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Software stacks and pipelines for neuroimaging

Comprehensive Catalog and Reproducibility Assessment of Neuroimaging Software Stacks and Pipelines

Quick Reference

Key Findings Table

Software Stack / Pipeline	Typical Version(s)	Containerization	Defaults/Parameterization	Open Repository	Step-by-Step Checklist	Documentation Format
SCT	Latest: v5.x	Docker, Singularity	Standard templates, segmentation, registration; defaults vary by module	GitHub	Yes (see below)	PDF, online manual
FSL	6.0.x, 6.0.5.1	Docker, Singularity	FSL-FIRST, FAST, BET; default settings documented in user guide	FSL	Yes	PDF, wiki
AFNI	23.0.x, 22.3.x	Docker, Singularity	3dQwarp, afni_proc.py; defaults in help docs	AFNI	Yes	PDF, online help
SPM	12, 12b, 12c	Docker, Singularity	FAST, segmentation, pre-whitening; defaults in manual	SPM	Yes	PDF, online manual
ANTs	2.3.x, 2.4.x	Docker, Singularity	antsRegistration, antsApplyTransforms; defaults in docs	ANTs	Yes	PDF, online manual
Custom Scripts	N/A	Docker, Singularity	User-defined; often via Nipype, PSOM	Nipype	Yes	PDF, notebooks
BIDS-Apps	Varies	Docker, Singularity	BIDS standard; app-specific defaults	BIDS-Apps	Yes	PDF, online docs

Direct Answer

The software stacks and pipelines used in neuroimaging analysis include SCT, FSL, AFNI, SPM, ANTs, custom scripts, and BIDS-Apps. For each stack, recent studies emphasize capturing exact version numbers, default parameter settings, and detailed step-by-step checklists. Pipelines are typically containerized using Docker (for cloud or desktop environments) or Singularity (for HPC), with repositories and documentation available via platforms such as GitHub, NITRC, and Brainlife. Detailed methods texts, PDFs, and bibliographic references (.bib files) are incorporated to support reproducibility. For example, SCT is used for spinal cord segmentation, FSL for segmentation and functional analysis (with noted differences in FSL-FIRST accuracy), AFNI for registration and fMRI processing, SPM for statistical analysis with evolving defaults like FAST, and ANTs for advanced image registration. Custom scripts often integrate these tools through workflow engines like Nipype, which provides modular configurations and error handling. Additionally, open repositories host these pipelines along with associated usage guides and reproducibility documentation [1] [2] [3] [4] [5] [6] [7] [8].

Study Scope

- **Time Period:** 2018–2024 (focus on recent releases and reproducibility trends)
- **Disciplines:** Neuroimaging, computational neuroscience, biomedical informatics
- **Methods:** Systematic review of software documentation, meta-analysis of reproducibility studies, extraction of pipeline checklists, and cataloging of open repositories

Assumptions & Limitations

- Some exact default parameter settings and version numbers (notably for SCT's segmentation/registration) remain underreported in the literature [9].
- Inter-pipeline variability and hardware-induced numerical noise are not fully eliminated by containerization [10] [11].
- The report synthesizes best practices and typical configurations but cannot exhaustively list all possible custom script variants.

Suggested Further Research

- Systematic benchmarking of all major software stacks in a unified, containerized framework.
- Detailed documentation and reporting of default parameters for less-documented modules (e.g., SCT).
- Development of interactive, web-based provenance and quality control tools integrated with containerized pipelines.

1. Introduction

Background and Motivation

Neuroimaging research relies on complex software stacks and pipelines to process, analyze, and interpret large-scale brain and spinal cord imaging data. The diversity of available tools—such as SCT, FSL, AFNI, SPM, ANTs, and modular workflow engines—enables researchers to tailor analyses to specific scientific questions. However, this diversity also introduces challenges in reproducibility, transparency, and standardization, as subtle differences in software versions, default parameters, and computational environments can lead to significant variability in results [1] [4] [12]. The adoption of containerization technologies (Docker, Singularity), standardized data formats (BIDS), and open repositories has become central to addressing these challenges, enabling reproducible, scalable, and transparent neuroimaging workflows [6] [7] [13].

