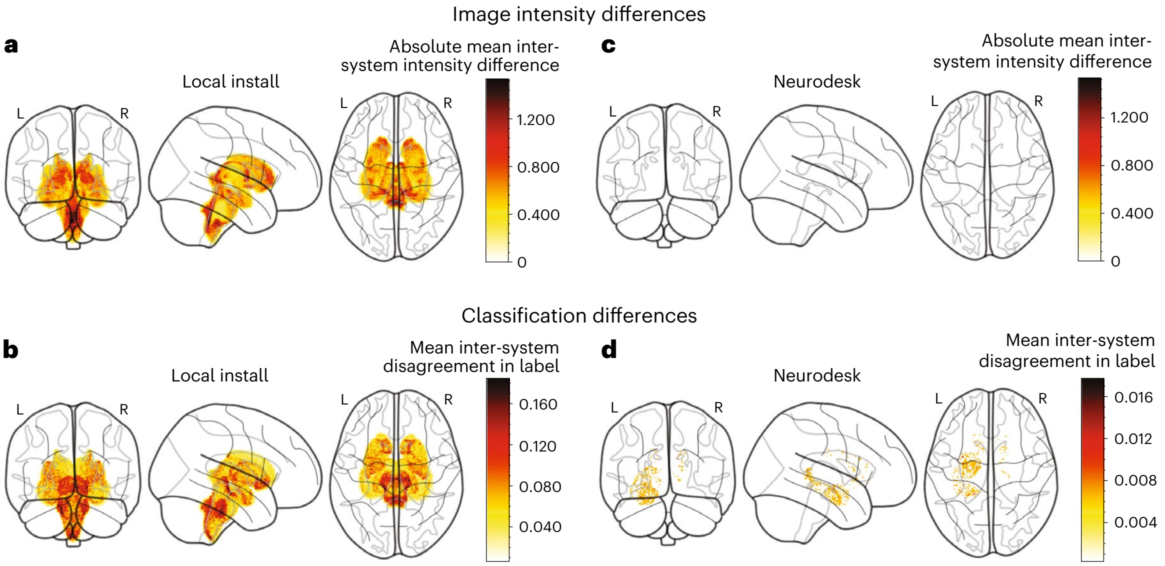

Fig. 2 | Inter-computer differences in an fMRI processing pipeline. **a**,**c**, Absolute mean inter-computer image intensity differences within subcortical structures after image registration with FSL-FLIRT. Projections are shown for locally installed software (**a**) and Neurodesk (**c**). **b**,**d**, Inter-system classification disagreement after image segmentation with FSL-FIRST, averaged across participants. Projections are shown for locally installed software (**b**) and Neurodesk (**d**) (note the difference in color scale range).

within and between projects. Containerized software reduces unnecessary computational variability between execution systems, making it possible to share analyses between laboratories and collaborate on large datasets without artificial differences between sites. Further, for developers, the effort to containerize and add one's software to Neurodesk may be minimal compared with testing software and supporting users across diverse computing platforms.

Studies have shown that subtle differences in hardware, firmware and software dependencies can systematically alter results across computing environments[19–21], meaning it is often impossible to replicate results even when given the original data, code and software version. This effect has been well described for functional magnetic resonance imaging (fMRI) processing pipelines[19]. To evaluate whether Neurodesk addresses these issues, we therefore set out to replicate and extend upon these findings; we ran four identical MRI analysis pipelines, in two separate computing environments, using software installed locally and through Neurodesk. We found meaningful differences in image intensity and subcortical tissue classification between the two computers for pipelines run on locally installed software (Fig. 2a,b), but not for pipelines run on Neurodesk (Fig. 2c,d). These results show that Neurodesk allows researchers to adhere to the highest possible reproducibility standards with minimal changes to their typical workflow. See the Supplementary Notes for the full results of this case study.

Neurodesk not only facilitates access to reproducible neuroimaging data analysis, but also makes sharing these workflows less burdensome. Neurocontainers are accessible within computational notebooks (for example, running FreeSurfer[22] within Google Colab), enabling researchers to share reproducible code and results alongside published manuscripts. Notably, this approach requires authors to ensure interoperability of the linked code and data, ensuring that readers do not need to spend time downloading large datasets from remote repositories, or overcome issues with executing notebooks due to insufficient cloud computing resources. Recent developments in reproducible preprints present an enriched publication path that simplifies the sharing of data and analysis code[23]. NeuroLibre, for example, hosts interactive notebooks and associated data, allowing readers to modify and re-execute code[24]. Neurocontainers are ideally suited for such integrated and reproducible approaches.

Neurodesk is also impactful as an educational tool in workshops and courses. The platform was first conceptualized during a 'hackathon'[25], an event where people with diverse skill sets collaborated on projects and developed research skills. Variability in analysis environments across attendees' computers presents a hurdle for neuroimaging training workshops such as this. Facilitators often spend considerable time troubleshooting software installations specific to unique computing environments. Neurodesk, which provides access to a standardized analysis environment with the requisite tools preinstalled with almost no set up, allows researchers to efficiently tackle complex scientific problems by eliminating technical troubleshooting. Moreover, Neurodesk is scalable to different class sizes and computational demands, can be accessed remotely and enables trainees to easily access their analyses after the workshop. Containerized platforms in other fields have made a substantial impact in this way, for example, the Galaxy platform for bioinformatics[26].

