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neuGRID

A GRID-BASED e-INFRASTRUCTURE FOR DATA ARCHIVING/ COMMUNICATION AND COMPUTATIONALLY INTENSIVE APPLICATIONS IN THE MEDICAL SCIENCES

Combination of Collaborative Project and Coordination and Support Action

Objective INFRA-2007-1.2.2 - Deployment of e-Infrastructures for scientific communities

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Dissemination Level		
PU	Public	X
PP	Restricted to other programme participants (including the Commission	
RE	Restricted to a group specified by the consortium (including the	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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1.0 – 1.3	All WP9 and project partners.	4/2/2009
1.4	Ronald van Schijndel, Ingrid Sluimer, Keith Cover (VUmc), Eva Örndahl (KI), Alberto Redolfi, Marco Lorenzi and Anna Caroli (FBF)	10/3/2009
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1.6	Giovanni Frisoni (FBF)	26/3/2009

Purpose and Intended Audience of this Document

D9.1 The User Requirements Specification forms a public deliverable and documents the requirements of the user communities in the project. This is written to be of use to clinical researchers, system designers, developers and maintainers from within and outside of the neuGRID consortium. If you wish to learn more about the project at a high-level then Sections 1, 3 and 4 will provide you with this. If on the other hand you are interested in the more detailed aims and requirements of the neuGRID infrastructure, then Section 5 covers these aspects. Section 7 has been created primarily for workpackage leaders and developers within the project and maps requirements to specific areas and tasks.

Executive Summary

The aim of the neuGRID project is to provide a user-friendly grid-based e-infrastructure, which will enable the European neuroscience community to carry out research that is necessary for the study of degenerative brain diseases. In order to achieve this goal, clinical researchers and computer scientists need to work together closely in order to determine the features that the infrastructure will provide to end users. This is challenging because the two communities are complex, have different terminologies and ways of working. Workpackage nine (WP9) was designed specifically to bridge the gap between the various stakeholders through a range of face-to-face meetings, telephone conferences and other activities in order to produce an agreed User Requirements Specification document that will drive the technical design and implementation phases of the project.

Key Objectives of WP9:

- **Conceptualisation**: to establish a common language and models among users, developers and the system deployment teams.

- **Elicitation**: to gather the end-user and developer requirements which are essential for the delivered software product to fulfil the clinical goals, the developers to understand the use-cases in which the software will be used, to understand constraints posed by legacy application and data.

- **Abstraction**: to represent the elicited and agreed requirements in the established conceptual framework.

- **Documentation**: to deliver a User Requirements Specification, that is accurate, reliable, complete and consistent. It will define functional, non-functional requirements and technical specifications known at this stage and their relationship to project objectives.

The requirements gathering process in neuGRID has benefited from enthusiastic support from the clinical researcher community. The requirements team organised elicitation sessions at FBF in Brescia, VUmc in Amsterdam and KI in Stockholm during the initial months of the project (please see Table 1 for further details.) The main purpose of these meetings was to work with researchers in order to identify the features that were necessary during their day to day work. This involved visiting research facilities and interacting with as many of the

clinical researchers as possible in order to hear their views. During each of the visits researchers presented their work and methods of analysis. By bringing computer scientists and clinical researchers together in this way, a common understanding of the problem domain was reached. The first series of planned meetings have now been completed and have been most productive in bridging the gap between system developers and clinical researchers. Initially meetings focused on the identification of some high-level stories and usage patterns. As these developed a range of use-cases were created and then prioritised. This provided a clear framework on which more detailed individual requirements could be based.

Date	Location	Content	Attendance
2008-02-04	Fatebenefratelli – Brescia, Italy	Initial series of requirements meetings and technical brainstorming on fundamentals of neuGRID system	ALL
2008-03-15	Karolinska Institute – Stockholm, Sweden	Second series of requirements meetings	FBF, UWE, MAAT, PRODEMA, KI
2008-05-15	VUmc – Amsterdam, The Netherlands	Third series of requirements meetings and in person technical brainstorming	FBF, UWE, MAAT, PRODEMA, VUmc
2008-09-02	Fatebenefratelli – Brescia, Italy	Fourth series of requirements meetings.	FBF, UWE, MAAT, PRODEMA, VUmc

Table 1: Requirements meetings held during the initial months of the project.

A major output of WP9 was the development and modelling of a group of stories which illustrate the end-to-end use of the neuGRID infrastructure. This has been of benefit in terms of describing the project and ensuring that important components are not overlooked. This led to a clear hierarchical conceptual framework being identified that linked high-level stories to more finely grained use-cases and to individual users requirements. This approach and the structure of the final user requirements specification were discussed and agreed to by project partners during project meetings. It was decided that the primary focus should be on the production of easily understandable models that are meaningful to both clinical researchers and software developers. The verification, prioritization and refinement of the constructed models has greatly benefited from the identified stakeholders at FBF, VUmc and KI.

1. Introduction

Analysis of the project scope and context (and associated users' requirements) is seen as an essential component of neuGRID that will ensure common understanding between the clinicians and those responsible for IT research and development from the outset of the development stage. It guides the development process involving multiple partners and will assist the test phase of the delivered components. *D9.1 User Requirements Specification* describes the requirements that need to be met for the project to achieve the goals described in the project proposal. It documents the scope of the project by reflecting the interests of all the major actors. This document establishes a hierarchical set of requirements which takes into account core project goals, the participating clinicians' views as well as constraints which ensure that focus on innovation in the promised areas is maintained from the outset.

The major outputs from this deliverable are the following:

(i) An agreed form of expression (“language”) of the concepts, including but not limited to textual and diagrammatic models.

(ii) The set of prioritized functional and non-functional specifications reflecting on the requirements of both the end-users and developers, expressed using the agreed conceptual framework.

(iii) A commitment to and a plan for reviewing the User Requirements Specification (URS) document as the project progresses.

A hierarchical conceptual framework has been created that links stories to more finely grained use-cases and to the users requirements. It was decided that the needs of the project place the main emphasis on producing easily understandable models that are clear to both researchers and software developers. This process began during the initial meetings with clinical researchers and discussions led to a set of stories being identified that spanned the problem domain and allowed use-cases to be grouped into areas of common purpose. Each story was modelled and thoroughly analysed to define the group of use-cases that were present in it. At this point the requirements team went through several cycles of review with clinical researchers, which resulted in a final frozen set of stories and use-cases that were agreed by all the project partners. Figure 1 shows the importance of review loops during the requirements gathering and within the wider system engineering process.

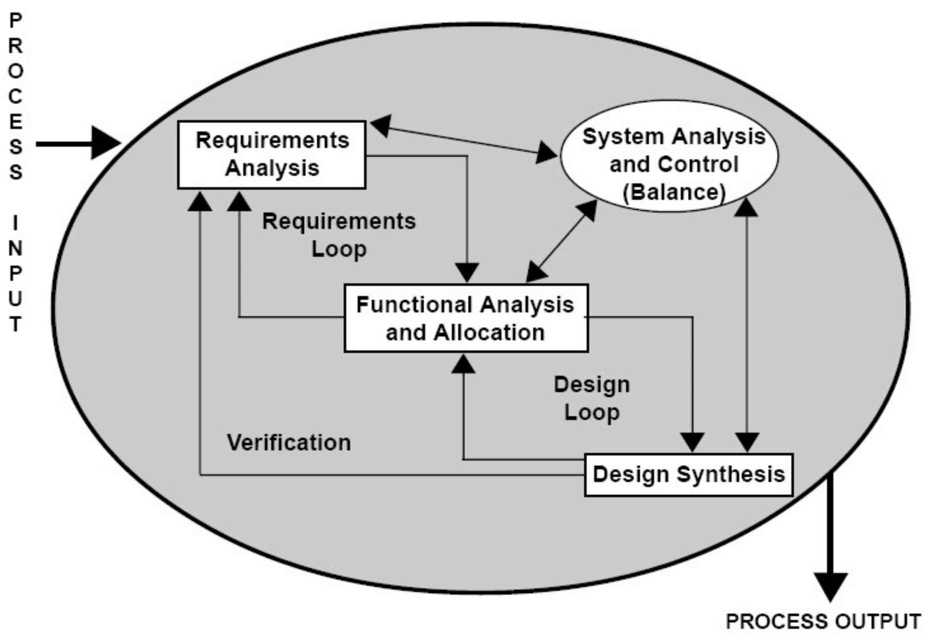


Figure 1: The Requirements Engineering Process, Image taken from [1].

