

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

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

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119 **Abstract**

120 Neuroimaging data analysis often requires purpose-built software, which can be challenging
121 to install and may produce different results across computing environments. Beyond being a
122 roadblock to neuroscientists, these issues of accessibility and portability can hamper the
123 reproducibility of neuroimaging data analysis pipelines. Here, we introduce the Neurodesk
124 platform, which harnesses software containers to support a comprehensive and growing suite
125 of neuroimaging software (<https://www.neurodesk.org/>). Neurodesk includes a browser-
126 accessible virtual desktop environment and a command line interface, mediating access to
127 containerized neuroimaging software libraries on various computing platforms, including
128 personal and high-performance computers, cloud computing and Jupyter Notebooks. This
129 community-oriented, open-source platform enables a paradigm shift for neuroimaging data
130 analysis, allowing for accessible, flexible, fully reproducible, and portable data analysis
131 pipelines.

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133

134 **Introduction**

135 Neuroimaging data analysis is a challenging enterprise. Aside from the
136 neuroscientific principles motivating the choice of analysis, building an analysis pipeline
137 requires advanced domain knowledge well beyond the researcher’s topic area; for example,
138 signal and image processing, computer science, software engineering, statistics, machine
139 learning, and applied physics. Researchers faced with this daunting task rely on multiple
140 specialized software packages used in custom pipelines to suit a specific aim. Researchers
141 with limited resources and software engineering teams often develop these packages,
142 resulting in little dedicated technical support. The required software packages are often
143 difficult to install and are inconsistently supported across computing environments²⁻⁴. They
144 often have conflicting dependencies tied to the specific operating system versions.
145 Consequently, researchers often spend considerable time installing and compiling bespoke
146 neuroimaging software, which can undermine scientific productivity and reproducibility. To
147 address these issues, we developed an open-source and community-oriented solution to
148 enable neuroscientists to develop neuroimaging analysis workflows in line with four guiding
149 principles: *Accessibility*, *Portability*, *Reproducibility*, and *Flexibility*.

150 Ideally, the software and code used in any scientific analysis workflow should be easily
151 *accessible* so that users can deploy the workflow without a substantial investment of time or
152 effort⁵. It should be *portable* so that analysis workflows can be tractably shifted between
153 operating system versions and computing environments and deliver identical results. Many
154 researchers prototype analysis pipelines using their local computers and later switch to
155 workstations and high-performance computing (HPC) clusters for processing datasets at
156 scale. Accessible and portable workflows allow for an optimized allocation of computing
157 resources while supporting shared development workloads amongst collaborators⁶.
158 Unfortunately, many neuroimaging data analysis workflows are currently neither readily
159 accessible nor portable⁷⁻⁹ because they rely on specialized tools purpose-built by a small
160 number of developers².

161 Beyond the productivity costs, the inaccessibility and instability of many
162 neuroimaging tools pose a wider threat to *reproducibility*¹⁰⁻¹⁷ with reproducibility defined as
163 “running the same software on the same input data and obtaining the same result”^{16,18,19}. The
164 transparency and openness promotion (TOP) guidelines, which have over 5,000 journals and

165 organizations as signatories, state that all reported results should be independently
166 reproduced before publication²⁰. However, this is impractical and too time-consuming to
167 implement at review⁸. Where analysis pipelines are ported, subtle differences in the
168 implementation of specific processing steps and software versions across computing
169 environments can systematically affect results²¹⁻²⁴. Thus, it is often impossible to reproduce
170 a prior study's results, even given the original data and analysis protocol^{14,21}. Controlling the
171 specific software version of a tool and its dependencies is key to reproducibility²⁵.

172 Unfortunately, many existing solutions lack the required *flexibility* for research
173 applications of neuroimaging data analysis²⁶. For example, single-install pre-programmed
174 analysis pipelines are a popular solution amongst clinicians, but researchers typically
175 custom-tailor analysis pipelines toward specific research questions²⁷⁻²⁹. The issues of
176 inaccessibility in neuroimaging software have been recognized by the NeuroDebian² and
177 NeuroFedora³⁰ projects, which provide a wide range of neuroimaging tools packaged for
178 Linux operating systems. However, most neuroscientists do not use Linux on their personal
179 computers and thus cannot access these packages³. Researchers often use dual-boot
180 computers or virtual machines to address this barrier. Still, these solutions are resource
181 intensive and force researchers to develop inflexible workflows due to the practical
182 limitations inherent in installing new tools. While compiled packages make installations
183 easier, applications still need to be installed on the host computer and suffer the usual
184 problems of conflicts between different software packages, software versions, or the required
185 libraries (software “dependencies”). Many researchers are also limited in flexibility by
186 institutional restrictions imposed on the installation of new software.

187 Applications with specific or conflicting dependencies are not unique to neuroscience.
188 This universal issue has led to the development of software containers: lightweight, portable
189 solutions for running and sharing individual applications. Software containers package
190 specific applications along with their dependencies. Container engines such as Docker and
191 Apptainer/Singularity allow applications to run on various computing environments while
192 eliminating concerns about conflicting or missing dependencies^{31,32}. These benefits make
193 software containers suited to tackle issues relating to developing the scientific analysis
194 workflows described above³³. However, despite the benefits of containerization, only a small
195 number of integrated neuroscience-specific or adaptable workflow systems support
196 containerized distributed computing^{6,34-36}. Although projects such as OpenNeuro³⁷,

197 Brainlife³⁸, Flywheel³⁹, Boutiques^{40,41}, XNAT⁴² and Qmenta⁴³ have improved the accessibility
198 and reproducibility of neuroimaging analyses, these projects still lack portability. At this
199 stage, no solution exists that universally addresses the issues of *Accessibility*, *Flexibility*,
200 *Portability*, and *Reproducibility*. Our objective is to change this with the development of
201 Neurodesk: a community-oriented open-source platform that harnesses software containers
202 to create an accessible and portable data analysis environment that allows users to flexibly
203 and reproducibly access a comprehensive range of neuroimaging tools.

204 **Results**

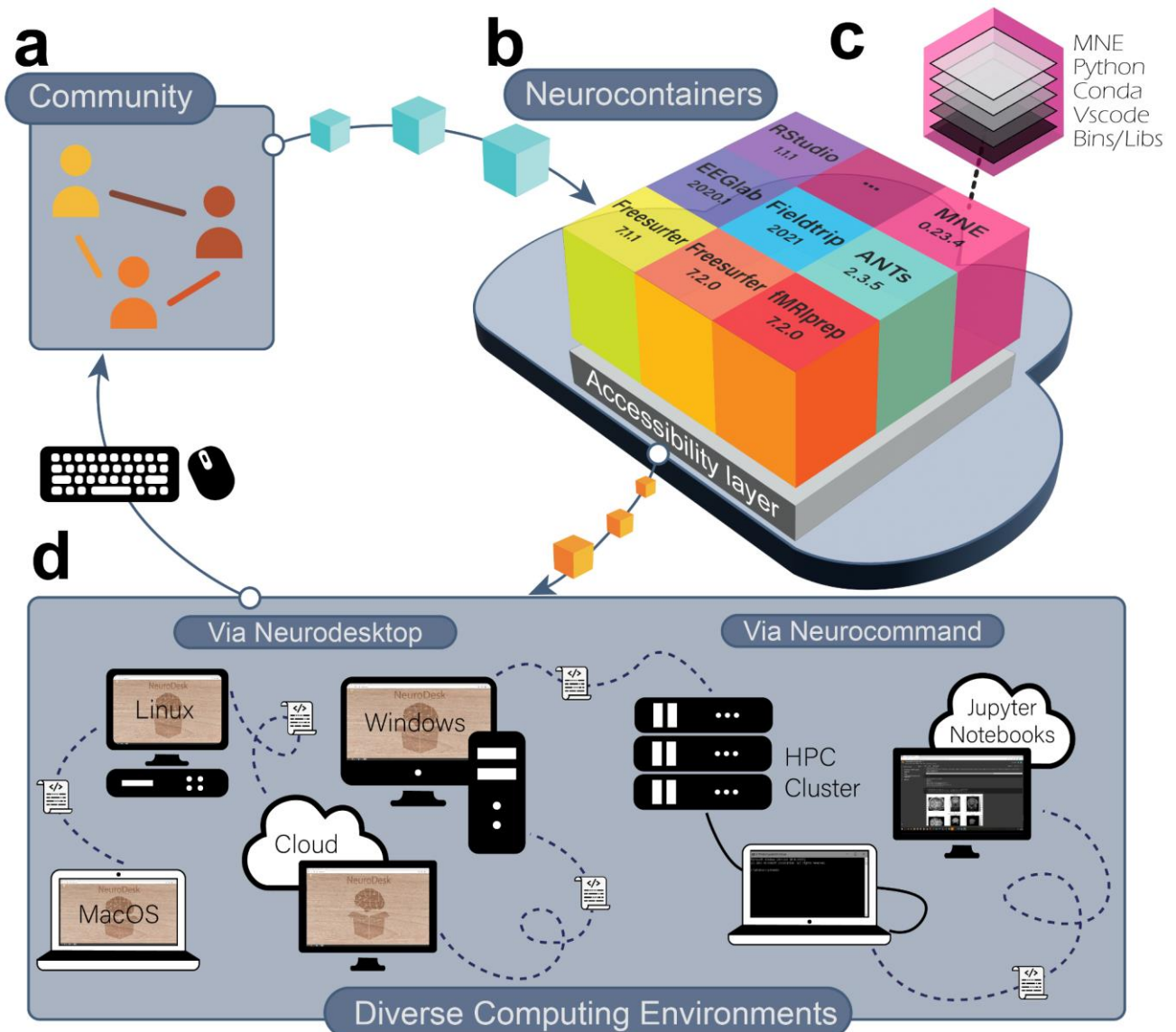
205 ***Overview of the Neurodesk Platform***