Neurodesk exists within a larger ecosystem of projects providing accessible, reproducible, flexible and portable neuroimaging analysis, and, where possible, seeks to interoperate with related platforms. While Neurodesk is not the only project to address any one of these principles, Neurodesk is unique in addressing all four principles. Projects such as NeuroDebian[1] and Neurofedora[27] increase accessibility for GNU/Linux operating systems, but offer limited support for portability or reproducibility. Other projects such as Brainlife[28], BIDSApps[29], Flywheel (https://flywheel.io/), XNAT[30], Code-Ocean[31], Qmenta (https://www.qmenta.com/), CBRAIN[32] and Biocontainers[33] all support reproducibility through containerization, but have different use-cases to Neurodesk. For example, Brainlife facilitates reproducible and traceable cloud-based analysis using community-contributed workflows. However, the platform is designed to allow users to run pre-coded analysis pipelines, rather than to flexibly access software to develop their own pipelines. To this end, the Neurodesk and Brainlife teams are increasing interoperability between the platforms by providing Brainlife development environments on Neurodesk, and running Neurodesk containers on Brainlife. Thus, in cases where flexibility is less important, Neurodesk can also be harnessed to support the complete workflow reproducibility offered by preprogrammed analysis pipelines with Brainlife. Similarly, we have integrated the 'BIDSApps' repository of containerized workflows, allowing users to access or adapt these workflows. In this way, users already accustomed to other platforms and tools will also benefit from the Neurodesk project.

Neurodesk has some limitations that warrant discussion. One area of ongoing development relates to the inclusion of proprietary and licensed software without compromising accessibility. Another challenge for a flexible platform with as wide a range of applications as Neurodesk is the project's long-term sustainability. Neurodesk's community-driven, continuous integration model provides a powerful and flexible way to address both of these expanded use-cases without depending on a single development team. We have developed multiple pathways for sustainability, including the federated support of the underlying hosting infrastructure, flexibility in the continuous integration and deployment infrastructure and a potential for a commercial model to offer tailored support for institutions and workshops.

The challenges of accessibility, portability, flexibility and reproducibility discussed here are not unique to neuroscience. In turn, Neurodesk's core foundation could be used to deploy software specific to any other discipline, and it is our sincere hope that this platform is adapted as such. The Neurodesk platform has the potential to improve the way scientists analyze data and communicate results. Specifically, Neurodesk allows any scientist, anywhere in the world, to conveniently access, develop and adapt their neuroimaging analysis tools, and apply them in a fully reproducible manner from any computing environment.

Online content

Any methods, additional references, Nature Portfolio reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41592-023-02145-x.