The next stage in the requirements gathering process was to make some initial decisions regarding the priority of use-cases. It was clear given the scope and budget of neuGRID that not all of the use-cases would be achievable during the course of the project. With this in mind it was decided that use-cases should be prioritized using a variant of the MoSCoW technique [2]. In this prioritization framework requirements are assigned one of the following levels of priority:

- M- MUST have this.
- S - SHOULD have this if at all possible.
- C - COULD have this if it does not affect anything else.
- W -WON'T have this time but WOULD like in the future.

The neuGRID prioritization framework is almost the same as this, but for clarity and brevity it was decided use-cases that definitely would not be implemented should be removed from the specification. Use-cases that were not included in the final specification are recorded in the minutes of the requirements meetings and will therefore remain accessible as the project continues. It was also thought sensible to prioritize use-cases at this stage and in this way because they would be used during the final requirements gathering stage as a foundation upon which individual user requirements would build. The following levels of priority were assigned to use-cases in the project:

- Essential (E): Those which are absolutely vital to the production of a functional infrastructure.
- Desirable (D): Those that whilst not vital, would provide important functionality to users.
- Optional (O): Those that might be useful but don't fit into the previous two categories and will probably be the last to be implemented if time / budget allows.

The prioritization of the use-cases was useful in stimulating debate and helping developers get acquainted with the requirements process that was underway. This also led to some additional use-cases being identified and some even being removed. Once the final set of use-cases and associated priorities had been agreed, they were frozen and the concentration was placed on the gathering of individual user requirements. The project as a whole felt that clinical researchers should play an active part in writing this part of the specification. Therefore an initial draft was circulated by the workpackage leader and this was then built upon by the end-users at FBF, KI and VUmc. This process was based on individual use-cases as a means of focusing in greater detail on smaller aspects of the system. For each uses-case the relevant user requirements were identified and described. The clinical researchers responded well to this task and produced a very comprehensive list of functional and in some cases even non-functional requirements.

In preparation for this deliverable the next stage was to take the final list of agreed requirements and assign them each an initial level of priority, in the same way as the use-cases had been prioritized earlier. In this respect the priority of the parent use-case from which a requirement came was a useful indicator of the level of priority that it should be given. That being said it was reasonably common for some requirements to be given a lower priority than their parent use-case. This was especially true for use-cases that had several requirements attached to them. The priorities that have been assigned during this phase of the project, are only initial indications and will necessarily evolve as the project progresses. In order for workpackage leaders and system designers to better understand how the current requirements and priorities may impact their work, an initial mapping between requirements and workpackages has been produced in Section 7 of this document. These will be revised and finalized during Task 9.5 in months 22-26 of the project.

2. Glossary of Terms Used

This section lists and briefly describes some clinical and technical terms that are subsequently used in the following sections of the document.

A		
	Actor	An indicative group of users or stakeholders in a system.
	Acquisition center	A Medical facility staffed with a clinical investigator (MD) qualified for performing clinical research. The center/site where the medical images and/or medical parameters are acquired.
	Administrator	A role in a computer system, which has complete privileges to perform any action permitted without any restrictions.
	ADNI Protocol	Set of roles which define the acquisition of the MR imaging sequences according to the Alzheimer Disease Neuroimaging Initiative (ADNI).
	Algorithm	A step-by-step problem-solving procedure.
	Anonymization	The process removing or obfuscating information from data which could be used to identify the concerned person or source.
B		
	Bandwidth	The maximum throughput, in bits per second, of a physical communication path in a digital communication system.
C		
	Clinical Biological Data	Data or measurements collected from clinical biological sources, which are commonly stored in files or databases.
	Cortical Thickness	Cortical Thickness refers to the quantitative measurement of the thickness of the human cerebral cortex.
	Core Lab	Center that collects data from various acquisition centers and checks for commitment to a given scan protocol, image quality and completeness of the acquired images. The DACS (Data Archiving and Computing Site) is synonymous with this concept.
D		
	Data Model	An abstract model that describes how data is represented, stored and accessed.
	Data Registration	The process of inputting new data to a data store
	Data Store	A repository where data is stored.
	Dependencies	In workflows or pipelines, dependencies refer to the tasks which provide input data to a specific task.
	DICOM	The Digital Imaging and Communications in Medicine (DICOM) is a standard for distributing and viewing almost any kind of medical image.

	Download	The process of copying remote data to a local data store.
E		
	Ethical Compliance	Guidelines required to be considered for aspects/actions eligibility.
F		
	Face Scrambling	An anonymization technique which obfuscates facial features of an image
	Field Inhomogeneities	A disturbance of the field homogeneity, because of magnetic material, technical problems or scanning at the edge of the field.
	fMRI	Functional Magnetic Resonance Imaging (fMRI) is a type of specialized MRI scan. It measures the haemodynamic response related to neural activity in the brain or spinal cord of humans or other animals. It is one of the most recently developed forms of neuroimaging.
	Functional Assessment Questionnaire Total Score	Psychiatric Rating Scales for dementia evaluation.
G		
	GDScale Total Score	Psychiatric Rating Scales for dementia evaluation.
	Global CDR	Psychiatric Rating Scales for dementia evaluation.
	Gradwarp	A system specific correction of image geometry distortion due to gradient non-linearity.
	Grid Computing	A form of distributed computing, where the system is created by forming a virtual organization over geographically distributed heterogeneous clusters. Grids can be both data centric and computation centric. In a data centric Grid, geographically distributed heterogeneous data sources are linked, and users can access and use data irrespective of location in the Grid. A Compute Grid, is a Grid which unifies the processing capabilities distributed in heterogeneous sites.
	GUI (Graphical User Interface)	A graphical user interface (GUI) is a human-computer interface that uses windows, icons and menus and which can be manipulated by a mouse.
I		
	Image	In the context of neuGRID, an image is a MRI brain scan.
	Image Acquisition	The process of acquiring a scan from a patient.
	Image Scrambling	The process of removing or obfuscating features from an image, in order to anonymize it.
	Inter-Slice Movement	Artifacts consisting in the misalignment between 2 or more slices within a stack and/or movement within a slice.
L		
	Linux	An Open Source Computer operating system, similar to Microsoft Windows, Mac OSX, Unix etc
	LONI	The Laboratory of Neuro Imaging (LONI) is a research centre dedicated to studying the relationship between brain structure and function using image data. It is based at the University of California, Los Angeles
	LORIS	The LORIS system (On-line Research Imaging System, formerly NeuBase) was originally implemented for the collection, management, and processing of the imaging data acquired in a multi-centre Alzheimer's Disease project

		(AddNeuroMed.)
M		
	MMSE Total Score	The mini-mental state examination (MMSE) is a brief 30-point questionnaire test that is used to screen for cognitive impairment. It is commonly used in medicine to screen for dementia. (source: http://encyclopedia.thefreedictionary.com/Mini+Mental+State+Examination.)
	Modality	Modality is used to describe the various classes of imaging devices used to image the internal structures of object. The modality is mostly differentiated by the physics used to create the image. For example Magnetic Resonance and Computed Tomogrphy are different modalities. (source http://www.angelfire.com/co2/whatdicom/yong.html.) This includes the various types of equipment or probes that are used to acquire images of the body.
	Modified Hachinski Total Score	Psychiatric Rating Scales for Dementia evaluation.
	MRI	Magnetic resonance imaging (MRI) is a medical imaging technique most commonly used in radiology to visualize the structure and function of the body. MR imaging uses a powerful magnetic field to align the nuclear magnetization of (usually) hydrogen atoms in water in the body. Radiofrequency fields are used to systematically alter the alignment of this magnetization, causing the hydrogen nuclei to produce a rotating magnetic field detectable by the scanner. This signal can be manipulated by additional magnetic fields to build up enough information to construct an image of the body.
N		
	Non-uniformity Correction	Non-uniformity Correction: A mathematical method for the automatic procedure that reduces residual intensity non-uniformity due to the wave or the dielectric effect (source http://www.fields.utoronto.ca/programs/scientific/08-09/mathoncology/courses/3_FreqTransforms.pdf.)
	NPI-Q Total Score	Psychiatric Rating Scales for Dementia evaluation.
P		
	PDF	The Portable Document Format (PDF) is a popular way to store and transmit electronic documents.
	Platform-independence	A property of a system, where the system is not tightly coupled with a specific platform.
	Pipeline	See definition for workflow.
Q		
	Quality Control	The process of ensuring that a certain system or product meets user requirements.
	Querying Language	A computer language used to query data or information from a data store.
	Quota	An allotment of a certain share from a resource. (i.e. Disk quota, bandwith quota.)
R		
	Research Set	A set of brain scans which will be used as input to a neuro-imaging pipeline.
S		