206 Here, we present Neurodesk, a platform facilitating *Accessibility*, *Portability*,
207 *Reproducibility*, and *Flexibility* for Neuroimaging data analysis (**Figure 1**). In developing
208 Neurodesk, we ensured that workflows developed on the Neurodesk platform remained
209 consistent with these four guiding principles across updates to users' local computing
210 environments. In this section, we introduce the available tools in the Neurodesk platform,
211 discuss how this addresses the issues raised above and report the results of an empirical
212 evaluation of reproducibility in Neurodesk. For further details of the rationale behind the
213 approaches adopted to achieve these results, please see the online methods.

214 At the core of Neurodesk are Neurocontainers, a collection of software containers that
215 package a comprehensive and growing array of versioned neuroimaging tools (**Figure 1b**).
216 The community contributes recipes based on the open-source project Neurodocker⁴⁴, a
217 continuous integration system builds the containers and uploads them to a container registry
218 (**Figure 1a**). Each 'Neurocontainer' includes the packaged tool and all dependencies required
219 to execute that tool, allowing it to run on various computing systems (**Figure 1c**). Because the
220 containers isolate dependencies, different Neurocontainers can provide different versions of
221 the same tool without conflicts. This mechanism allows researchers to seamlessly transition
222 between different software versions across projects or within a single analysis pipeline. A
223 newly developed accessibility layer enables researchers to use software directly through the
224 cloud or download containers for offline use without the need to install software on a local
225 system (**Figure 1b**).

226 There are two options for interfacing with Neurocontainers: The first is
227 Neurodesktop, a remote desktop and browser-accessible virtual desktop environment that
228 can launch any of the containerized tools from the application menu (**Figure 1d**). Analyzing
229 neuroimaging data through Neurodesktop has the look and feel of working on one's local
230 computer. For more advanced users and HPC environments, Neurocommand enables
231 interfacing with Neurocontainers through the command line (**Figure 1d**). These interfaces
232 can be deployed across almost any computing hardware and modern operating system,
233 meaning that analysis pipelines developed using the Neurodesk platform are reproducible
234 and can range from local computers to cloud and HPC environments. Neurocontainers even
235 work inside Jupyter Notebooks, so researchers developing analysis pipelines using
236 Neurodesk can share the reproducible code and results alongside published manuscripts
237 (**Figure 1d**).

238



239

240 **Figure 1.** The Neurodesk platform. (a) The Neurodesk platform is built by and for the scientific community, enabling
 241 anyone to contribute recipes for new software containers to the repository. (b) Recipes contributed by the community
 242 are automatically used to build software containers and stored in the Neurocontainers repository. (c) Each software
 243 container packages a tool together with all the required runtime dependencies. The packaged software can therefore
 244 run identically in any supported computing environment. (d) Neurodesk provides two layers of accessibility: 1.
 245 Neurodesktop is a browser-accessible virtual desktop environment, allowing users to interact with the containerized
 246 software. 2. Neurocommand is a command-line interface that allows users to run the same software containers
 247 programmatically. These interfaces allow users to reproduce the same analysis pipelines across various computing
 248 environments.

249

250

251 ***How to use Neurodesk: Accessibility, Flexibility & Portability***

252 A core aim behind Neurodesk is to provide a platform that makes building and
253 running reproducible analysis pipelines accessible to all researchers. The platform website
254 (<https://Neurodesk.org/>) is user-friendly and open to community contributions via pull
255 requests. The website contains automatically updating information about the software
256 included through continuous integration. As such, there is always up-to-date documentation,
257 lists of currently available applications, and release history. The website also hosts clear
258 instructions and guidance for accessing and interacting with Neurodesk from various
259 computing environments and tutorials on using various software packages.

260 Besides ensuring that users have access to thorough and up-to-date documentation,
261 additional steps ensure that Neurodesk makes reproducible neuroimaging data analysis
262 *accessible*. Neurodesk works in almost any computing environment and brings the same
263 dependencies to all supported platforms. This portability extends to the Neurodesktop
264 graphical user interface (GUI), which provides the same desktop environment across all
265 supported computing environments. Containerized analyses look, feel, and run the same way
266 across different computing environments. Thus, researchers reading or reviewing
267 manuscripts with open-source data and code can use Neurodesk to replicate the *exact*
268 pipeline using the reported tool versions without requiring to install additional software.

269 For a data analysis environment to be *portable*, such that it can easily shift between
270 computing environments, it also needs to be lightweight with a small storage footprint. To
271 this end, our accessibility layer harnesses the CernVM File System (CVMFS)⁴⁵. The CVMFS
272 layer allows accessing the software from a remote host without installation, so only those
273 parts of a container actively used are sent over the network and cached on the user's local
274 computer. Users can access terabytes of software without downloading or storing it locally.
275 The Neurodesk platform has several CVMFS nodes worldwide, providing low latency and
276 direct access to Neurocontainers. Thus, to use Neurodesk, users only install the required
277 container engine and access the Neurocontainer of their choice. For Neurodesktop, which
278 facilitates access to all tools in the Neurocontainers repository, the download is only ~1GB.

279 Anticipating that installing a third-party container engine software may be a barrier
280 to entry for some researchers, there is an entirely cloud-based solution; 'Neurodesk Play'
281 (<http://play.neurodesk.org>). Neurodesk Play is accessible globally, allowing anyone to use a

282 cloud-based graphical desktop environment for neuroimaging data analysis and teaching.
 283 Neurodesktop can also run on institutional or cloud computing resources enabling access to
 284 large amounts of computing resources or datasets. For example, Neurodesk is freely available
 285 as a national service on the Nectar Research Cloud Virtual Desktop Service provided by the
 286 Australian Research Data Commons (ARDC).

287 *Long-Term Sustainability of the Neurodesk Platform*

288 Neurodesk has a wide selection of tools available spanning many domains of
 289 neuroimaging data analysis. **Table 1** shows the tools available at the time of publication,
 290 though this list is growing rapidly. Users can find a full and up-to-date list at
 291 <https://Neurodesk.org/applications/>. Neurodesk employs a two-pronged approach to staying
 292 up-to-date with new neuroimaging tools and new versions of already included software: a.)
 293 The Neurodesk maintainers add tools as they become aware of new developments or
 294 community members request the addition of new packages. The Neurodesk GitHub
 295 repository (<https://github.com/NeuroDesk>) has an active discussion forum where developers
 296 respond to requests for new software containers. b.) In addition to this developer-centric
 297 route to new software containers, we actively encourage contributions from the research
 298 community. A core aim for developing the Neurodesk platform was to build a community-
 299 driven project that is not contingent on a specific team of developers. As such, we provide a
 300 template and detailed instructions for creating build scripts for new software containers.