References

1. Halchenko, Y. & Hanke, M. Open is not enough. let's take the next step: an integrated, community-driven computing platform for neuroscience. *Front. Neuroinform.* **6**, 22 (2012).
2. Hanke, M. & Halchenko, Y. Neuroscience runs on GNU/Linux. *Front. Neuroinform.* **5**, 8 (2011).
3. Niso, G. et al. Open and reproducible neuroimaging: from study inception to publication. *NeuroImage* **263**, 119623 (2022).
4. Wilkinson, M. D. et al. The FAIR Guiding Principles for scientific data management and stewardship. *Sci. Data* **3**, 160018 (2016).
5. Kurtzer, G. M., Sochat, V. & Bauer, M. W. Singularity: scientific containers for mobility of compute. *PLoS ONE* **12**, e0177459 (2017).
6. Van Gorp, P. & Mazanek, S. SHARE: a web portal for creating and sharing executable research papers. *Procedia Comput. Sci.* **4**, 589–597 (2011).
7. Poline, J. -B. et al. Is neuroscience FAIR? a call for collaborative standardisation of neuroscience data. *Neuroinformatics* **20**, 507–512 (2022).
8. Silberzahn, R. et al. Many analysts, one data set: making transparent how variations in analytic choices affect results. *Adv. Methods Pract. Psychol. Sci.* **1**, 337–356 (2018).
9. Tapera, T. M. et al. FlywheelTools: data curation and manipulation on the Flywheel platform. *Front. Neuroinform.* **15**, 678403 (2021).
10. Routier, A. et al. Clinica: an open-source software platform for reproducible clinical neuroscience studies. *Front. Neuroinform.* **15**, 689675 (2021).
11. Abe, T. et al. Neuroscience cloud analysis as a service: an open-source platform for scalable, reproducible data analysis. *Neuron* **110**, 2771–2789 (2022).
12. Goodman, S. N., Fanelli, D. & Ioannidis, J. P. A. What does research reproducibility mean? *Sci. Transl. Med.* **8**, 341ps12–341ps12 (2016).
13. Nosek, B. A. et al. Replicability, robustness, and reproducibility in psychological science. *Annu. Rev. Psychol.* **73**, 719–748 (2022).
14. Plesser, H. E. Reproducibility vs. replicability: a brief history of a confused terminology. *Front. Neuroinform.* **11**, 76 (2018).
15. Nosek, B. A. et al. Promoting an open research culture. *Science* **348**, 1422–1425 (2015).
16. Boettiger, C. An introduction to Docker for reproducible research. *ACM SIGOPS Oper. Syst. Rev.* **49**, 71–79 (2015).
17. Trunov, A. S., Voronova, L. I., Voronov, V. I. & Ayrapetov, D. P. Container cluster model development for legacy applications integration in scientific software system. in *2018 IEEE International Conference 'Quality Management, Transport and Information Security, Information Technologies' (IT QM IS)* 815–819 https://doi.org/10.1109/ITMQIS.2018.8525120 (2018).
18. Thomas, T. et al. Jupyter Notebooks—a publishing format for reproducible computational workflows. In *Positioning and Power in Academic Publishing: Players, Agents and Agendas* (eds Loizides, F. & Schmid, B.) 87–90 (IOS Press, 2016).
19. Glatard, T. et al. Reproducibility of neuroimaging analyses across operating systems. *Front. Neuroinform.* **9**, 12 (2015).
20. Gronenschild, E. H. et al. The effects of FreeSurfer version, workstation type, and Macintosh operating system version on anatomical volume and cortical thickness measurements. *PLoS ONE* **7**, e38234 (2012).
21. Krefting, D. et al. Reliability of quantitative neuroimage analysis using freesurfer in distributed environments. In *MICCAI Workshop on High-Performance and Distributed Computing for Medical Imaging* (2011).
22. Fischl, B. FreeSurfer. *NeuroImage* **62**, 774–781 (2012).
23. DuPre, E. et al. Beyond advertising: new infrastructures for publishing integrated research objects. *PLoS Comput. Biol.* **18**, e1009651 (2022).
24. Karakuzu, A. et al. NeuroLibre: a preprint server for full-fledged reproducible neuroscience. Preprint at *OSF* https://doi.org/10.31219/osf.io/h89js (2022).
25. Gau, R. et al. Brainhack: developing a culture of open, inclusive, community-driven neuroscience. *Neuron* **109**, 1769–1775 (2021).
26. Afgan, E. et al. The Galaxy platform for accessible, reproducible and collaborative biomedical analyses: 2018 update. *Nucleic Acids Res.* **46**, W537–W544 (2018).
27. Sinha, A. et al. Comp-NeuroFedora, a free/open source operating system for computational neuroscience: download, install, research. *BMC Neurosci.* **21**, 1 (2020).
28. Hayashi, S. et al. brainlife.io: a decentralized and open source cloud platform to support neuroscience research. Preprint at *arXiv* https://doi.org/10.48550/arXiv.2306.02183 (2023).
29. Gorgolewski, K. J. et al. BIDS apps: improving ease of use, accessibility, and reproducibility of neuroimaging data analysis methods. *PLoS Comput. Biol.* **13**, e1005209 (2017).
30. Herrick, R. et al. XNAT Central: open sourcing imaging research data. *NeuroImage* **124**, 1093–1096 (2016).
31. Staubitz, T., Klement, H., Teusner, R., Renz, J. & Meinel, C. CodeOcean—a versatile platform for practical programming excercises in online environments. In *2016 IEEE Global Engineering Education Conference (EDUCON)* 314–323 https://doi.org/10.1109/EDUCON.2016.7474573 (2016).
32. Sherif, T. et al. CBRAIN: a web-based, distributed computing platform for collaborative neuroimaging research. *Front. Neuroinform.* **8**, 54 (2014).
33. da Veiga Leprevost, F. et al. BioContainers: an open-source and community-driven framework for software standardization. *Bioinformatics* **33**, 2580–2582 (2017).

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Methods

How to use Neurodesk: accessibility, flexibility and portability

The Neurodesk platform's website (https://www.neurodesk.org/) is user-friendly and open to community contributions. The website contains information about the included software and is automatically updated through continuous integration. Therefore, there is always up-to-date documentation, lists of currently available applications and a release history. The website also hosts clear instructions for accessing and interacting with Neurodesk from various computing environments and tutorials on using various software packages.

Neurodesk makes reproducible neuroimaging data analysis accessible in almost any computing environment and brings the same dependencies to all supported platforms. This portability extends to the Neurodesktop graphical user interface, which provides the same desktop environment across all supported computing environments. Containerized analyses look, feel and run the same way across different computing environments. Thus, researchers reading or reviewing manuscripts with open data and code can use Neurodesk to replicate the exact pipeline using the reported tool versions without being required to install additional software.

For a data analysis environment to be portable, such that it can easily shift between computing environments, it also needs to be lightweight with a small storage footprint. To this end, our accessibility layer harnesses the CernVM File System (CVMFS)[34]. The CVMFS layer allows accessing the software from a remote host without installation, so only parts of a container that are actively used are sent over the network and cached on the user's local computer. Users can access terabytes of software without explicitly downloading or storing it locally. The Neurodesk platform has several CVMFS nodes worldwide, providing low latency and direct access to Neurocontainers. Thus, to use Neurodesk, users only install the required container engine to access the Neurocontainer of their choice. The current release of Neurodesktop, which facilitates access to all tools in the Neurocontainers repository, is less than 1.6 GB in download size.