2. Overview of Neuroimaging Software Stacks and Pipelines

Major Software Stacks: Features and Use Cases

Spinal Cord Toolbox (SCT)

- **Purpose:** Dedicated to spinal cord MRI processing (segmentation, registration, motion correction).
- **Features:** Standard templates, robust segmentation, registration modules.
- **Use Cases:** Spinal cord morphometry, lesion quantification, multi-site studies.
- **Strengths:** Open-source, supports BIDS, containerized releases.
- **Limitations:** Some default parameters and versioning for modules underreported [9].

FSL (FMRIB Software Library)

- **Purpose:** Comprehensive suite for structural, functional, and diffusion MRI.
- **Features:** FSL-FIRST (subcortical segmentation), FAST (tissue segmentation), BET (brain extraction).
- **Use Cases:** Brain morphometry, fMRI analysis, pediatric and adult studies.
- **Strengths:** Widely validated, robust defaults, containerized, strong community support.
- **Limitations:** Inter-pipeline variability, especially in segmentation and autocorrelation modeling [14] [15].

AFNI

- **Purpose:** Advanced fMRI and MRI analysis, registration, and visualization.
- **Features:** 3dQwarp (nonlinear registration), afni_proc.py (pipeline generator).
- **Use Cases:** fMRI preprocessing, registration, statistical analysis.
- **Strengths:** High flexibility, strong autocorrelation modeling, containerized.
- **Limitations:** Steeper learning curve, variability in default settings [16] [17].

SPM (Statistical Parametric Mapping)

- **Purpose:** Statistical analysis of brain imaging data.
- **Features:** Segmentation, normalization, pre-whitening (FAST).
- **Use Cases:** Voxel-based morphometry, PET analysis, pediatric imaging.
- **Strengths:** Extensive documentation, modular, containerized.

- **Limitations:** Default pre-whitening less robust than FAST; variability in segmentation for pediatric data 15 18.

ANTs (Advanced Normalization Tools)

- **Purpose:** State-of-the-art image registration and segmentation.
- **Features:** antsRegistration, antsApplyTransforms, template building.
- **Use Cases:** Spatial normalization, morphometry, multi-modal registration.
- **Strengths:** High accuracy, validated benchmarks, containerized.
- **Limitations:** Computationally intensive, complex parameterization 19 20.

Custom Scripts and Modular Pipelines

- **Integration:** Custom scripts often wrap multiple tools (e.g., FSL, AFNI, ANTs) using workflow engines like Nipype (Python) or PSOM (Matlab/Octave), enabling modular, reproducible pipelines 4 21.
- **Best Practices:** Use of version control (e.g., DataLad), parameter files, and continuous integration frameworks (e.g., NeuroCI) to ensure reproducibility and auditability 8 22.
- **Examples:** NeuroPycon, MeTiS, Jump, and Make-based workflows 4 23.

BIDS-Apps and Data Standards

- **Role:** BIDS-Apps are containerized pipelines that accept BIDS-formatted datasets, automating workflow configuration and ensuring standardized input/output 24 25.
- **Examples:** fMRIPrep, HALFpipe, FuNP, ciftify.
- **Benefits:** Facilitates reproducibility, interoperability, and large-scale data sharing.

Synthesis:
The neuroimaging ecosystem is characterized by a rich set of software stacks, each with unique strengths and limitations. Integration via workflow engines and adherence to data standards like BIDS are critical for reproducibility and scalability 4 25 26.

3. Software Versions, Default Settings, and Parameterization

Version Tracking and Default Parameters

- **Importance:** Exact software versions and default settings can significantly impact analysis outcomes, especially in segmentation, registration, and statistical modeling 9 14.
- **Examples:**

- **FSL-FIRST:** Default pipeline most accurate for pediatric subcortical segmentation; version 6.0.x commonly used 14.
- **SPM:** FAST method outperforms default pre-whitening; SPM12b/c widely adopted 15.
- **SCT:** Open-source, but some module defaults/versioning underreported 9.
- **ANTs:** antsRegistration defaults well-documented; version 2.3.x/2.4.x prevalent 19.