301

302 **Table 1.** Tools currently available in Neurodesk (retrieved from
 303 <https://Neurodesk.org/applications/>). Note that each tool has been listed under only one
 304 category, though some may span multiple categories.

Category	Tool
Editors and Programming	VS Code, Gedit, Emacs, Vim, Python, Git, Julia, Matlab, ROOT, RStudio
Data Synchronization Tools	Rsync, Rclone, Nextcloud client, Owncloud client, Globus personal connect

Workflows	Nipype ⁴⁶ , ASLPrep ⁴⁷ , fMRIPrep ⁴⁸ , MRIQC ⁴⁹ , QSMxT ⁵⁰
Data Organization	dcm2niix ⁵¹ , BIDScoin ⁵² , BIDStools ⁵³ , Convert3D ⁵⁴
Diffusion MRI	Diffusion Toolkit ⁵⁵ , DSI Studio ⁵⁶ , MRtrix ⁵⁷ , MRtrix3Tissue ⁵⁸ , TrackVis ⁵⁵
Rodent Imaging	AIDAmri ⁵⁹ , RABIES ⁶⁰
Spectroscopy	LCModel ⁶¹ , MRSIProc ⁶²
Structural and/or Functional Imaging	AFNI ⁶³ , ANTs ⁶⁴ , ASHS ⁶⁵ , BART ⁶⁶ , CAT12 ⁶⁷ , CLEAR-SWI ⁶⁸ , CLEAR-SWI ⁶⁸ , Conn ⁶⁹ , Connectome Workbench ⁷⁰ , FatSegNet ⁷¹ , FreeSurfer ⁷² , FSL ⁷³ FSL, HD-BET ⁷⁴ , LASHiS ⁷⁵ , LayNii ⁷⁶ , MINC ⁷⁷ , MRIttools ⁷⁸ , NiftyReg ⁷⁹ , NiiStat ⁸⁰ , OSH-yX ⁸¹ , Palm Alpha ⁸² , PhysIO ⁸³ , ROMEO ⁸⁴ , Slicer ⁸⁵ , Spinal Cord Toolbox ⁸⁶ , SPM ⁸⁷ , TGVQSM ⁸⁸
Electroencephalography (EEG) and/or Magnetoencephalography (MEG)	Brainstorm ⁸⁹ , EEGLAB ⁹⁰ , FieldTrip ⁹¹ , MNE ⁹² , Sigviewer ⁹³
Machine Learning and Statistics	R ⁹⁴ , Deep Retinopy ⁹⁵ , Delphi ⁹⁶
Visualization and Image Editing	ImageMagick ⁹⁷ , GIMP ⁹⁸ , itk-SNAP ⁵⁴ , MRICron ⁹⁹ , MRICroGL ^{100,101} , SicerSALT ¹⁰² , Surf Ice ^{103,104}

306 ***Reproducibility in Neurodesk***

307 Scientific progress fundamentally depends on the peer review process - scientists must
308 be able to critically assess reported findings and conclusions based on a clear and thorough
309 methodological description¹⁸. Well-documented experimental code is the most thorough
310 description of any analysis pipeline. However, differences in computing environments and
311 dependencies mean that access to this source code does not guarantee the capability to run
312 the code nor the same result^{19,105}. Reproducibility has therefore come to represent a minimum
313 standard by which to judge scientific claims^{16,18,19}. Unfortunately, scientific reproducibility is
314 often not attainable due to differences in the outcomes of neuroimaging pipelines across
315 different computing environments, as previously documented^{21,106,107}. Glatard et al. (2015)
316 demonstrated this effect for several MRI analysis pipelines, showing that differences in the
317 implementation of floating-point arithmetic across operating systems accumulated
318 throughout long analysis pipelines and led to meaningful differences in the results²¹.
319 Neurodesk solves this issue using containerized software, which guarantees the same
320 runtime dependencies across computing environments. To evaluate this claim, we replicated
321 Glatard et al.'s analyses using Neurodesk vs. locally installed software across different
322 operating systems. We discuss in the online supplements why differences between library
323 versions affect the results.

324 *Methodological approach.* The widely used FMRIB Software Library (FSL) 6.0.5.1⁷³ was
325 installed both locally and within Neurodesk on two separate computers (System A, System B)
326 which were running different Linux distributions. This resulted in four unique computing
327 environments (see **Table 2**). Glatard et. al's FSL-based analyses, namely the brain extraction
328 (Brain Extraction Tool [FSL-BET]), tissue classification (FMRIB's Automated Segmentation
329 Tool [FSL-FAST]), image registration (FMRIB's Linear Registration Tool [FSL-FLIRT]), and
330 subcortical tissue segmentation (FMRIB's Integrated Registration and Segmentation Tool
331 [FSL-FIRST]) were replicated in each of these environments using 157 T1-weighted magnetic
332 resonance images (MRI) from the International Consortium for Brain Mapping (ICBM)¹⁰⁸.
333 Each analysis was run twice within each environment to verify that there was no intra-
334 environment variability. To evaluate the reproducibility of the analysis environment using
335 locally installed vs. Neurodesk software, we compared the outputs for each installation type
336 across computers (System A vs. System B). For intra- and inter-environment comparisons, we
337 first compared file checksums. When two files produced different checksums, we quantified

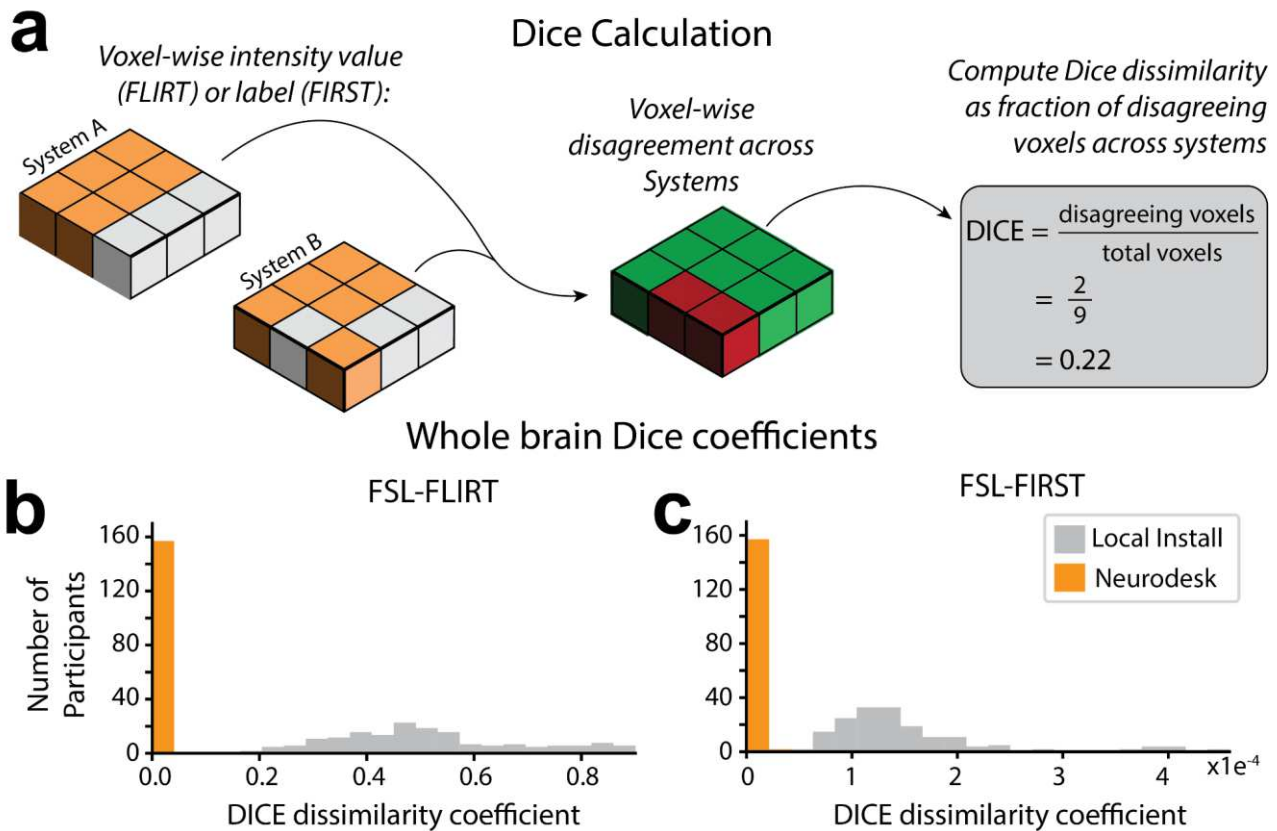
338 the pairwise differences across systems by computing Dice dissimilarity coefficients across
 339 images (**Figure 2a**). Note that there were never any intra-system differences in checksums
 340 (i.e., all analyses were deterministic, resulting in identical outcomes when run twice in the
 341 same computing environment). The code used to implement these analyses is available and
 342 re-executable through Neurodesk Play at: <https://osf.io/e6pw3/>.