Anticipating that installing a third-party container engine software may be a barrier to entry for some researchers, there is an entirely cloud-based solution: 'Neurodesk Play' (https://play.neurodesk.org/). Neurodesk Play is accessible globally, allowing anyone to use a cloud-based graphical desktop environment for neuroimaging data analysis and teaching. Neurodesk play instances are Binderhub[35] instances deployed based on the zero-to-binderhub guide, coupled with the full suite of Neurocontainers delivered via CVMFS. Neurodesktop can also run on institutional or cloud computing resources enabling access to large amounts of computing resources or datasets. For example, the Australian Research Data Commons (ARDC) provides Neurodesk on their Virtual Desktop Service freely available to anyone with an Australian Access Federation account.

The accessibility, flexibility and portability of this platform can be best assessed through its utility to users. We, therefore, display up-to-date usage statistics for the platform on our website (https://www.neurodesk.org/docs/overview/metrics/). Further, the platform has already been referenced in several peer-reviewed studies[36–39].

Long-term sustainability of the Neurodesk platform

Neurodesk has a wide selection of tools available spanning many domains of neuroimaging data analysis. Extended Data Table 1 shows the tools available at the time of publication, although this list is growing rapidly as the community and developers contribute software through recipes created using the open-source Neurodocker project[40]. These recipes can be based on the Neurodebian project[1]. Users can find a full and up-to-date list at https://www.neurodesk.org/applications/. Neurodesk uses a two-pronged approach to staying up to date with new neuroimaging tools and new versions of already included software: (1) The Neurodesk maintainers add tools as they become aware of new developments or community members request the addition of new packages. The Neurodesk GitHub organization (https://github.com/NeuroDesk/) has an active discussion forum where developers respond to requests for new software containers. (2) In addition to this developer-centric route to new software containers, we actively encourage contributions from the research community. A core aim for developing the Neurodesk platform was to build it as a community-driven project that is not contingent on a specific team of developers. As such, we provide a template and detailed instructions for creating build scripts for new software containers. Moreover, we aim to ensure long-term executability of the containers by storing the containers in different formats: docker, podman, singularity/apptainer and an unpacked chroot environment. This comes with the benefit of increased accessibility for users and the advantage that when technology progresses and standards change over the years, users will still be able to execute the software through standard GNU/Linux kernel tools (chroot and mount)[41–99].

Reporting summary

Further information on research design is available in the Nature Portfolio Reporting Summary linked to this article.

Data availability

The data that support the findings of the case study are available from the ICBM database (https://www.loni.usc.edu/). There are restrictions that apply to the availability of these data, which were used under approved permission for the current study, and thus are not publicly available but are available from ICBM upon request. Source data are provided with this paper.

Code availability

The code for this project is publicly available on GitHub, across multiple repositories under the https://github.com/NeuroDesk/ organization. It has also been archived on Zenodo at https://doi.org/10.5281/zenodo.8053090. The code is licensed under the MIT License.
All stages of development, from the initial conception as a hackathon project, through to the most current iteration of Neurodesk, with up-to-date community-built Neurocontainer recipes, are documented publicly across the project's GitHub repository and the platform's website; which contains descriptions of how code is organized on the GitHub repository, and how to contribute to the project (https://www.neurodesk.org/).
Any issues can be logged at https://github.com/orgs/NeuroDesk/discussions/. Contributions can be made by any community member with a GitHub account and the eagerness to create pull requests.

References

34. Blomer, J. et al. Micro-CernVM: slashing the cost of building and deploying virtual machines. *J. Phys. Conf. Ser.* **513**, 032009 (2014).
35. Jupyter, P. et al. Binder 2.0—reproducible, interactive, sharable environments for science at scale. in *Proceedings of the 17th Python in Science Conference* 113–120 https://doi.org/10.25080/Majora-4af1f417-011 (2018).
36. Atilgan, H. et al. Functional relevance of the extrastriate body area for visual and haptic object recognition: a preregistered fMRI-guided TMS study. *Cereb. Cortex Commun.* **4**, tgad005 (2023).
37. Chang, J. et al. Open-source hypothalamic-ForniX (OSHy-X) atlases and segmentation tool for 3T and 7T. *J. Open Source Softw.* **7**, 4368 (2022).
38. Stewart, A. W. et al. QSMxT: robust masking and artifact reduction for quantitative susceptibility mapping. *Magn. Reson. Med.* **87**, 1289–1300 (2022).
39. Biondetti, E. et al. Multi-echo quantitative susceptibility mapping: how to combine echoes for accuracy and precision at 3 Tesla. *Magn. Reson. Med.* **88**, 2101–2116 (2022).