	Service	An independent, self contained module in a Service oriented Architecture. It provides a single functionality, which is exported via standardized interfaces (WSDL) and communicates via standardized communication protocols, mainly SOAP.
	System Maintenance	The modification of a system to correct faults, to improve performance, or to adapt the system to a changed environment or changed requirements.
	Service Oriented Architecture (SOA)	Service Oriented Architecture is an architecture which uses loosely coupled ad-hoc collection of independent services. Each service is self contained and provides a specific piece of functionality. This architecture is popular in large-scale distributed systems, primarily because it is robust, scalable, extensible and potentially resistant to failure.
	SOAP	Simple Object Access Protocol, a standardized means of inter-communications between services and clients in a SOA.
	Source Code	The human readable logic of a computer program.
	Story	A high-level model of several user requirements.
U		
	Upload	The process of copying data from a local data store to a remote data store.
	User Collections	Lists of images collected by the neuGRID users.
	Use-case	An abstract model of a user requirement.
W		
	Webinar	A webinar is a collaborative meeting, analogous to a seminar, where the participants attend from remote locations linked by the Internet.
	Workflow	The defined series of tasks within an organization to produce a final outcome.
	WSDL	Web Service Description Language, the standardized means of describing and exporting service functionality in a SOA.

3. The Actors In neuGRID

A key part in analyzing the requirements for any system is identifying the types of users that will make use of it in some way. This allows the requirements team to ensure that they do not miss out features that a small number of members within a wider user community may desire. By modeling the ways in which the Actors interact with the system that is being designed, a range of important conclusions can be drawn. Practically speaking, this may mean ensuring that representative members from each group of Actors are present during requirements elicitation sessions and that they review any specifications that are produced. This Section briefly describes the Actors that have been identified in neuGRID and gives some profiles of projects members from within the neuGRID consortium that are members of these groups.

Research Leaders

Team leaders who need to monitor the progress, resource usage and perhaps distribute research studies to a research team.

Example Profile

Dr. Frisoni is a Neurologist and Vice-Scientific Director of IRCCS-Fatebenefratelli Hospital Brescia (Italy). His main research interests are focussed on the exploitation of intensive computational neuroanatomy algorithms in translational neuroscientific research and in the dissemination of new brain image analysis tools to clinical neuroscientists and clinical physicians. He works with his team to carry out research and communicate findings to the wider community through publications and other scholarly activities.

Example publications:

1. Frisoni GB et al. Neuroimaging tools to rate regional atrophy, subcortical cerebrovascu. Ashburner J, Frisoni GB, et al., Computer-assisted imaging to assess brain structure in healthy and diseased brains. Lancet Neurol 2003;2:79-88.
3. Frisoni GB, et al., Detection of grey matter loss in mild Alzheimer's disease with voxel based morphometry. J Neurol Neurosurg Psychiatry 2002;73:657-64.
4. Frisoni GB, et al., In vivo neuropathology of the hippocampal formation in AD: a radial lar disease, and regional cerebral blood flow and metabolism: consensus paper of the EADC. J Neurol Neurosurg Psychiatry 2003;74:1371-81.
2 mapping MRbased study. Neuroimage. 2006;32:104-10.
5. Frisoni GB, et al., The topography of grey matter involvement in early and late onset Alzheimer's disease. Brain. 2007;130:720-30.

Researchers

Individual members of the research team who will use neuGRID during their day-to-day research work. These may interact with the system in different ways depending on their experience and the nature of the research that they are carrying out. Broadly speaking the following groups of users has been identified:

Basic User

This group represents users who have a certain level of computing expertise, but are mainly content to use software as it was installed and are not inclined to customize environments to their needs. They expect a reasonably straightforward user interface through which they can carry out their day to day tasks.

Example Profile:

Olof is a PhD student at K.I. with Professor Wahlund since 2007. His research area is the anatomy and volumetry of the frontal lobe. His main research project involves frontal lobe dementia, which can be investigated by the shrinking of various small structures in the brain such as the putamen and caudate. A typical day at SMILE for Olof involves using the Hermes system to manually trace the 3D outline of the brain structures of interest, sometimes importing more images into the system (the material consists of 600 patients being scanned at intervals of a year or so) to work on. Even though Olof has studied some "computer science", he knows very little. He can navigate inside a Windows system (but not add a printer, for instance) and do some basic tasks on a Linux system (cd, ls -- grep is the limit of his knowledge). The Hermes system has GUI:s with buttons (and a unix platform which the average user needs not bother with, usually), which he handles expertly. Olof also knows how to run FSL and FreeSurfer, but cannot write scripts at all, on any platform.

Intermediate User

This user is similar to the Basic user but requires a little more flexibility in the way that they work and want to have more control over their environment. They may wish to extend existing workflows or make some changes to settings or the way in which they are configured.

Example Profile:

Michela is a PhD student at IRCCS-FBF with Dr. Frisoni since 2004. Her research area is the control, pre-processing and post-processing of diffusion tensor images (DTI) with specific tools for the analysis of the weighted images. A typical day for Michela involves the usage of the FDT (FMRIB's Diffusion Toolbox that is part of FSL system) to perform scanner pre-processing (e.g. averaging of multiple acquisitions, removal of images affected by large artifacts). These initial steps are usually done manually by Michela. Then, in order to correct stretches and shears due to current distortion in the images she runs different command line utilities. A probabilistic diffusion model of the corrected data is generated and finally a probabilistic tractography map is outputted for each image. Michela is an end user that is able to run programs from the command line shell and knows how to write bash scripts or simple programs in a language such as Matlab, Perl or Python on a range of different platforms.

Advanced User

This group of users wants full control over their work environment. They may wish to construct new tools or adapt existing ones for other purposes. It is likely that such users have a high degree of experience and probably a good understanding of computing techniques. The flexibility to do what they want is paramount to this group of users and they do not wish to be constrained in their work by the system. They may also perform tasks that are covered by the Basic and Intermediate user roles from time to time.

Example Profile:

Researchers at VUmc performed volume changes over time for the brain and the hippocampi of MCI patients. For this reason the hippocampi where manually outlined at baseline. The mask for the hippocampi were converted into Analyze to combine them with the original images. For the brain volume change and the change in hippocampi volume the brains on follow up were registered to BL. The Fluid algorithm of the dementia research group of London (DRG) was separated from its surrounding GUI and executed on the hippocampi and the whole brain. This resulted in a relational comparison between the brain volume change, the hippocampi volume change and the MMSE values of the used data. To perform this analysis a number of scripts were used. Some existing programs of other research centre were slightly modified and used in a fashion that better matched the used data.

Pipeline Developers

The developers of new research pipelines need to integrate them within the system in order to provide facilities to researchers. These are very technical users and share some similarities with the Advanced User. Given the cutting-edge nature of their work, it is likely that they may go beyond this profile and may require access to development and debugging tools. They will also require a good degree of flexibility from the system.

Example Profile:

Alex is a researcher with a long track record in the development and validation of image processing algorithms and pipelines for the quantitative analysis of brain MRI. Typically the development of novel algorithms relies on rapid prototyping and testing cycles, in which algorithm or parameter changes are implemented, executed, and their results observed. This requires relatively low-level, “hands-on” access to the system, with the ability to rapidly modify modules in a pipeline and/or modify the pipeline itself, and execute immediate tests. For thorough testing and validation though, an algorithm or pipeline may need to be run on tens or hundreds (or even more) cases; and/or collection of scans may need to be processed using a range of parameter values in order to establish optimal parameter values. This latter case requires the ability to process large numbers of scans and/or a set of scans with a possibly large range of pipeline configurations.

Image / Data Input Managers

Managers and administrators that work to upload and manage the data stored within the system.