343 **Table 2.** Computing environments used to run analyses.

	System A		System B	
	Local	Neurodesk	Local	Neurodesk
Applications	FSL 6.0.5.1	FSL 6.0.5.1	FSL 6.0.5.1	FSL 6.0.5.1
Glibc version	2.31	2.23	2.28	2.23
OS	Ubuntu 20.04	Ubuntu 16.04.7	AlmaLinux 8.5	Ubuntu 16.04.7
Hardware	12th Gen Intel(R) Core(TM) i7-12700		AMD EPYC 7542 32-Core Processor	

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347 **Figure 2.** Discrepancies in image registration and tissue segmentation. (a) Calculation of the Dice
 348 dissimilarity coefficients; for each image, the voxel-wise disagreement in image intensity (FLIRT) or
 349 label (FIRST) calculated on System A vs System B was expressed as a proportion of the total number
 350 of voxels for each participant. (b) Histograms of Dice dissimilarity coefficients for image intensity
 351 calculated with FSL-FLIRT on Neurodesk vs. Local Install. To calculate these Dice coefficients,
 352 “disagreement” meant a voxel had a different intensity after image registration on System A vs.
 353 System B. Thus, the Dice coefficient of 0 for every participant whose images were registered using
 354 Neurodesk, means that the image intensity of each participant was matched across systems at every
 355 voxel. (c) Histograms of Dice dissimilarity coefficients for subcortical structure labels calculated using
 356 FSL-FIRST on Neurodesk vs. Local Install. To calculate these Dice coefficients, “disagreement” meant
 357 a voxel had different labels (e.g., amygdala, hippocampus, etc.) after image segmentation on System
 358 A vs. System B. Note that these Dice coefficients are much smaller than for image registration. This
 359 is expected because there are 73 times more “classes” for the image registration task, which uses
 360 image intensity (Range: 0 – 1903) as a class, than the classification task, which has labels for 15
 361 structures. However, while both Neurodesk and the local system show strong agreement across
 362 systems overall, these distributions are completely non-overlapping, with Neurodesk showing much
 363 greater reliability across systems.

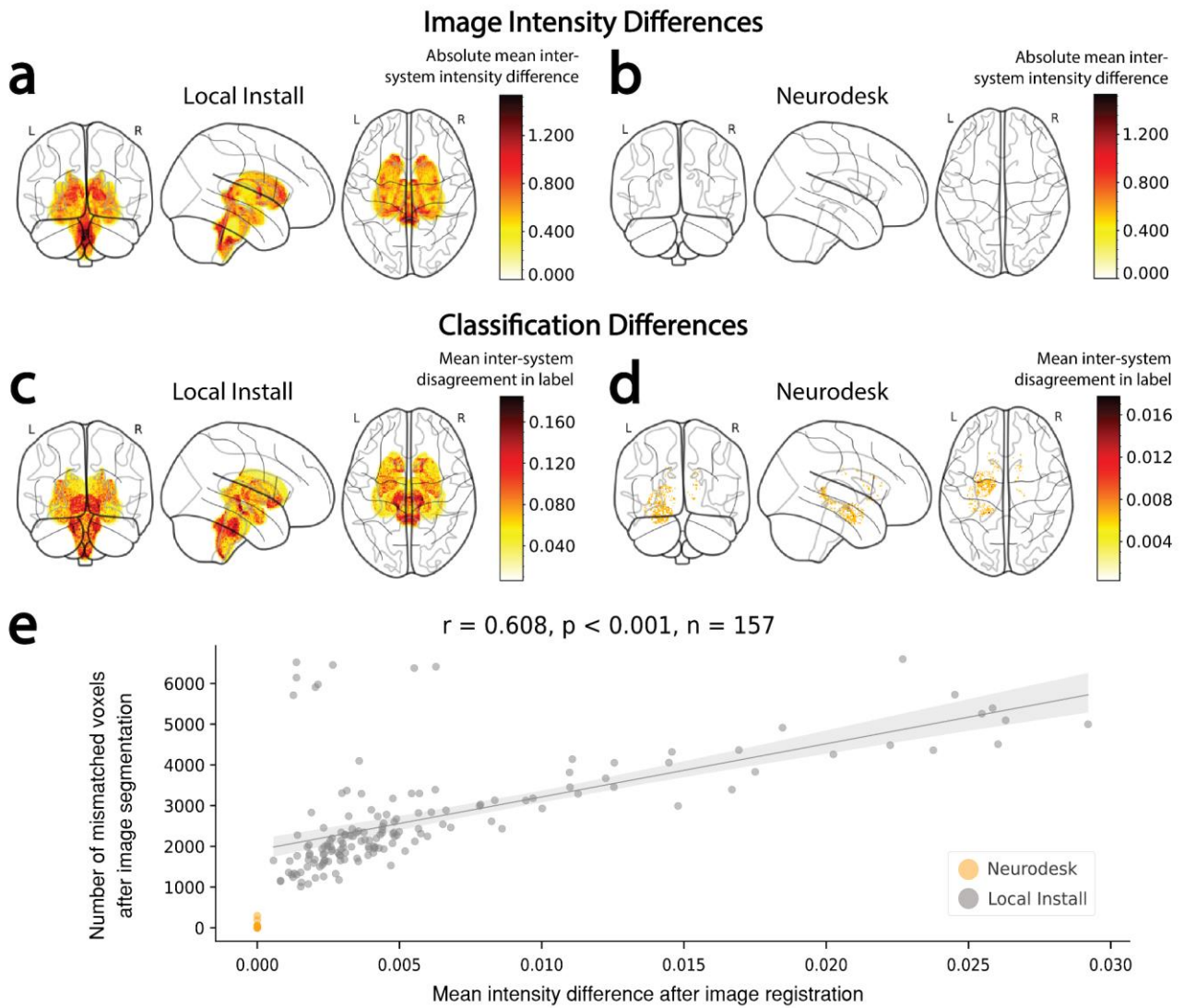
364

365 *Brain extraction and tissue classification.* Skull stripping and brain tissue segmentation
366 were done by running FSL BET and FAST on raw images. The pipeline was fully reproducible
367 up to this stage because the file checksums were identical across all computing
368 environments.

369 *Image registration.* FSL FLIRT was applied to register the images to the standard MNI-
370 152 T1 1 mm template using 12 degrees of freedom. When run through Neurodesk, the
371 outputs of this processing step had identical file checksums across computing systems for all
372 images. However, file checksums for local installations of FSL did not match across systems.
373 Dice dissimilarity coefficients for each image were computed to quantify the pairwise
374 differences in image intensity across systems (**Figure 2a**). Voxel-wise agreement in image
375 registration for Neurodesk was perfect (Dice dissimilarity coefficient; Range: 0.00, M = 0.00,
376 SD = 0.00). However, there were many voxels with differing intensity across local installations
377 (Dice dissimilarity coefficient; Range: 0.19 – 0.90, M = 0.51, SD = 0.17, **Figure 2b**). These high
378 Dice dissimilarity coefficients for the local installation indicate differences across many
379 voxels, however, the magnitude of these differences in image intensity was subtle (inter-
380 system intensity difference; M = 1.88, SD = 1.97; where $intensity \in Z: intensity \in [0,1903]$,
381 **Figure 3a, b**).