40. Kaczmarzyk, J. et al. ReproNim/neurodocker: 0.9.5. https://doi.org/10.5281/zenodo.7929032 (2023).
41. Gorgolewski, K. et al. Nipype: a flexible, lightweight and extensible neuroimaging data processing framework in Python. *Front. Neuroinform.* **5**, 13 (2011).
42. Adebimpe, A. et al. ASLPrep: a platform for processing of arterial spin labeled MRI and quantification of regional brain perfusion. *Nat. Methods* **19**, 683–686 (2022).
43. Esteban, O. et al. fMRIPrep: a robust preprocessing pipeline for functional MRI. *Nat. Methods* **16**, 111–116 (2019).
44. Esteban, O. et al. MRIQC: Advancing the automatic prediction of image quality in MRI from unseen sites. *PLoS ONE* **12**, e0184661 (2017).
45. Li, X., Morgan, P. S., Ashburner, J., Smith, J. & Rorden, C. The first step for neuroimaging data analysis: DICOM to NIfTI conversion. *J. Neurosci. Methods* **264**, 47–56 (2016).
46. Zwiers, M. P., Moia, S. & Oostenveld, R. BIDScoin: a user-friendly application to convert source data to brain imaging data structure. *Front. Neuroinform.* **15**, 770608 (2022).
47. Gorgolewski, K. J. et al. The brain imaging data structure, a format for organizing and describing outputs of neuroimaging experiments. *Sci. Data* **3**, 160044 (2016).
48. Yushkevich, P. A. et al. User-guided segmentation of multi-modality medical imaging datasets with ITK-SNAP. *Neuroinformatics* **17**, 83–102 (2019).
49. Wang, R., Benner, T., Sorensen, A. G. & Wedeen, V. J. Diffusion toolkit: a software package for diffusion imaging data processing and tractography. *Proc. Intl Soc. Mag. Reson. Med.* **15**, 3720 (2007).
50. Yeh, F. -C. Population-based tract-to-region connectome of the human brain and its hierarchical topology. *Nat. Commun.* **13**, 4933 (2022).
51. Tournier, J. -D., Calamante, F. & Connelly, A. MRtrix: diffusion tractography in crossing fiber regions. *Int. J. Imaging Syst. Technol.* **22**, 53–66 (2012).
52. Pallast, N. et al. Processing pipeline for atlas-based imaging data analysis of structural and functional mouse brain MRI (AIDAmri). *Front. Neuroinform.* **13**, 42 (2019).
53. Desrosiers-Gregoire, G. et al. Rodent Automated Bold Improvement of EPI Sequences (RABIES): a standardized image processing and data quality platform for rodent fMRI. Preprint at *bioRxiv* https://doi.org/10.1101/2022.08.20.504597 (2022).
54. Hangel, G. et al. Ultra-high resolution brain metabolite mapping at 7T by short-TR Hadamard-encoded FID-MRSI. *NeuroImage* **168**, 199–210 (2018).
55. Cox, R. W. AFNI: what a long strange trip it's been. *NeuroImage* **62**, 743–747 (2012).
56. Avants, B. B., Tustison, N. & Johnson, H. Advanced Normalization Tools (ANTS). *Insight J.* **2**, 1–35 (2009).
57. Wisse, L. E. M. et al. Automated hippocampal subfield segmentation at 7T MRI. *Am. J. Neuroradiol.* **37**, 1050–1057 (2016).
58. Gaser, C. et al. CAT—a computational anatomy toolbox for the analysis of structural MRI data. Preprint at *bioRxiv* https://doi.org/10.1101/2022.06.11.495736 (2022).
59. Eckstein, K. et al. Improved susceptibility weighted imaging at ultra-high field using bipolar multi-echo acquisition and optimized image processing: CLEAR-SWI. *NeuroImage* **237**, 118175 (2021).
60. Whitfield-Gabrieli, S. & Nieto-Castanon, A. Conn: a functional connectivity toolbox for correlated and anticorrelated brain networks. *Brain Connect* **2**, 125–141 (2012).
61. Marcus, D. S. et al. Human Connectome Project informatics: quality control, database services, and data visualization. *NeuroImage* **80**, 202–219 (2013).
62. Estrada, S. et al. FatSegNet: a fully automated deep learning pipeline for adipose tissue segmentation on abdominal dixon MRI. *Magn. Reson. Med.* **83**, 1471–1483 (2020).
63. Jenkinson, M., Beckmann, C. F., Behrens, T. E. J., Woolrich, M. W. & Smith, S. M. FSL. *NeuroImage* **62**, 782–790 (2012).
64. Isensee, F. et al. Automated brain extraction of multisequence MRI using artificial neural networks. *Hum. Brain Mapp.* **40**, 4952–4964 (2019).
65. Shaw, T., York, A., Ziaei, M., Barth, M. & Bollmann, S. Longitudinal Automatic Segmentation of Hippocampal Subfields (LASHiS) using multi-contrast MRI. *NeuroImage* **218**, 116798 (2020).
66. Huber, L. R. et al. LayNii: a software suite for layer-fMRI. *NeuroImage* **237**, 118091 (2021).
67. Vincent, R. D. et al. MINC 2.0: a flexible format for multi-modal images. *Front. Neuroinformatics* **10**, 35 (2016).
68. Grussu, F. et al. Multi-parametric quantitative in vivo spinal cord MRI with unified signal readout and image denoising. *NeuroImage* **217**, 116884 (2020).
69. Winkler, A. M., Ridgway, G. R., Webster, M. A., Smith, S. M. & Nichols, T. E. Permutation inference for the general linear model. *NeuroImage* **92**, 381–397 (2014).
70. Kasper, L. et al. The PhysIO toolbox for modeling physiological noise in fMRI data. *J. Neurosci. Methods* **276**, 56–72 (2017).
71. Dymerska, B. et al. Phase unwrapping with a rapid opensource minimum spanning tree algorithm (ROMEO). *Magn. Reson. Med.* **85**, 2294–2308 (2021).
72. Fedorov, A. et al. 3D slicer as an image computing platform for the quantitative imaging network. *Magn. Reson. Imaging* **30**, 1323–1341 (2012).
73. De Leener, B. et al. SCT: Spinal Cord Toolbox, an open-source software for processing spinal cord MRI data. *NeuroImage* **145**, 24–43 (2017).
74. Ashburner, J. Computational anatomy with the SPM software. *Magn. Reson. Imaging* **27**, 1163–1174 (2009).
75. Langkammer, C. et al. Fast quantitative susceptibility mapping using 3D EPI and total generalized variation. *NeuroImage* **111**, 622–630 (2015).
76. Klein, S., Staring, M., Murphy, K., Viergever, M. A. & Pluim, J. elastix: a toolbox for intensity-based medical image Registration. *IEEE Trans. Med. Imaging* **29**, 196–205 (2010).
77. Shamonin, D. et al. Fast parallel image registration on CPU and GPU for diagnostic classification of Alzheimer's disease. *Front. Neuroinform.* **7**, 50 (2014).
78. Civier, O., Sourty, M. & Calamante, F. MFCSC: novel method to calculate mismatch between functional and structural brain connectomes, and its application for detecting hemispheric functional specialisations. *Sci. Rep.* **13**, 3485 (2023).
79. Tadel, F., Baillet, S., Mosher, J. C., Pantazis, D. & Leahy, R. M. Brainstorm: a user-friendly application for MEG/EEG analysis. *Comput. Intell. Neurosci.* **2011**, 879716 (2011).
80. Brunner, C., Delorme, A. & Makeig, S. Eeglab—an open source MATLAB toolbox for electrophysiological research. *Biomed. Tech.* **58**, 1 (2013).
81. Oostenveld, R., Fries, P., Maris, E. & Schoffelen, J. -M. FieldTrip: open source software for advanced analysis of MEG, EEG, and invasive electrophysiological data. *Comput. Intell. Neurosci.* **2011**, 156869 (2011).
82. Gramfort, A. et al. MNE software for processing MEG and EEG data. *NeuroImage* **86**, 446–460 (2014).
83. Brunner, C., Breitwieser, C. & Müller-Putz, G. R. Sigviewer and Signalserver—open source software projects for biosignal analysis. *Biomed. Eng. Tech.* **58**, 1 (2013).
84. Ihaka, R. & Gentleman, R. R: a language for data analysis and graphics. *J. Comput. Graph. Stat.* **5**, 299–314 (1996).
85. Ribeiro, F. L., Bollmann, S. & Puckett, A. M. Predicting the retinotopic organization of human visual cortex from anatomy using geometric deep learning. *NeuroImage* **244**, 118624 (2021).