Example Profile:

Anna is a PhD student at IRCCS-FBF with Dr. Frisoni since 2004. She is a key figure in the neuGRID Data Archiving and Computation Centers (DACS). Her main task will be to ensure the correct uploading of both images and data from the data collecting sites (DCS). She will have to maintain contact with the "data input managers" in the other neuGRID core labs in order to adopt procedures for standard data handling. Before the upload of each data set she will perform a quality control procedure. A key aspect of the data input Manager is to organize the available data for use by the neuGRID community providing different levels of access and maintaining data integrity. She will ensure proper data management and the saving of local mirror copies of data. Finally, she has a deep knowledge of MySQL because the data management will be conducted through the LORIS relational database system.

The data managers at VUmc are collecting data from various sites. From each site firstly a dummy run is requested. This dummy run is checked for image quality and commitment to the scan protocol (both by the data manager and a Radiologist). After one or more rounds to establish the best acquisition parameters, scan parameters are frozen. After the successful dummy procedure the site can send images to VUmc. Each scan is checked whether it fulfils the parameters agreed on at the dummy run, whether the image quality is good enough, whether the required patient information (random codes) are in the file header and for other quality indicators. After these checks the data can further be anonymized and will be sent to an image archive.

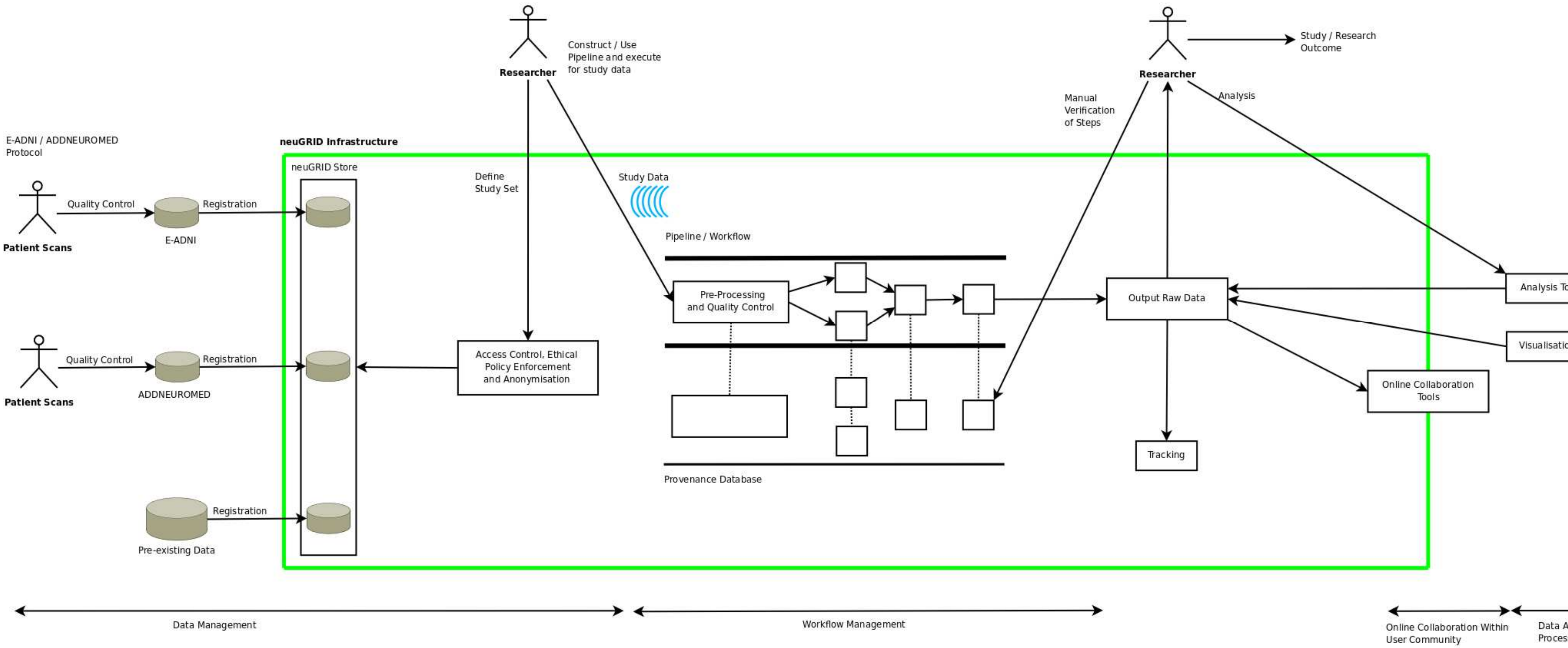
System Administrators

Technical support operators, who are responsible for installing, monitoring and generally administrating the system.

Example Profile:

Marco is a graduate in Mathematics and has started his PhD at IRCCS-FBF with Dr. Frisoni from December 2006. Marco will maintain and operate the neuGRID computer system and its network. He is usually charged with installing, supporting, and maintaining servers or other computer systems. This entails a good knowledge of operating systems and applications, as well as hardware and software troubleshooting. An important thing is that he must also have a detailed knowledge of the purposes for which people use the neuGRID platform and most importantly, he has strong problem solving skills. Marco has already demonstrated a blend of technical skills and responsibility.

4. Description of an End-To-End Example



This Section describes a potential end-to-end example of the use of the neuGRID platform. This sets the scene for the following Section in which the requirements are specified, by identifying the key stages in the operation of the infrastructure. In neuGRID, users may pass through the following stages to carry out their analysis on a set of images:

1. Data registration into the neuGRID Store, data management and quality control.
2. Data access, querying and browsing.
3. Workflow development, execution and management.
4. Validation of results and workflows using the provenance data.
5. Sharing workflows, histories and results.
6. Visualization of the results.

The first stage in the analysis cycle is to register images in the neuGRID store that have been collected from the hospital data acquisition system or have been imported from other research projects. For example, a new acquisition center may wish to make use of the neuGRID infrastructure to share data within the wider research community. Existing data is thus put through a process which enforces quality control, formatting and ethical compliance. Finally the data is integrated with the neuGRID standard data model, which enables other researchers to access it and carry out their research. As new data sets are acquired they go through an initial local quality control step before passing through the same system-wide quality control, formatting, ethical compliance and data model integration processes that the pre-existing data goes through.

The role of the second stage in the analysis process is to make the data browsable through automated querying tools. Therefore, an appropriate data access mechanism needs to be put in place. For example, a researcher may be interested in a rare form of a disease and wants to do a statistically meaningful analysis. Unfortunately the researcher's institution does not have sufficient images to make this possible. The user will interact with the system using the neuGRID store, to search for and to identify an appropriately large set of images from a group of hospitals that match the required criteria. At this stage access controls and ethical policies are fully enforced to protect sensitive data. The researcher then uses the system to submit the study set for analysis through a workflow.

Once the data has been imported into the neuGRID system and users are able to access and query it, they may like to carry out studies and data analyses to find results of interest. Workflow development is a methodology that can be used to represent user preferences for an automatic analysis of data and this is the third stage in the analysis chain. Users may create workflows and then execute them more quickly on the distributed resources provided by the Grid. The workflow development and execution is an important stage in the analysis life cycle in the neuGRID project. For example, a researcher may wish to run a comparative analysis using a study set of 3000 MRI scans stored in geographically distributed medical centres. It is important that the results are generated in a timely fashion as the researcher may have a number of different studies to carry out that week. The user may as the available data grows interact with the system to choose a study set of perhaps 3000 images, selects the pipeline or workflow through which the analysis will take place and starts the analytical process. Users do not have to use the workflows and study samples that have been developed previously, they can also construct new workflows. For example, a new image analysis methodology may be developed and a researcher may wish to build a workflow to run it. Using an interactive creation tool the user can construct a workflow and specify some initial settings. The user may also create a record which describes the workflow and gives other users information about its purpose and access controls. The system allows different versions of the workflow to be created, tested and released when they are ready for use by other researchers.

Simply creating and executing workflows is not enough on its own however. It is important that results, as and when required, should be reproduced and reconstructed using past information. The maintenance of the history of workflow specifications and their evolution between different stages is known as provenance and may help in the verification of results using audit trail information. For example, a workflow yields some surprising and possibly significant results. A researcher may wish to confirm that the results are accurate and identify any mistakes that may have been made. By analysing all the intermediary image sets and workflow execution logs the user is able to manually verify that the results were incorrect. It may be found that the error was due to a specific group of images interacting badly within the workflow. The user can then annotate the workflow so that other users are warned if they attempt a similar analysis.