382 *Subcortical tissue segmentation.* Differences in image intensity across local installations
383 were widespread yet subtle. In line with Glatard et. al's approach, we next asked whether
384 these differences impacted subcortical tissue segmentation (using FSL FIRST); the next step
385 in the analysis pipeline. File checksums for the segmentation outputs matched for 0% of
386 images when run using the local installation and for 93% of images when run with Neurodesk.
387 Computation of the Dice dissimilarity coefficients for each type of installation revealed that
388 while differences were small, they had non-overlapping ranges. Indeed, differences were
389 much less prevalent for the Neurodesk installations (Dice dissimilarity coefficient; Range:
390 $0.00 - 2.20 \times 10^{-5}$, M = 3.43×10^{-7} , SD < 0.01) compared with the local installations (Dice
391 dissimilarity coefficient; Range: $5.80 \times 10^{-5} - 4.59 \times 10^{-4}$, M = 1.46×10^{-4} , SD < 0.01, **Figure 2c**). On
392 average, there were 426 times more voxel-wise disagreements across systems for the locally
393 installed software than for Neurodesk. This difference can be visualized by comparing the
394 3D projections of the mean inter-system differences in classification across participants
395 (**Figure 3c, d**). These projections illustrate that differences for locally installed software were

396 widespread across all subcortical structures (**Figure 3c**), while any subtle differences for
 397 Neurodesk were limited to a few voxels (**Figure 3d**).



398

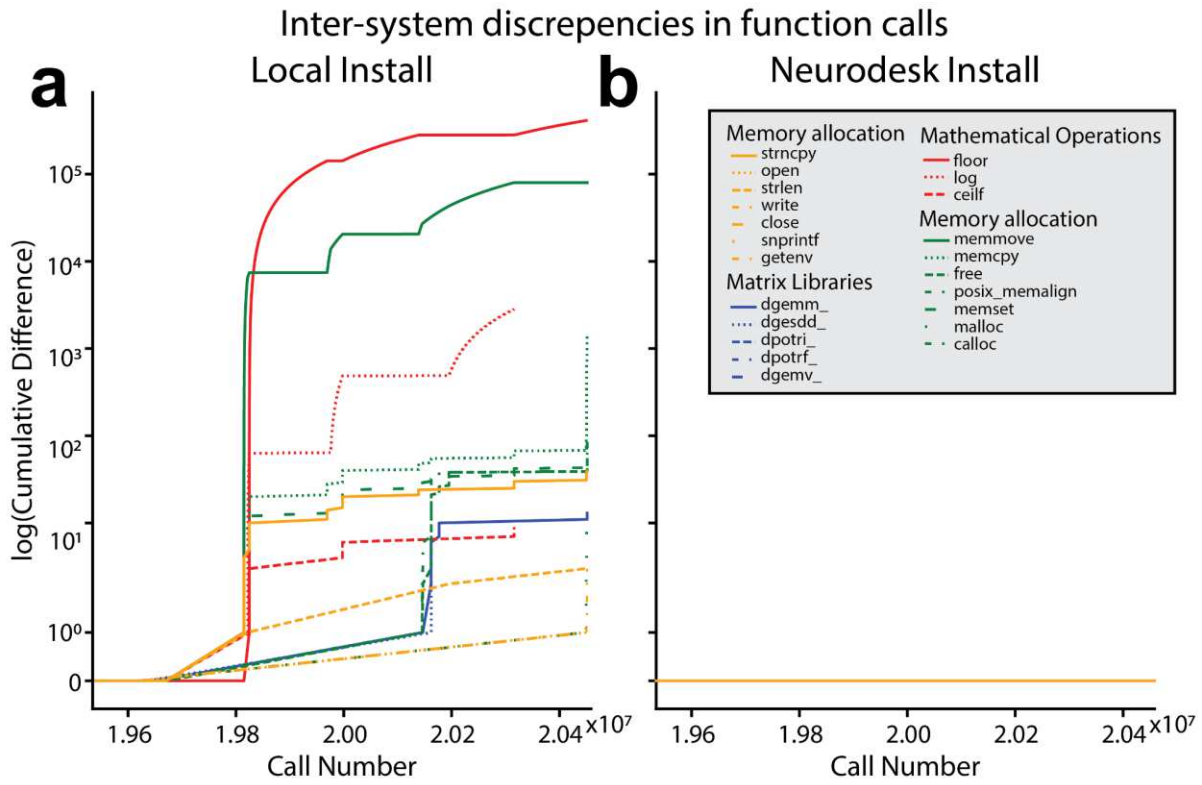
399 **Figure 3.** Inter-system differences in image intensity in subcortical structures and subsequent
 400 classification of these subcortical structures. (**a,b**) Absolute voxel-wise differences in image intensity
 401 within subcortical structures after image registration with FSL-FLIRT on each system (i.e.
 402 $|Intensity_{system A} - Intensity_{system B}|$), averaged across participants. Projections are shown for image
 403 registration performed (**a**) using locally installed software, and (**b**) using Neurodesk (for which there
 404 were no intersystem differences). (**c,d**) Inter-system disagreement in subcortical structure labels
 405 after image segmentation with FSL-FIRST, averaged across participants. Projections are shown for
 406 image segmentation performed (**c**) using locally installed software and (**d**) using Neurodesk. (**e**)
 407 Scatter plot showing the mean inter-system image intensity differences across all voxels within the
 408 classified subcortical structures vs. the number of voxels subsequently classified with different labels
 409 across systems. For analyses performed with locally installed software, participants with larger
 410 differences in image intensity typically also had more prolific disagreement in labels between systems

411 (Pearson's $r = 0.608$, $p < 0.001$). This trend could not be assessed for Neurodesk, as there were no
412 differences in image intensity across systems.

413 *Understanding inter-system differences in image registration and tissue classification.*
414 Differences in tissue classification were at least partially attributable to differences in
415 registered image intensity earlier in the pipeline. Indeed, there was a strong positive
416 correlation between the magnitude of each participant's inter-system differences in
417 registered image intensity and inter-system classification mismatches (Pearson's $r = 0.608$, p
418 $< .001$, **Figure 3e**). Thus, larger inter-system differences after the FSL FLIRT analysis were
419 associated with larger inter-system differences after the subsequent FSL FIRST analysis.

420 We next replicated Glatard et al.'s findings by showing that the remaining variability
421 in inter-system differences for tissue classification, as well as the differences for image
422 registration, could be attributed to a combination of differences in floating point
423 representation and differences in underlying dependencies across systems. Tracing the calls
424 to dynamically linked system libraries revealed many differences for the local installations,
425 but complete congruence between Neurodesk installations (**Figure 4**, see online methods).
426 This begs the question - why were there still minor differences in the classification of
427 subcortical structures for Neurodesk? The most likely explanation is that floating point
428 calculations can produce different results on different processors due to different
429 implementations of the floating point arithmetic instructions¹⁰⁹. Reasons include whether 64
430 (SIMD, GPU) or 80 bit (x87 FPU) precision is used internally, reduced rounding for fused
431 multiply-add, or if negative zero and positive zero are considered equal. Critically, these
432 differences are minor, which is likely why the differences in classification across systems for
433 Neurodesk were subtle.

434 Overall, these results demonstrate that differences in dependencies across computing
435 environments can lead to slight differences in the outcomes of computational analyses. This
436 can snowball across successive processing steps to cause potentially meaningful differences
437 in results across computing environments, especially when investigating subtle effects.
438 Minimizing differences at each stage of the analysis can enhance overall accuracy and
439 reliability. Critically, Neurodesk eliminates this source of variability by facilitating access to
440 containerized software. This allows researchers to reproduce the same result from different
441 computing environments.



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Figure 4. Cumulative difference in the numbers of system library calls between System A and System B for the analysis run using the (a) locally installed and (b) Neurodesk version of FSL FIRST. Note that calls to *floorf()* were excluded from the plot as they occurred earlier in time and the discrepancies for *floorf()* far outnumbered those for any other function from the locally installed tool.