86. Mishra, P., Lehmkuhl, R., Srinivasan, A., Zheng, W. & Popa, R. A. Delphi: a cryptographic inference service for neural networks. In *29th USENIX Security Symposium (USENIX Security 20)* 2505–2522 (2020).
87. Still, M. *The definitive guide to ImageMagick*. vol. 1 (Springer, 2006).
88. Rorden, C. & Brett, M. Stereotaxic display of brain lesions. *Behav. Neurol.* **12**, 191–200 (2000).
89. Rorden, C. rordenlab/MRIcroGL: version 20-July-2022 (v1.2.20220720) https://doi.org/10.5281/ZENODO.7533834 (2022).
90. Vicory, J. et al. SlicerSALT: Shape AnaLysis Toolbox. In *Shape in Medical Imaging* (eds. Reuter, M. et al.) vol. 11167, 65–72 (Springer International Publishing, 2018).
91. Rorden, C. & Hanayik, T. neurolabusc/surf-ice: version 6-October-2021 (v1.0.20211006). https://doi.org/10.5281/ZENODO.7533772 (2021)
92. Bumgarner, J. R. & Nelson, R. J. Open-source analysis and visualization of segmented vasculature datasets with VesselVio. *Cell Rep. Methods* **2**, 100189 (2022).
93. Cusack, R. et al. Automatic analysis (aa): efficient neuroimaging workflows and parallel processing using Matlab and XML. *Front. Neuroinform.* **8**, 90 (2015).
94. Liem, F. & Gorgolewski, C. F. BIDS-Apps/baracus: v1.1.2. https://doi.org/10.5281/ZENODO.1018841 (2017).
95. Kim, Y. et al. BrainSuite BIDS App: containerized workflows for MRI analysis. Preprint at *bioRxiv* https://doi.org/10.1101/2023.03.14.532686 (2023).
96. Glasser, M. F. et al. The minimal preprocessing pipelines for the Human Connectome Project. *NeuroImage* **80**, 105–124 (2013).
97. Smith, S. M. et al. Resting-state fMRI in the Human Connectome Project. *NeuroImage* **80**, 144–168 (2013).
98. Trott, O. & Olson, A. J. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J. Comput. Chem.* **31**, 455–461 (2010).
99. Eberhardt, J., Santos-Martins, D., Tillack, A. F. & Forli, S. AutoDock Vina 1.2.0: new docking methods, expanded force field, and Python bindings. *J. Chem. Inf. Model.* **61**, 3891–3898 (2021).