Sometimes it may not be enough to reproduce the results. It may also be necessary to validate and, if required, reproduce the workflow that has been used to obtain the results. This makes users confident not only in the results that have been produced but also in the process that led them to generate these results. For example, a user may create a new workflow and run it on a test data set. At each stage in the execution of the workflow, the intermediary images or data are stored and a full provenance track is kept. After results have been produced, the user can examine the provenance to check that each stage of the analysis was completed correctly. The raw results can then be exported into the user's preferred analysis tool and the whole process can be added to the researcher's history for future reference. Initially the new workflow may produce some poor results during testing. The researcher therefore can inspect the logs of the workflow execution and locate the problem. The user can then interact with the system to make changes to the relevant settings and re-run the test study. This time the process may run correctly and meaningful results may be produced. Without the mechanism to validate workflows, it would not be possible to correct the process and generate accurate results. Therefore the validation of results and workflows are two significant requirements that should be addressed in the neuGRID system.

Once a workflow has been developed and verified, a user should be able to share it with other researchers in the field. The user may make the workflow available to a team or group of users from a partner institution or project. This will save time, effort and resources from other teams and they will not have to reinvent the pipelines which have been produced by their peers or partners. Users may also be able to share results and histories of their analysis processes. For example, a user might interact with the system to search existing studies and to compare, contrast and validate their results against research from other groups. This process helps the researcher to identify an error in their methodology and prevents them from making any embarrassing claims. A researcher could have carried out a similar study six months ago and may be worried that it too, might have been influenced by a similar error. The user can look up their research history and identify the appropriate study. The original process can be re-run on the original data set using the stored settings and pipeline configuration. This allows the researcher to confirm that the previous results were correct.

This abstract example has proven useful in describing the system components within neuGRID and to a wider audience. It is also important however, to understand how more detailed examples of real research processes can enrich this conceptual framework. The remainder of this Section will consider a real-world use-case in greater detail and show how this is useful in identifying potential requirements.

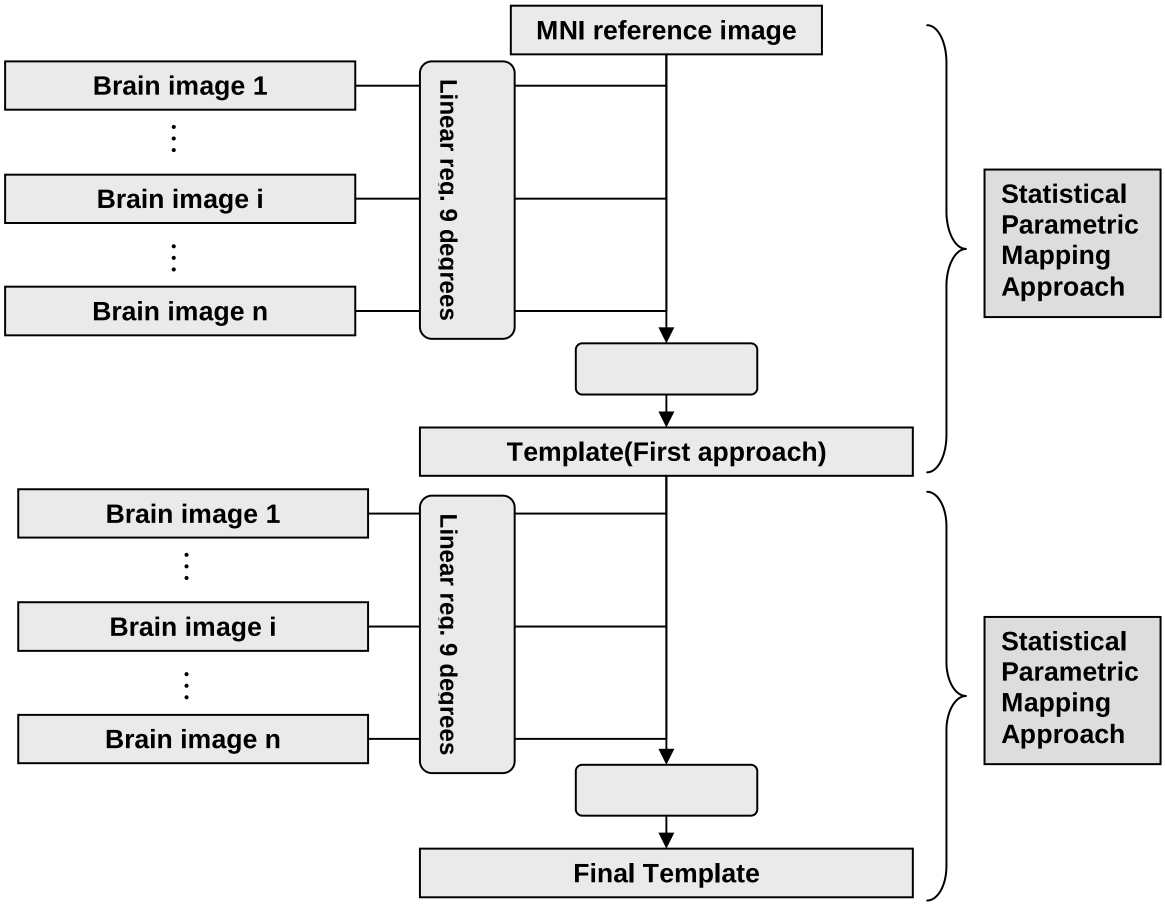


Figure 3: The VBM analysis process.

A Real Research Example

A VBM analysis of Alzheimers and Frontal Lobe Dementia patients is calculated using a template based on the given patients groups. Before the pipeline is used it is first tested on the multiplanar reformations (MPR) scans of Alzheimers and MCI patients of the ADNI data. When the pipeline appears to work correctly on the ADNI data the pipeline is used for a set of Alzheimers and Frontal Lobe Dementia patients that does not yet reside on neuGRID. At the end when the results looks promising the data and pipeline are share with the neuGRID community. This process is shown in figure 3.

The pipeline used consists of two parts:

- The creation of the template.

- The VBM analysis

1. Creation of the template.

The template creation is done by registering/aligning all scans to the MNI template (a template that comes with FSL in the Nifti file format) using 9 degrees of freedom. All images registered to this template are re-aligned together to create a new template. This new template is now used as template instead of the MNI template. A final template is build using the template of the first iteration.

2. The VBM analysis itself.

The VBM analysis is a regular VBM analysis on the data.

Steps necessary:

1. Select a list of MCI and Alzheimer patients of the ADNI dataset.

2. Register/Align (9 degrees of freedom) the selected scans to the MNI template which comes with FSL (in the Nifti file format).

3. Re-aligned all registered images to create the template.

4. Register/Align (9 degrees of freedom) the selected scans to the template generated in the first run and re-aligned the registered images to create the final template.

5. Perform a VBM analysis through the Statistical Parametric Mapping Approach on the selected scans using the template generated to compare MCI with Alzheimers.

6. Validate whether the pipeline works correctly.

7. Upload a new set of scans of Alzheimers and Frontal Lobe Dementia patients to be used as a private date set to neuGRID and use this scans to generate a template of these new dataset (using step 2 up to 4) and run a VBM analysis on the scans.

8. Make the uploaded dataset public.

9. Make the generate pipeline public.

Indicative User Requirements:

- The user should be able to generate a pipeline.

- The user should be able to test a pipeline with existing data.

- The user should be able to test a pipeline on their own data.

- A user has to be able to upload an initial template (e.g. MNI template in .mnc file format).

- It should be possible to convert the original Dicom files (of ADNI) Into Nifti.

- It should be possible to use the registration program Flirt (FSL) to register a set of images to a given template.

- It should be possible to perform image calculations (for example through the “avwmaths” program of FSL).

- It should be possible to perform quality control on the registrations.

- It should be possible to realign all registrations into a new image.

- It should be possible to use a generated image (first approach template) as a new template for registration.

- It should be able to perform a VBM analysis on the data.

- The user should be able to make its data public to a given community.

- The user should be able to make its pipeline public to a given community.

It is clear that detailed examples like this are useful in capturing a well rounded set of requirements. During requirements meetings, such examples have been presented to the requirements team by clinical researchers and the implications for neuGRID discussed. This has been of great benefit in compiling the requirements specification that is considered in the following Section.