449 **Discussion**

450 Neuroimaging data analysis pipelines are often challenged with limitations in
451 *Accessibility, Flexibility, Portability* and *Reproducibility*. Neuroscientists may hold back from
452 exploring new tools or spend excessive amounts of time installing software (and
453 dependencies) in new computing environments, only to find that the same analysis pipeline
454 produces different results. We developed Neurodesk to address these challenges by building
455 an open-source and community-oriented platform for reproducible neuroimaging data
456 analysis. Neurodesk allows scientists to flexibly create fully reproducible and accessible data
457 analysis pipelines in various computing environments. By providing an accessibility layer for
458 software containers, the Neurodesk platform allows for convenient portability across
459 computing environments. Finally, by keeping the platform open-source and utilizing
460 continuous integration and deployment, we have democratized the Neurodesk platform and
461 set a path toward a sustainable ecosystem for neuroimaging data analysis.

462 The Neurodesk platform has the potential to transform neuroimaging data analysis,
463 because it allows for truly reproducible data analysis and is highly accessible. Scientists strive
464 to uphold scientific principles to the highest possible standard. However, looming deadlines
465 and the pressure to publish often force individual researchers to find a balance between these
466 ideals and the practical constraints imposed by resource limitations. Neurodesk can allow all
467 researchers to adhere to the highest possible reproducibility standards with minimal changes
468 to their typical development pipelines. Reducing unnecessary computational variability
469 between execution systems makes it possible to share analyses between labs and collaborate
470 on large datasets without potentially obscuring effects or introducing artificial differences
471 between sites. Neurodesk enables researchers to not only access a comprehensive suite of
472 neuroimaging data analysis software, but also contribute developments into the future for an
473 ever-increasing suite of packages. Hence, researchers can flexibly take advantage of open
474 datasets, reproduce reported analyses, switch between neuroimaging modalities across
475 projects, and apply complementary analysis methods alongside their primary approach. By
476 harnessing Neurodesk together with cloud computing technologies, published manuscripts
477 can also include links to Jupyter Notebooks, therefore democratizing the reproducibility of
478 key analyses. The ease with which Neurodesk allows analysis pipelines to be shared and
479 reproduced across computing environments also has particular relevance for distributed
480 research groups and collaborative, multi-site projects. Thus, the Neurodesk platform not only

481 facilitates access to reproducible neuroimaging data analysis but also makes developing and
482 sharing these workflows less burdensome.

483 Neurodesk is not the first platform to address the limited accessibility and
484 reproducibility available for many neuroimaging data analysis tools. Indeed, software
485 distribution mechanisms like NeuroDebian² have made great progress in making
486 neuroimaging software more accessible, while projects such as OpenNeuro³⁷, Brainlife³⁸,
487 Flywheel³⁹, XNAT⁴², Code-Ocean¹¹⁰, Boutiques^{40,41} and Qmenta⁴³ have greatly improved the
488 accessibility and reproducibility of neuroimaging analyses. However, all current existing
489 solutions have lacked portability and flexibility. Many existing solutions require users to
490 upload datasets to their platforms, and developing custom pipelines on these platforms
491 requires substantial platform-specific knowledge. However, even users already accustomed
492 to these specifics may still benefit from the Neurodesk project as Neurodesk's containers are
493 interoperable with other platforms.

494 Neurodesk has been developed as a research tool to facilitate the analysis of
495 neuroimaging data. However, the platform may have a significant impact as an educational
496 tool for workshops, summer schools, and 'hackathons'¹¹¹. The Neurodesk platform was first
497 conceptualized during a 'hackathon' event, during which neuroscientists from around the
498 globe gathered in hubs to collaborate on short-term projects, attend workshops, and develop
499 critical research skills. One of the greatest hurdles for organizers and attendees of such
500 events is the diversity in computing environments across researchers. When delivering a
501 workshop or tutorial, facilitators often spend a large portion of the allocated time
502 troubleshooting installations or issues specific to unique computing environments.
503 Neurodesk addresses these issues by allowing access to identical computing environments
504 with requisite tools pre-installed. This functionality allows groups of researchers to
505 efficiently tackle complex problems by eliminating Sisyphean troubleshooting. The Galaxy
506 platform, for example, has made a significant impact in this way by providing a containerized
507 solution for bioinformatics and social science¹¹². Aside from educational applications,
508 Neurodesk can also aid research software developers wishing to make their tools more
509 accessible. The effort to containerize and add one's software to Neurodesk may be minimal
510 compared to the burden of testing across multiple computing platforms and fielding support
511 queries from end-users running software in diverse environments.

512 Neurodesk currently has limitations that warrant discussion. The first limitation is
513 that the software containers in the Neurodesk platform currently do not support the ARM
514 CPU architecture, which will become increasingly common as Mac users update their
515 hardware. This stems from limitations in the underlying software applications, which
516 currently need more support for this processor architecture. However, tool developers are
517 rapidly adapting tools for this architecture, and we are convinced that this problem will be
518 addressed for the most used applications in the future. Further limitations may arise as
519 Neurodesk is applied across more diverse use-cases by the broader research community. A
520 pertinent example relates to the use of proprietary and licensed software. This is an area of
521 active development as the Neurodesk community investigates how to integrate such software
522 without compromising the accessibility principle. A strength of Neurodesk is that the
523 community-oriented, continuous integration model provides a powerful and flexible way to
524 address such expanded use-cases without depending on a single development team. This
525 relates to a potential limitation of any such platform - the project's long-term sustainability.
526 The Neurodesk platform was funded to be sustainable and supported by the community, but
527 for this to be successful, the project needs constant maintenance. We, therefore, developed
528 multiple pathways for sustainability, including the federated support of the underlying
529 hosting infrastructure, flexibility in the continuous integration and deployment
530 infrastructure, and a potential for a commercial model to offer tailored support for
531 institutions and workshops.

532 The challenges to accessibility and reproducibility posed by neuroimaging data
533 analysis software are not unique to neuroscience. While we have chosen to containerize
534 software designed for neuroimaging datasets, the principles governing the design of the
535 Neurodesk platform can be unrestricted to this field of research. This open-source platform
536 could be used to deploy software specific to any other discipline, and it is our sincere hope
537 that this platform is adapted to other disciplines struggling with similar issues. The
538 Neurodesk platform has the potential to improve the way scientists analyze data and
539 communicate results profoundly. For the first time, this platform allows any scientist,
540 anywhere in the world, to conveniently access their data analysis tools and apply them in a
541 fully reproducible manner from any computing environment. We are excited to see what new
542 insights such technology can enable.

543

Online methods

544 Neurodesk's open-access code and documentation

545 All stages of development, from the initial conception as a hackathon project, through to
546 the most current iteration of Neurodesk, with up-to-date community-built Neurocontainer
547 recipes, are documented publicly:

548 <https://www.neurodesk.org/> - Platform website which includes 'Getting Started' tutorials for
549 new users of various skill levels.

550 <https://github.com/NeuroDesk> - Public GitHub repository, where Issues can be logged, and
551 contributions can be made by any community member with a GitHub account and the
552 eagerness to create pull requests.

553 Data Availability

554 The data that support the findings of this study are available from the International
555 Consortium for Brain Mapping (ICBM) database (www.loni.usc.edu/ICBM). The ICBM
556 project (Principal Investigator John Mazziotta, M.D., University of California, Los Angeles)
557 is supported by the National Institute of Biomedical Imaging and BioEngineering. ICBM is
558 the result of efforts of co-investigators from UCLA, Montreal Neurologic Institute,
559 University of Texas at San Antonio, and the Institute of Medicine, Juelich/Heinrich Heine
560 University - Germany. There are restrictions that apply to the availability of these data,
561 which were used under approved permission for the current study, and so are not publicly
562 available, but available from ICBM upon request.

563 Code Availability

564 The code for this study is available on the GitHub repository at
565 <https://github.com/NeuroDesk> with no restrictions on access. The code is licensed under
566 the MIT License.

567

568 **Frequently Asked Questions**

569 ***How could researchers build an analysis pipeline and share this with other researchers using***
570 ***Neurodesk?***

571 We provide a Jupyter Notebook to showcase how different tools can be used in a fully
572 reproducible and shareable analysis pipeline: [https://github.com/NeuroDesk/example-](https://github.com/NeuroDesk/example-notebooks/blob/main/nipype_module_example.ipynb)
573 [notebooks/blob/main/nipype_module_example.ipynb](https://github.com/NeuroDesk/example-notebooks/blob/main/nipype_module_example.ipynb). In this example, we demonstrate the
574 use of FSL and AFNI on a publicly available dataset. We used the open-source nipype
575 workflow system to execute analyses on this data, enabling complex analyses to be built,
576 shared, and executed identically in another Neurodesk installation.