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Competing interests

The authors declare no competing interests.

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Extended Data Table 1 | Tools currently available in Neurodesk

Category	Tool
Editors and Programming	VS Code, Gedit, Emacs, Vim, Python, Git, Julia, Matlab, ROOT, RStudio
Data Synchronisation Tools	Rsync, Rclone, Nextcloud client, Owncloud client, Globus personal connect
Workflows	Nipype[42], ASLPrep[43], fMRIPrep[44], MRIQC[45], QSMxT[39]
Data Organisation	dcm2niix[46], BIDScoin[47], BIDStools[48], Convert3D[49]
Diffusion MRI	Diffusion Toolkit[50], DSI Studio[51], MRtrix[52], MRtrix3Tissue (www.3Tissue.github.io), TrackVis[50]
Rodent Imaging	AIDAmri[53], RABIES[54]
Spectroscopy	LCModel (http://s-provencher.com/lcmodel.shtml), MRSIProc[55]
Structural and/or Functional Imaging	AFNI[56], ANTs[57], ASHS[58], BART (https://mrirecon.github.io/bart/) , CAT12[59], CLEAR-SWI[60], Conn[61], Connectome Workbench[62], FatSegNet[63], FreeSurfer[22], FSL[64], HD-BET[65], LASHiS[66], LayNii[67], MINC[68], MRItools[69], NiftyReg (https://www.nitrc.org/projects/niftyreg/), NiiStat (https://www.nitrc.org/projects/niistat/), OSHy-X[38], Palm Alpha[70], PhysIO[71], ROMEO[72], Slicer[73], Spinal Cord Toolbox[74], SPM[75], TGVQSM[76], elastix[77,78], mfcsc[79]
Electroencephalography (EEG) and/or Magnetoencephalography (MEG)	Brainstorm[80], EEGLAB[81], FieldTrip[82], MNE[83], Sigviewer[84]
Machine Learning and Statistics	R[85], Deep Retinopy[86], Delphi[87]
Visualisation and Image Editing	ImageMagick[88], GIMP (www.gimp.org), itk-SNAP[49], MRIcron[89], MRIcroGL[90], SicerSALT[91], Surf Ice[92] , VesselVio[93]
BIDS App	Automatic Analysis[94], BARACUS[95], BrainSuite[96], HCPPipelines[97,98], MRtrix3_connectome (https://github.com/bids-apps/MRtrix3_connectome)
Molecular biology	MGLTools (https://ccsb.scripps.edu/mgltools/), AutoDock Vina[99,100]

The Neurodesk development team uses a broad definition of what constitutes a 'tool' and is guided by the community in what level of granularity would most flexibly facilitate neuroimaging data analysis on a case-by-case basis. Note that each tool has been listed under only one category, although some may span multiple categories. An up-to-date table can be retrieved from https://www.neurodesk.org/applications/. Details on the tools are available in refs. 41–99.

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☐	☒	Estimates of effect sizes (e.g. Cohen's *d*, Pearson's *r*), indicating how they were calculated

Our web collection on statistics for biologists contains articles on many of the points above.

Software and code

Policy information about availability of computer code

Data collection	No data analysis software were used.
Data analysis	Data analysis for the case-study reported in supplementary materials was performed using the FMRIB Software Library (FSL) 6.5.0.1. The code and instructions on how to reproduce the reported analysis through Neurodesk Play (https://www.neurodesk.org/) are available on the Open Science Framework: https://osf.io/e6pw3/. All code underlying the Neurodesk project used to analyse data is openly available on Github: https://github.com/NeuroDesk.

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The data that support the findings of this study are available from the International Consortium for Brain Mapping (ICBM) database (www.loni.usc.edu/ICBM). The

ICBM project (Principal Investigator John Mazziotta, M.D., University of California, Los Angeles) is supported by the National Institute of Biomedical Imaging and BioEngineering. ICBM is the result of efforts of co-investigators from UCLA, Montreal Neurologic Institute, University of Texas at San Antonio, and the Institute of Medicine, Juelich/Heinrich Heine University - Germany. There are restrictions that apply to the availability of these data, which were used under approved permission for the current study, and so are not publicly available, but available from ICBM upon request.