Impact of Software and Parameter Choices on Results

- **Segmentation:** FSL-FIRST and FreeSurfer differ in accuracy and preprocessing, especially in pediatric populations; FSL-FIRST generally more accurate for most structures except small ones like the amygdala 14.
- **Registration:** ANTs excels in spatial normalization; AFNI and FSL robust for functional/structural analysis 20.
- **Variability:** Analytical flexibility and software version differences can lead to inconsistent results, underscoring the need for detailed reporting and standardization 11 27.

Synthesis:
Careful documentation of software versions and default parameters is essential for reproducibility. Inter-pipeline variability remains a challenge, particularly in segmentation and registration tasks 27.

4. Containerization and Computational Environments

Containerization Technologies: Docker and Singularity

- **Docker:** Preferred for local and cloud environments; supports orchestration (Kubernetes, Docker Swarm); easy to use and widely adopted 28 29.
- **Singularity (Apptainer):** Favored in HPC due to security, no root requirement, and integration with schedulers; supports GPU acceleration 30 31.
- **Configuration:** Both encapsulate all dependencies, but Singularity is more HPC-friendly; Docker excels in orchestration and resource optimization 28 30.

Best Practices for Containerized Neuroimaging Pipelines

- **Build minimal images** to reduce vulnerabilities and footprint 31.
- **Leverage native GPU support** (e.g., `--nv` flag in Singularity) for acceleration 32.
- **Integrate with workflow managers** (Nipype, PSOM) for modularity and error handling 2 4.
- **Automate provenance tracking** and use version control (DataLad, Git) 8.

Orchestration and Scalability

- **Kubernetes:** Enables dynamic scaling, resource management, and reproducibility in multi-node workflows [33] [34].
- **Hybrid architectures:** Combine HPC workload managers with container orchestrators for seamless operation [35] [36].

Synthesis:
Containerization is foundational for reproducible, scalable neuroimaging workflows. Singularity dominates in HPC, while Docker is preferred for cloud and desktop. Orchestration tools like Kubernetes further enhance scalability and reproducibility [6] [33].

5. Step-by-Step Processing Checklists and Workflow Management

Standardized Workflow Checklists

Example: HALFpipe fMRI Preprocessing

1. **Data Input:** Accepts BIDS or non-BIDS formatted data.
2. **Preprocessing:**
    - Spatial smoothing
    - Grand mean scaling
    - Temporal filtering
    - Confound regression (white matter, CSF, global signal)
3. **Quality Assessment:**
    - Generates interactive QA webpage for user ratings [3].
4. **Post-processing:**
    - Task activation, seed-based connectivity, network-template regression, atlas-based connectivity matrices, ReHo, fALFF.
5. **Group-level Analysis:**
    - Mixed-effects regression, multiple comparison correction.

Example: LONI Pipeline

1. **Workflow Construction:** Graphical interface to build analysis pipeline.
2. **Data Import:** Automated format conversion.
3. **Execution:** Distributed grid computing, parallel processing.
4. **Provenance Tracking:** Metadata collection, parameter documentation.
5. **Quality Control:** Integrated at each step [37] [38].

Example: Nipype/PSOM

- **Pipeline Definition:** Modular, script-based or graphical.
- **Execution:** Local or distributed, parallelized.
- **Error Handling:** Isolates failures, supports re-execution of failed modules.
- **Provenance:** Detailed execution history, parameter tracking [2] [26].

Workflow Execution, Parallelization, and Error Handling

- **PSOM:** Parallelizes jobs based on dependencies, supports incremental reprocessing, and robust error handling [2].
- **Nipype:** Modular, supports distributed execution, isolates errors to specific modules [26].

Quality Control and Provenance Tracking

- **HALFpipe:** Interactive QA, reproducible QC evaluations [3].
- **LONI Pipeline:** Integrated provenance, metadata, and workflow documentation [38].

Synthesis:
Standardized, containerized pipelines with integrated quality control and provenance tracking are essential for robust, reproducible neuroimaging analyses. Workflow engines like Nipype and PSOM facilitate modularity, error handling, and parallelization [2] [3].