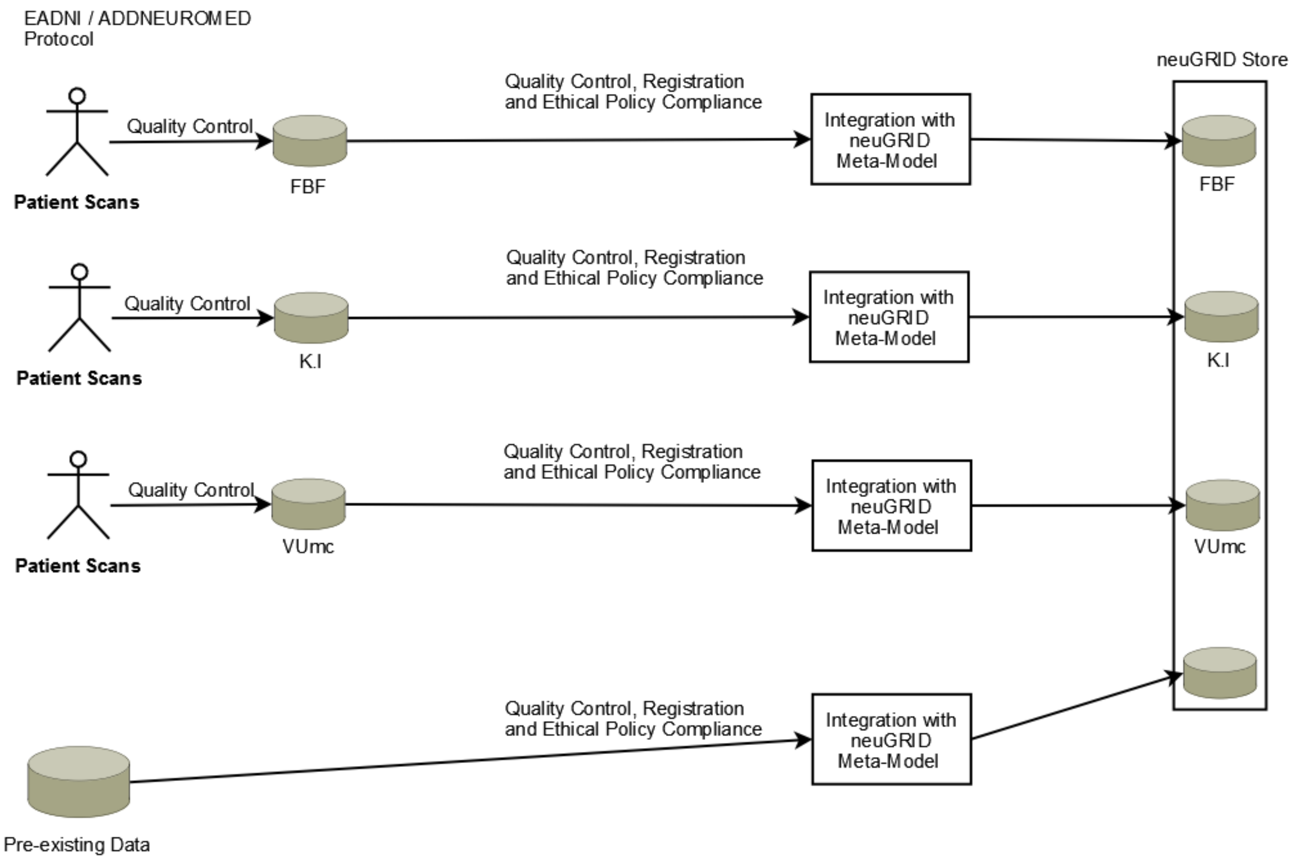
5. The User Requirements

Each segment of the user requirements specification begins with a Story. The relevant Use-cases that are contained within it are described and then broken down further to form individual user requirements. The numbering scheme allows the hierarchical relationships between Stories, Use-cases and Requirements to be easily traced. The high-level Stories are indicated by the S prefix and Use-cases are given the prefix U. Individual Requirements are denoted by the R prefix. The prioritization scheme focuses on Essential, Desirable and Optional requirements and is based on the variation of the MoSCoW technique [1] that was described in Section 1. Essential requirements are those which are absolutely vital to the production of a functional infrastructure. Desirable requirements are those that whilst not vital, would provide important functionality to users and a reasonable proportion of these should be implemented. Optional requirements are those that might be useful but don't fit into the previous two categories and will probably be the last to be implemented if time / budget allows.

Where E = Essential D = Desirable O = Optional.

S1. Data Registration into the neuGRID Store, Management and Quality Control:

A new acquisition center wishes to make use of the neuGRID infrastructure to share data within the wider research community. Existing data is put through a process which enforces quality control, formatting and ethical compliance. Finally the data is integrated with the neuGRID standard data model, which enables other researchers to access it and carry out their research. As new data sets are acquired they go through an initial local quality control step before passing through the same system-wide quality control, formatting, ethical compliance and data model integration processes that the pre-existing data goes through.



Indicative Use-cases:

U1.1 Perform quality control, ethical compliance (including appropriate anonymisation) and upload the new data sets into the system.

User Requirements:

R1.1.1	An interface is required for the upload of images and data sets into data stores. This should allow images to be imported into the "storage area" (drag and drop or lists of file names.)	D
R1.1.2	A basic QC viewer which allows comparison between different sets of images. It should be possible to show a DICOMDump of at least one image from each series to check for any information that has leaked through the anonymization steps.	E
R1.1.3	The ability to record the outcome of manual QC validation.	D
R1.1.4	A tool to delete images of inferior quality from a set.	E
R1.1.5	Provide software to those uploading data into neuGRID that enables the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and anonymization.)	E
R1.1.6	The ability to adapt to new ethical policies is necessary.	D
R1.1.7	Logs should be kept outlining exactly what was uploaded and by whom. A	E

	tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	
R1.1.8	A means of preventing duplicate data upload.	D
R1.1.9	The ability to visualize image(s) metadata (Acquisition Plane, Acquisition type and Field strength.)	D
R1.1.10	The ability to visualize image field inhomogeneities, subject position and artifacts.	D
R1.1.11	The possibility to perform corrective steps on images.	D
R1.1.12	Security and authentication of users should be enforced before images can be uploaded.	E
R1.1.13	Documentation should be provided that defines quality control and ethical compliance.	E
R1.1.14	The system should allow new anonymization methods to be applied as privacy standards evolve.	D
R1.1.15	Quality control should be done automatically where possible (number of images in series ranges of TE and TR values, pixel sizes, used coils etc.)	D
R1.1.16	It should be possible to do some manual quality control: visual inspection on Signal Noise Ratio, movement artifacts, inter-slice movement (for interleaved scanned series) etc. to assist the visual inspection process, an orthogonal view should be provided so that checks can be made for missing slices and artifacts between the slices.	E
R1.1.17	Something similar to the Linux/Unix strings command should be executed on at least one image in each series, to check for hidden patient information.	E
R1.1.18	If face scrambling is required, a surface rendering tool should be available and used to show the effect of the face scrambling.	O
R1.1.19	It should be possible to trace back data on neuGRID to the original data (perhaps at the core labs)	D
R1.1.20	When data is uploaded into the neuGRID storage area access restrictions should be specified.	E

U1.2 For pre-existing data, perform quality control, ethical compliance (including appropriate anonymisation), format standardisation and upload the data sets into the system.

User Requirements

R1.2.1	An interface is required for the upload of images and data sets into data stores. This should allow images to be imported into the “storage area” (drag and drop or lists of file names.)	D
R1.2.2	A Basic QC viewer which allows comparison between different sets of images is necessary.	E
R1.2.3	A tool for deleting images of inferior quality from a set is required.	e
R1.2.4	Provide software to enable the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and anonymization.)	E

R1.2.5	Logs should be kept outlining exactly what was uploaded and by whom. A tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	E
R1.2.6	A means of preventing duplicate data upload.	D
R1.2.7	The ability to visualize image(s) metadata (Acquisition Plane, Acquisition type and Field strength.)	D
R1.2.8	The ability to visualize image field inhomogeneities, subject position, artifacts.	D
R1.2.9	The possibility to perform corrective steps on images. The possibility to perform specific correction steps for each kind of acquisition: Gradwarp and Non-uniformity correction for MRI images. Realigning, unwarping and slice timing correction for fMRI images. Pre-processing steps for PET images with particular attention to the ADNI protocols (http://www.loni.ucla.edu/ADNI/Data/ADNI_Data.shtml .)	D
R1.2.10	Security and authentication of users before images can be uploaded or managed. There should be a certificate-based system to identify users and to perform access control.	E
R1.2.11	Documentation should be provided for performing appropriate quality control and ethical compliance on data sets.	E
R1.2.12	Provide software for format conversion.	D
R1.2.13	The system should allow new anonymization methods to be applied as privacy standard evolve.	D

U1.3 Standardize all uploaded data to comply with the neuGRID data model.