577 ***Will running my analyses on Neurodesk be slower than if they were run locally, especially if I'm***
578 ***on a slower internet connection?***

579 The internet bandwidth will only affect your analysis speed the first time you use a
580 new tool. Neurodesk uses the CernVM File System (CVMFS), meaning that only the
581 specific part of a currently used container will be downloaded over the internet. Once
582 downloaded, these will be cached locally, meaning that software will operate at the same
583 speed as it would when running locally (see **table S1**). Although there is a container
584 initialization time that could impact performance in comparison to a non-containerized
585 workflow, there is evidence that in some cases, containerized analysis pipelines may run
586 even faster than locally installed software due to efficiency gains in accessing files¹¹³.

587 ***Where are Neurodesk containers stored, and will the performance differ from country to***
588 ***country?***

589 Neurodesk containers are distributed globally via CVMFS and accessed from the
590 fastest server according to your location. We aim to get mirror servers as close as possible
591 to all users so that CVMFS can automatically use the fastest available mirror server.

592 ***Are there any security concerns regarding using the Neurodesk platform in a web browser? For***
593 ***example, could there be any risks that compromise data processed on Neurodesk?***

594 The underlying container technology in Neurodesk ensures that applications are
595 isolated with the least privileges to minimize the impact of malicious software. Interacting
596 with the web from within a Neurodesktop poses a similar risk to any system with access to

597 the internet, so all precautions would apply. Neurodesktop can be shut down, deleted and
598 started fresh with minimal effort, which means recovery is significantly simpler than a
599 native installation in a similar scenario. To ensure data security, it is essential for users who
600 run Neurodesk on a cloud provider or in their local network to follow security best practices
601 and secure the port Neurodesktop is running on via firewall rules. For an in-depth review of
602 the potential security concerns of containerizing scientific data analysis software, see Kaur
603 et al. (2021)¹¹⁴.

604 ***Can I store processed data in Neurodesk?***

605 Neurodesktop allows host directories to be mounted for local data access, and these
606 directories can then be accessed from the Neurocontainers. Data can also be accessed via
607 access clients and the web inside a Neurodesktop instance running for example on a cloud
608 provider. Upon installation of Neurodesk on a local PC or HPC, users have the option of
609 mounting an existing local directory or utilizing the automatically created and locally
610 stored directory, ~/neurodesktop-storage. This directory is permanently stored on the local
611 host and will remain even if Neurodesktop is deleted, ensuring that the data remains on the
612 local host and does not leave their PC. It is important to note that the data remains on the
613 user's computer if Neurodesk is running locally, but Neurodesk can also run in a cloud
614 environment where data is stored remotely and users need to ensure that their use case is in
615 line with their ethics and data agreements.

616 ***Can you provide more technical detail on how the Neurodesk desktop virtual environment has
617 been built?***

618 Neurodesktop is a Docker container packaging a linux desktop environment that
619 delivers neuroscience applications via CVMFS, distributed via singularity containers. It
620 uses Apache Guacamole with underlying remote-desktop protocol (RDP) or virtual network
621 computing (VNC) remote desktop protocols to deliver a desktop experience in the browser,
622 including copy, paste and file transfer functionality.

623 ***Why are there different types of containers (i.e. Docker, Singularity) in Neurodesktop? Are there
624 any conflicts between Docker and Singularity?***

625 Docker and Singularity containers are both used in Neurodesktop for different,
626 complementary purposes. Docker is used to containerize the Neurodesktop environment

627 due its cross-platform support and ability to run singularity containers within. Singularity,
628 which is used for the individual application containers (Neurocontainers), is preferred by
629 most high-performance computing (HPC) platforms, where multi-user security and
630 scheduling are of particular concern and can also be used indirectly via wrapper scripts and
631 lmod; a system which manages environment configurations for different software packages.

632 ***Are there any financial costs associated with keeping Neurodesk running, and if so, how will***
633 ***these be met for the foreseeable future?***

634 The long-term sustainability of Neurodesk has been planned according to three
635 possible financial scenarios. 1) *No further funding*: In this case, Neurodesk will be minimally
636 maintained such that all the open-access containers will still be accessible. However,
637 Neurodesk Play (the cloud-based no-install version of Neurodesktop) will no longer be
638 accessible and the software distribution via CVMFS Neurodesk may run more slowly
639 outside of Australia. 2) *Marginal Funding*. Neurodesk will be maintained with its current
640 functionality, but with less focus on the development of new features. 3) *Sufficient funding*.
641 The Neurodesk team is working on a not-for-profit business model in which additional
642 financial costs involved in extending Neurodesk's current functionality could be covered by
643 charging a nominal fee to manage the resources required to deploy Neurodesk in
644 combination with Jupyterhub in the cloud for organizations or for workshop and teaching
645 purposes. Note that Neurodesk (Neurodesktop, Neurocommand, and the Neurocontainers)
646 will always remain open-source and open-access under the MIT license, which enables
647 commercial use. Any fee would be used to reduce the administrative load and technical
648 challenges for workshop organizers and participants, such that workshop participants can
649 access a fully maintained and cloud-based Neurodesktop environment.

650 ***Neurodesk is open-source, such that anyone is able to contribute containerized software to the***
651 ***platform. Are there any protocols in place to verify that this software is working as expected***
652 ***before it is made available to the community?***

653 There is a feature to include a functional test within each tool's container. This test
654 can be run automatically after each container is built. However, such automated tests can
655 only cover a subset of potential problems and we also rely on issues reported by users on
656 GitHub and manual testing of new containers when releasing new versions.

657 *The software I need is not available in Neurodesk, and I don't feel confident in my ability to*
658 *contribute a container to the Neurodesk repository. Is there a way I can request that it be*
659 *added?*

660 Users can submit a GitHub issue to request new tools by providing the following
661 information: name and version of the tool, preferred Linux distribution, Linux commands
662 for installing the tool, any GUI applications and commands to start them, test data to
663 include, reference to paper, link to documentation, and commands for testing the tool.

664 *How do I get help if I encounter an issue with Neurodesk?*

665 There is an active discussion forum on GitHub with a Q&A section. If your question
666 has not already been addressed there, please raise a new issue.

667 **Reproducibility in Neurodesk**

668 To investigate our claims that the Neurodesk platform's containerized tools lead to
669 more reproducible results than locally installed software, we sought to conceptually
670 replicate the results reported by Glatard et al. (2015) using Neurodesk vs locally installed
671 software across different operating systems. The first steps in Glatard et al.'s analysis
672 pipeline were brain extraction and tissue classification.

673 *Brain extraction and tissue classification.* FSL BET and FAST were run on raw MRI
674 images to extract voxels containing brain tissue and classify tissue types, respectively. The
675 file checksums for the outputs of these processing steps were identical across all computing
676 environments, verifying that the implementation of the processing pipeline was
677 reproducible across systems for both Neurodesk and local installation. After these steps,
678 image registration and tissue classification were performed with FSL-FLIRT and FSL-
679 FIRST, respectively. These analysis steps did lead to differences in results across systems,
680 and are thus reported in the main text.

681 *Understanding inter-system differences in image registration and tissue classification.*
682 Given that the image registration and tissue classification steps led to inter-system
683 differences, we sought to understand the cause of these differences. FSL utilizes dynamic
684 linking to shared system libraries such as libmath and LAPACK, which are loaded at
685 runtime. Thus, while the same version of FSL was installed in all four computing
686 environments, differences in image processing still emerge for analyses run on locally

687 installed software. This is due to differences in dependencies across systems, a problem
688 addressed by Neurodesk. To better understand how such differences might emerge, calls to
689 these libraries were recorded for a representative image using 'ltrace'. The libraries called
690 during the FLIRT and FIRST analyses could be categorized into four main classes:
691 mathematical operations, matrix operations, memory allocation, and system operations.
692 Interestingly, Glatard et al., who used older software versions than we investigated here,
693 found that image processing differences across systems resulted largely from differences in
694 floating point representation in the mathematical functions *expf()*, *cosf()*, and *sinf()*. They also
695 found inter-system differences in the control-flow of the programs, indicated by differences
696 in the number of library calls to mathematical functions such as *floorf()*. Here, differences in
697 floating point representation were less severe, as these were only present for the *sinf()*
698 function. However, the number of calls made to several functions differed across the local
699 FSL installations, indicating that the inter-system differences in the control flow of the
700 processing pipeline remain an issue for reproducibility (**Table S1**). The *floorf()* function
701 represented the most prevalent difference in library calls. There were over 13 000 additional
702 calls to this function made on System B relative to System A for the FLIRT analysis, and
703 approximately 5.5 million additional calls for the FIRST analysis. Overall, the FIRST
704 analysis had greater discrepancy in calls overall. After accounting for the additional calls to
705 *floorf()*, which occurred early in the FIRST analysis pipeline, mismatches in the sequence of
706 system calls to several other functions remained (**Figure 4a**). However, all remaining
707 mismatches across systems occurred in memory allocation functions. Importantly, there
708 was no difference in floating point representation or the number of system calls to shared
709 libraries across systems for the Neurodesk implementation of FSL (**Figure 4b**), while
710 maintaining a similar runtime as local installation on the same hardware (**Table S1**).