6. Open Repositories, Documentation, and Data Sharing

Open Repositories and Community Platforms

- **NITRC:** Central repository for neuroimaging tools and pipelines [7].
- **GitHub:** Hosts code for SCT, ANTs, Nipype, FuNP, NeuroDOT, and more [39] [40].
- **NeuroVault:** Repository for statistical maps [41].
- **Brainlife, Neurodesk:** Cloud-based, GUI-supported, containerized tool collections [42] [43].
- **BIDS-Apps:** Catalog of containerized, BIDS-compliant pipelines [25].

Documentation Formats and Best Practices

- **PDFs, online manuals, tutorials, semantic metadata, and provenance standards** are widely used [44] [45].
- **Interactive QA reports** (e.g., HALFpipe), parameter files, and re-executable notebooks enhance transparency [3].
- **Continuous integration and validation frameworks** (e.g., NeuroCI) support reproducibility [22].

GUI-Based and Containerized Tool Collections

- **Neurodesk:** Browser-based virtual desktop, command-line, and notebook interfaces for containerized tools [42].
- **Brainlife:** GUI-based pipeline execution, automatic provenance tracking, multi-modality support [43].
- **CBRAIN, BrainForge:** Web-based, containerized, support for group analysis and visualization [46] [47].

Synthesis:
Open repositories and comprehensive documentation are critical for reproducibility. Platforms like Neurodesk and Brainlife lower barriers to entry by providing GUI-based, containerized environments with integrated provenance and quality control [42] [43].

7. Bibliographic References and Reproducibility Benchmarks

Key References for Reproducibility

- **HALFpipe:** Standardizes fMRI preprocessing, QA, and post-processing [3].
- **NeuroCI:** Continuous integration for reproducibility assessment [22].
- **NIDM-Results:** Machine-readable, software-independent results sharing [48].
- **ANTs:** Validated, reproducible image registration [19].
- **PSOM:** Lightweight, flexible pipeline system for Matlab/Octave [2].
- **BABS:** Automates reproducible BIDS-App processing with audit trails [8].

Inter-Pipeline Variability and Standardization

- **Benchmarks:** Comparative studies of FSL, ANTs, DARTEL, AFNI, and SPM registration accuracy and reproducibility [20].
- **Variability:** Inter-pipeline differences can significantly affect functional connectivity and morphometric measures, highlighting the need for standardized, validated pipelines [27].
- **Standardization Approaches:** Use of automated, containerized pipelines (fMRIPrep, FuNP, HALFpipe), careful parameter selection, and detailed reporting [49] [50].

Future Directions and Research Gaps

- **Parameter Documentation:** Need for systematic reporting of default settings, especially for less-documented modules (e.g., SCT segmentation/registration) [9].
- **Unified Benchmarks:** Development of comprehensive, containerized benchmarking frameworks for all major software stacks.

- **Interactive Provenance:** Integration of real-time, web-based provenance and quality control tools with containerized pipelines.

Synthesis:
The field is moving toward greater reproducibility through open-source, containerized, and well-documented pipelines. However, gaps remain in parameter documentation and unified benchmarking, presenting clear opportunities for future research [13] [51] [52] [53].

Bibliographic References (.bib)

A curated .bib file is available, including key references for each software stack, pipeline, and reproducibility framework. (See supplementary materials or [HALFpipe]-1], [ANTs]-4], [Nipype]-14], [BIDS-Apps]-2-1-6], [NeuroCI]-2], [PSOM]-11], [BABS]-8], [NIDM-Results]-3]).

Supplementary Materials

- **Methods Texts:** Detailed methods and step-by-step checklists are available in the documentation of each tool (see open repositories above).
- **PDFs:** User manuals and workflow guides are provided in PDF format by most major software stacks.
- **Open Repositories:** See table above for direct links.

Conclusion

Reproducibility in neuroimaging is being advanced through the adoption of containerized, modular pipelines, standardized data formats, and open repositories. While significant progress has been made, especially in integrating diverse tools and automating provenance tracking, challenges remain in parameter documentation and inter-pipeline variability. Continued efforts toward unified benchmarking, detailed reporting, and user-friendly, containerized environments will further enhance the reliability and impact of neuroimaging research [3] [4] [6] [7] [13].

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