Human research participants

Policy information about studies involving human research participants and Sex and Gender in Research.

Reporting on sex and gender	This study made use of an existing dataset, and thus no sex or gender data were specifically recorded. As the focus of the analyses were on reproducibility in general, no sex or gender specific analyses were performed.
Population characteristics	The ICBM dataset aimed to broadly sample the population. While specific population data are not available for each subject, the curators of the dataset have stated that data were sampled from "geographical locations as disparate as Japan and Scandinavia and spanning the age range from 18 to 90 years. Special efforts have been made to obtain a wide range of racial and ethnic diversity"
Recruitment	Participants for the ICBM dataset used were originally recruited by advertisement, and then selected according to a series of inclusion criteria to ensure uniformity in the dataset. The effects of these recruitment protocols has been evaluated in detail here: Mazziotta, J. C., Woods, R., Iacoboni, M., Sicotte, N., Yaden, K., Tran, M., ... & International Consortium for Brain Mapping (ICBM. (2009). The myth of the normal, average human brain—the ICBM experience:(1) subject screening and eligibility. Neuroimage, 44(3), 914-922.
Ethics oversight	As per the original curators of the ICBM dataset, "All subjects who participated in this project as well as all of the screening materials, exclusion criteria and procedures for applying them were approved by the UCLA Institutional Review Board. All subjects signed an informed consent describing the process, risks and benefits. They were also given a Subject's Bill of Rights."

Note that full information on the approval of the study protocol must also be provided in the manuscript.

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Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Sample size	This case study aimed to replicate that reported by: Glatard, T., Lewis, L. B., Ferreira da Silva, R., Adalat, R., Beck, N., Lepage, C., ... & Evans, A. C. (2015). Reproducibility of neuroimaging analyses across operating systems. Frontiers in neuroinformatics, 9, 12. We used the same dataset as the original study, thus sample size was determined as that matching the study we sought to replicate, which was the full size of the dataset (157 participants).
Data exclusions	No data were excluded.
Replication	This case study was, in itself, a replication of an existing study (see above). Further, the experiment was run twice on each operating system to verify intra-system reproducibility.
Randomization	Randomization is not relevant to this study, as all factors were within-subjects (i.e. each subject's data was analysed using each computing system).
Blinding	Blinding is not relevant to this study, as data were structural images, and all images were subjected to all analysis conditions.

Reporting for specific materials, systems and methods

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Materials & experimental systems

n/a	Involved in the study
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☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☐	☒ MRI-based neuroimaging

Magnetic resonance imaging

Experimental design

Design type	Resting state
Design specifications	Structural scans (e.g. no functional imaging of behavioral task).
Behavioral performance measures	No behavioral task.

Acquisition

Imaging type(s)	Structural
Field strength	T3
Sequence & imaging parameters	These are described in detail in the manuscript describing the collection of the dataset used: Mazziotta, J. C., Toga, A., Evans, A., Fox, P., Lancaster, J., & Woods, R. (2000). A probabilistic approach for mapping the human brain: the International Consortium for Brain Mapping (ICBM). In Brain mapping: the systems (pp. 141-156). Academic Press.
Area of acquisition	Whole-brain

Diffusion MRI ☐ Used ☒ Not used

Preprocessing

Preprocessing software	Analyses were run using the FMRIB Software Library (FSL) 6.0.5.135. Brain extraction (Brain Extraction Tool [FSL-BET]), tissue classification (FMRIB's Automated Segmentation Tool [FSL-FAST]), image registration (FMRIB's Linear Registration Tool [FSL-FLIRT]), and subcortical tissue segmentation (FMRIB's Integrated Registration and Segmentation Tool [FSL-FIRST]) were performed using the default settings.
Normalization	N/A. All analyses were performed on the results of preprocessing pipelines.
Normalization template	N/A. All analyses were performed on the results of preprocessing pipelines.
Noise and artifact removal	N/A. All analyses were performed on the results of preprocessing pipelines.
Volume censoring	N/A. All analyses were performed on the results of preprocessing pipelines.

Statistical modeling & inference

Model type and settings	N/A. All analyses were performed on the results of preprocessing pipelines.
Effect(s) tested	We evaluated the consistency of results (DICE similarity coefficient) between Neurodesk and natively installed software. No statistical tests were performed on this effect, as Neurodesk typically was so reproducible as to have 0 or nearly 0 variance across systems. Results were reported as summary statistics.

Specify type of analysis: ☒ Whole brain ☐ ROI-based ☐ Both

Statistic type for inference (See Eklund et al. 2016)	N.A - No statistical tests were performed on the main effect of interest, as Neurodesk typically was so reproducible as to have 0 or nearly 0 variance across systems. Results were reported as summary statistics.
Correction	N/A- No statistical tests were performed on the main effect of interest, as Neurodesk typically was so reproducible as to have 0 or nearly 0 variance across systems. Results were reported as summary statistics.

Models & analysis

n/a	Involved in the study
☒	☐ Functional and/or effective connectivity
☒	☐ Graph analysis
☒	☐ Multivariate modeling or predictive analysis