User Requirements

R1.3.1	Define a set of image data rules for neuGRID. A checklist should be provided which itemizes the image parameters that need to be removed or added to the set to make it comply with the neuGRID standard data model (e.g. date of birth missing in images XX)	E
R1.3.2	A form/tool to allow complementary information to be written to the uploaded set, perhaps with a reporting mechanism.	D
R1.3.3	The ability to remove parameters not included in neuGRID standard.	E
R1.3.4	The presence of an Image Data Archive web menu interface to establish the suitability of images before being uploaded/used in the neuGRID data store.	D
R1.3.5	Quality control needs to be done both locally (each centre should only upload high quality/usable images) and centrally (all uploaded images should undergo quality control with a unified criteria).	E
R1.3.6	Provide software to check if uploaded data sets conform to the neuGRID data model, and provide tools for conversion if required. There should be tools to convert a given data set to the neuGRID data model. This could be supplied to the core labs, neuGRID users or both.	D

U1.4   Manage stored data.

U1.4.1. Check and control system capacity.

User Requirements

R1.4.1.1.	The ability to control and manage the system through a simple graphical interface.	D
R1.4.1.2.	Provide tools and software to monitor system storage capacities and user quotas.	E
R1.4.1.2.1	Set quotas.	E
R1.4.1.2.2	Edit quotas.	E
R1.4.1.2.3	Delete quotas.	E
R1.4.1.2.4	Interact with users when storage reaches quota limits (possibly e-mail users with warnings.)	D

U1.4.2. Backup data.

User Requirements

R1.4.2.1	Manage backup data	E
R1.4.2.2.	Provide a means to backup data storage resources	E
R1.4.2.3	The ability to ask to users to save data not yet backed up, in an iterative way	D

U1.4.3. Perform system maintenance.

User Requirements

R1.4.3.1.	The possibility to follow a step-by-step predefined GUI-based wizard for the performance of system maintenance.	D
R1.4.3.2.	Provide a manual for performing system maintenance	D
R1.4.3.3.	A means of communicating periods of service downtime to users	D
R1.4.3.4.	Mechanisms for recovering from system failure should be provided.	D
R1.4.3.5.	A maintenance mode with the ability to take the system off-line for a period	D
R1.4.3.6.	A system dashboard could be provided to give an overall picture of status of the infrastructure at any given point in time.	D

U1.4.4. Query the stored data.

User Requirements

R1.4.4.1.	The ability to search for images based on subject and image-related criteria including: type of illness, date of birth, etc...	E
R1.4.4.2.	View images, form image collections (user collections) and download images in several file formats.	D
R1.4.4.3	The possibility to use two different research modalities: BASIC	D

	(Subject_ID, Sex, Age, Modality, Series description) or ADVANCED (Diagnosis, MMSE Score, GD Scale Score, TE, TR, Slice thickness and more) with different fields / levels of search.	
R1.4.4.4	The ability to store and manage user defined data collections.	D
R1.4.4.5	The querying language should be user friendly and querying interface should be operable by both technical and non-technical users.	E

U1.4.5. Search and view records of the quality control, anonymisation and format conversion processes that have been applied to data sets as they are entered into the system.

User Requirements

R1.4.5.1.	Search QC records for images that pass a given set of QC parameters.	D
R1.4.5.2.	View the QC records, sorted after parameter of choice (not just QC parameters.)	D
R1.4.5.3.	Search and view the record of format conversions that have been applied to an image/image set at upload.	D
R1.4.5.4.	The ability to display the QC results directly to the users with the subject image.	D
R1.4.5.5.	The anonymization process shouldn't be visible to the final user. This step could be done within the neuGRID consortium and should not be accessible (except for special privileges) by the end users of neuGRID.	E
R1.4.5.6.	neuGRID system images should be uploaded and stored as DICOM images. The image conversion process is something that has to be done during the different pipelines and, consequently, is something that could be checked by the user that uploaded the original image or a data input manager. In the case there isn't a DICOM definition for a given type of image (e.g. MEG images), data can be uploaded in the original file format (but should be fully anonymized). But there is no promise that all the workflows will work on it.	D
R1.4.5.7.	Provide provenance information related to modifications made to a data set. Provenance information may include modifications made for quality control, ethical compliance, anonymization, any format conversions that were necessary and related information.	E

U1.4.6. Handle potentially corrupted data sets.

User Requirements

R1.4.6.1.	A copy of the initial data should be kept safely.	E
R1.4.6.2.	No seriously corrupted or unusable data should remain in the neuGRID data store.	E
R1.4.6.3.	Provide tools to detect corrupted data sets, and to recover them as required.	D
R.1.4.6.4.	Once data has been made available to users, ensure that it remains unaltered (with the exception of legal requirements) even if it has some degree of corruption. Any improvements to the data are handled by making a new version available to users while still keeping the old version	E

	available to users. It should be clear to users which is the most up to date version.	
R1.4.6.5	Delete corrupted data	E
R1.4.6.6	Locate origin of corrupted data and handle the possibility of systemic problems	D

U1.4.7. Remove data from the system.

User Requirements

R1.4.7.1.	Select data sets or groups (R1.4.8.3) to be removed as defined within authorization levels.	E
R1.4.7.2.	An automatic report of removal to be sent to the uploaded site contact email.	D
R1.4.7.3.	Provide functionality to delete data sets from the data store.	E
R1.4.7.4.	Provide functionality to delete data sets from the user collections (R1.4.4.4.)	E

U1.4.8. Track / determine the history of a piece of data.

User Requirements

R1.4.8.1	Select a data set that fits a certain criteria.	D
R1.4.8.2	Generate an itemized list of when and by whom a data file in the set has been used in a workflow.	D
R1.4.8.3	Generate a list of which workflows have been applied to a data set, and sort sets into groups (group A had workflow X used on them, group B workflow Y, group C workflow X+Y.)	D
R1.4.8.4	To capture information on which kind of studies and analysis data has been used.	D
R1.4.8.5	To collect different clinical results in which some particular information was used.	D
R1.4.8.6	The possibility to define the roles of specific data in the AD pathology.	D
R1.4.8.7	The possibility to create a list of publications and view where neuGRID has played a part in the research.	D
R1.4.8.8	Data set specific provenance data should contain information related to the history of the piece of data.	E
R1.4.8.9	Allow a user to opt out of making tracking information public to other users for a given period	E

U1.5. Control the security of the stored data.

U1.5.1. Implement new and edit existing access control strategies.

User Requirements

R1.5.1.1.	Sort data sets into groups to which a certain access control is set.	E
R1.5.1.2	Edit the access control of a group of data (see 1.5.2.2.)	E

R1.5.1.3.	Sort and edit access control for a named individual/ or group of researchers. Provide tools to administrators to define user specific access control policies (at the project and individual levels.)	E
R1.5.1.4	A supervisor or responsible person should define both the access level and the policies that pertain to gaining access to the data stored inside neuGRID.	E
R1.5.1.5.	Provide secure access to data storage resources.	E
R1.5.1.6.	There should be a possibility to give individual users special access to a certain data set.	D

U1.5.2. Configure a set of ethical rules that relate to and govern the use of particular data sets.