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716 **Table S1.** Differences in the execution of tissue segmentation (FIRST) and image registration (FLIRT)
 717 pipelines. Runtime refers to the CPU time spent on system and library calls within a pipeline.

	Local		Neurodesk	
FIRST (# of calls)	System A	System B	System A	System B
floor	553,308	553,962	553,341	553,341
floorf	48,406,500	53,942,784	51,928,356	51,928,356
log	2,820	3,138	3,024	3,024
FLIRT (# of calls)	System A	System B	System A	System B
floorf	41,347,920	41,334,549	41,342,544	41,342,544
Runtime (n=8)	System A	System B	System A	System B
Average (mins)	4.88	5.39	5.73	5.47
Standard Deviation (mins)	0.07	0.19	0.20	0.15

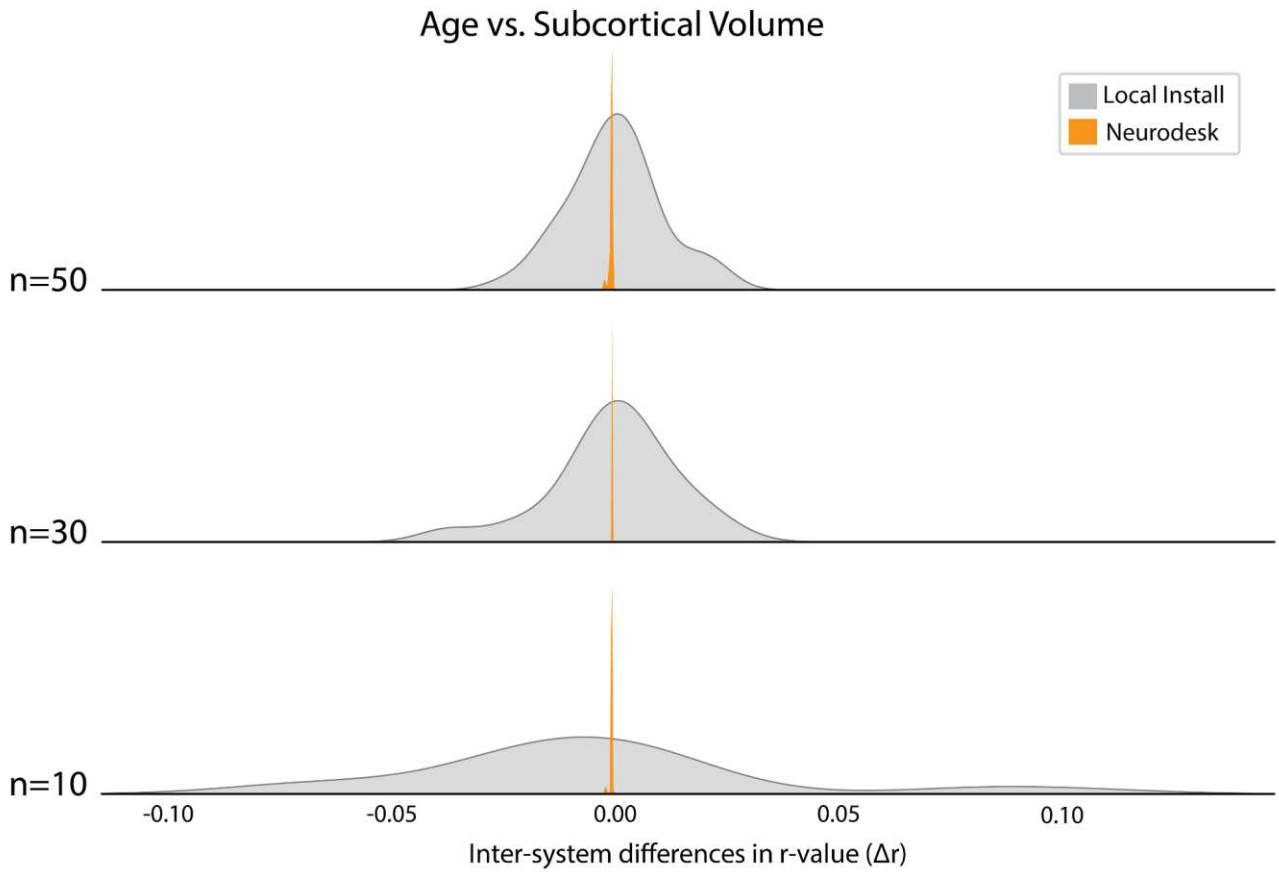
718

719 *Understanding the practical implications of inter-system differences.* The local installations led
 720 to inter-system differences in tissue classification orders of magnitude larger than in
 721 Neurodesk. However, it is difficult to know how voxel-wise differences of this scale might
 722 actually affect test statistics i.e. could there actually be a different conclusion about the
 723 research question if the same analysis on the same data runs on a different computer? To
 724 address these questions, we performed a permutation test to examine the impact of inter-
 725 system differences in tissue classification (using FSL FIRST) on correlations between
 726 subcortical structure volumes and age.

727 On each system (A,B), for both Neurodesk and local installations, we computed the volume
 728 of each subcortical structure in the left hemisphere, right hemisphere, and the whole
 729 structure by participant. We performed permutation tests for each of these volumes (9999
 730 permutations each). On each permutation, we performed a Pearson correlation of volume

731 vs. participant age, and calculated the differences in the values of the correlation
732 coefficients across the two systems. These permutation tests were repeated for three
733 different sample sizes ($n=10, 30, 50$), such that each permutation for each sample size
734 represented a different randomly selected group of participants. Critically, for each sample-
735 wise permutation, the same sample was used for each of the two systems, such that the test-
736 statistic difference always represented inter-system differences rather than inter-sample
737 differences. Thus, the distribution of test statistic differences for each sample size
738 represents 209979 permuted samples (7 subcortical structures (Putamen, Amygdala,
739 Thalamus, Pallidum, Caudate Nucleus, Hippocampus, Accumbens.) x 3 methods (left
740 hemisphere, right hemisphere, both) x 9999 subject-wise permutations).

741 The analysis showed that as sample size decreased, the inter-system coefficient differences
742 for the local installations increased in magnitude (Local installation: $N=50, \Delta r = -0.02 - 0.02$ |
743 $N=30, \Delta r = -0.04 - 0.03$ | $N=10, \Delta r = -0.08 - 0.11$; **Figure S1**). By contrast, the inter-system test
744 statistic differences for Neurodesk were negligible and did not scale with sample size
745 (Neurodesk: $N=50, \Delta r = -1.74 \times 10^{-3} - 2.59 \times 10^{-4}$ | $N=30, \Delta r = -3.75 \times 10^{-5} - 1.89 \times 10^{-4}$ | $N=10, \Delta r = -$
746 $1.52 \times 10^{-3} - 0$; **Figure S1**). Thus, the minor differences in image processing with locally
747 installed software can meaningfully impact the reliability of test statistics, especially when
748 statistical power is already low. It is therefore crucial to consider both sample variability
749 and system variability when conducting these types of analyses.



750

751 **Figure S1.** Permutation test results showing inter-system differences in r-values for the correlation
752 between age and volume of subcortical structures, organized by sample size ($n = 10, 30, 50$).

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