User Requirements

R1.5.2.1.	Compose ethical agreements in writing which accompany a chosen data set/group.	E
R1.5.2.2.	Unless the relevant conditions are agreed to in writing by a user, an ethically restricted set cannot be used.	E
R1.5.2.3.	Log the users who use such a set (see 1.4.8.2) with a flag that they have agreed to be bound by the ethical agreement.	E
R1.5.2.4.	Define different agreements and set different rules for public, academic, research, and industrial neuGRID users.	D
R1.5.2.5.	All users should accurately provide requested information regarding who will use neuGRID data and the analyses that are planned.	E
R1.5.2.6.	All users should be requested to cite neuGRID as the source of their results in published work.	E
R1.5.2.7.	Provide tools to configure and define ethical rules applying on stored data sets.	D
R1.5.2.8.	There should be a description of the ethical rules (used informed consent for this data set etc.) for a given data set.	E

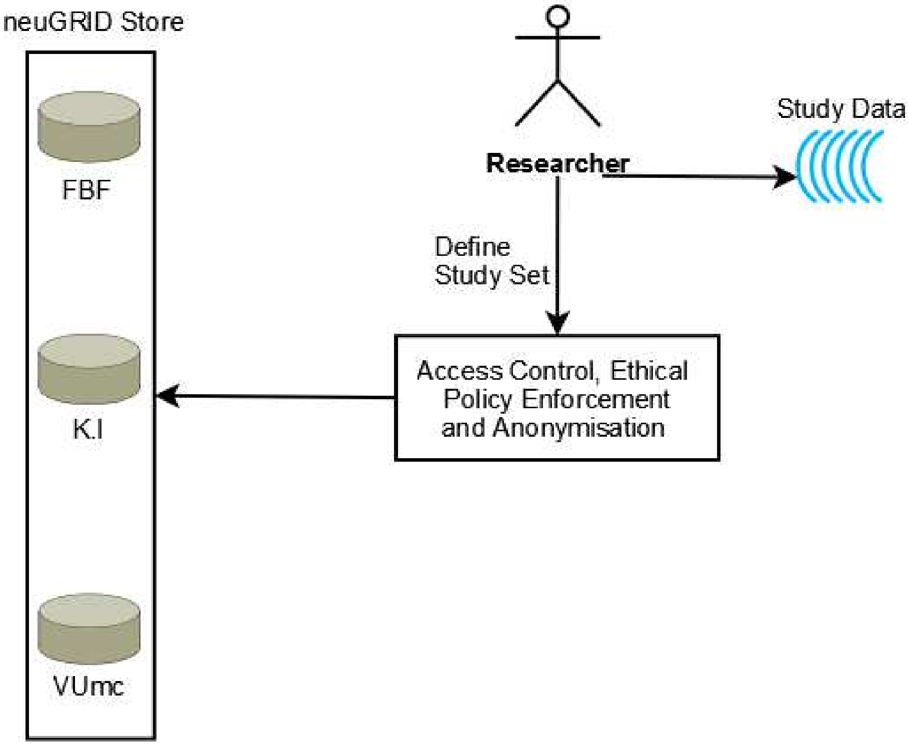
U1.5.3. Temporarily upload a private dataset to neuGRID.

User Requirements

R1.5.3.1	A user may wish to check whether an existing workflow also works for a private dataset which holds a rare subset of patients MRI scans. A way of temporarily uploading the private dataset to neuGRID is therefore required.	E
R1.5.3.2	The dataset in R1.5.3.1 should be accessible to existing pipelines, uploaded batch scripts (e.g. bash) or linux executables.	D
R1.5.3.3	A temporary dataset should be accessible for a given period of time and then be removed from the system.	D

S2. Data Access:

A researcher is interested in a rare form of a disease and wants to be able to do a statistically meaningful analysis. Unfortunately the researcher's institution doesn't have enough images to make this possible. The user interacts with the system using the neuGRID store, to search for and identify an appropriately large set of images from a group of hospitals that match the required criteria. At this stage access controls and ethical policies are fully enforced to protect sensitive data. The researcher then uses the system to submit the study set for analysis through a workflow.



Indicative Use-cases:

U2.1 Authenticate a user and enforce access control / ethical policies. E

User Requirements

R2.1.1.	Download neuGRID interaction tool bundle (unless web-based?). A signed usage agreement could be put in place.	E
R2.1.2.	Fill in requested neuGRID user data (institute, name etc) and store as “My profile” under “My account”.	E
R2.1.3.	The possibility to become part of a group of researchers (start a new group, be invited to an existing one).	D
R2.1.4.	Sensitive individual data sets will generate specific access agreements to be signed (1.5.2.2), which will be stored under “My account”	E
R2.1.5.	All the neuGRID users must be registered. They will fill an on-line form in which neuGRID staff will provide both a specific user_ID and a password.	E
R2.1.6.	Provide a global security model, which enables individual researchers from collaborating institutes to access other institutes’ data sets. There should be a certificate-based system to identify users and to perform access control.	E
R2.1.7.	Allow institutes to define local access control policies.	D
R2.1.8.	It is necessary to have access controls at the Project and Individual data set levels.	E

U2.2 Search for a group of images or data that matches a given criteria. E

User Requirements

R2.2.1.	Select a set of properties with which to generate data subsets from the database.	E
R2.2.2.	Generate feedback about the data sets (lists), which can be sorted after for instance QC parameters, type of camera etc.	D
R2.2.3.	Fine-tune the property set interactively.	D
R2.2.4.	Store the final property set under a label under “My account”/”My search property sets”.	D
R2.2.5.	Store the resulting data sets (lists of data generated by applying the property set on the data base) under “My account”/”My data sets”.	D
R2.2.6.	Provide a global search utility which searches distributed neuGRID data stores based on user defined criteria. Researchers should be able to search for a certain type of patients based on medical information as well on imaging information. For instance patients with Mild Cognitive Impairment with a given range of MMSE values which have had a T1 MPR sequence with a pixel size smaller equal 1.5 mm in each direction. The range of fields that can be used for searching should include:	E
R2.2.6.1.	Subject information: Subject Id, Sex, Research Group, Age, Weight.	E
R2.2.6.2.	Project specific information.	D
R2.2.6.3.	Clinical assessment information: MMSE Total Score, GDScale Total Score, Global CDR, Modified Hachinski Total Score, NPI-Q Total Score, Functional Assessment Questionnaire Total Score.	D
R2.2.6.4.	Study information: Study date, Visit.	E
R2.2.6.5.	Image information: Original (Choose Modality, Series Description, Acquisition type, Weighting, Slice Thickness, TE, TR, Acquisition Plane, Manufacturer, Field Strength) – Pre-processed (Series Description, Image File Type, Anatomic Structure, Tissue Type, Laterality, Registration/Space) – Post Processed (Series Description, Image File Type, Anatomic Structure, Tissue Type, Laterality, Registration/Space.)	E
R2.2.7.	Metadata will need to be stored for images to enable search functionality, this will identify images and the search will be performed on the metadata.	E

U2.3 Define and group the data that comprises a set for use in research. E

User Requirements

R2.3.1.	Combine labelled property sets into meta-sets.	E
R2.3.2.	Store the meta-sets under a label under “My account”/”My search property sets”.	D
R2.3.3.	Store the resulting data sets (lists) under a label under “My account”/”My data sets”.	D
R2.3.4.	Note prominently which property sets/meta-sets/data lists are bound by which ethical agreements.	D
R2.3.5.	Provide an interface which allows users to define groups of search results for research purposes.	E

U2.4 Visualize a research set. D

User Requirements

R2.4.1.	The ability to basically visualize data which includes:	E
R2.4.1.1.	Clinical biological data (e.g.: Tau, Ab1-42, P-Tau 181P , Tau/Ab1-42 P-Tau181P/Ab1-42) regarding the group of patients considered in a specific study.	E
R2.4.1.2.	Imaging data (DTI, 3dT1, T2, PD, fMRI, PET) regarding the group of patients considered in a specific study.	E
R2.4.2.	The provision of a summary of a user's research sets in list form under "My account"/"My data sets".	D
R2.4.3.	View condensed lists of clinical biological data and the imaging data set properties (44 images with a 3 T camera, 1445 of different patients in 1943 etc.) under "My account"/My data sets"	D
R2.4.4.	The possibility to generate some descriptive statistics about the parameters that have been chosen using a basic statistical package that is integrated within the infrastructure.	D
R2.4.4.1.	Provide appropriate visualization tools that are integrated in the search utility.	D
R2.4.4.2.	User should be able to visualize data sets with or without download.	D
R2.4.5.	An image viewer should be provided that provides a convenient browsing mechanism for users.	E

U2.5 Store a research set for future use. O

User Requirements

R2.5.1	A research set can be generated again using the saved property sets, or accessed from the saved data set lists.	O
R2.5.2	Each user has the possibility to view and download his/her own "User Collection" for local back up.	O
R2.5.3	Create a structured environment with directories and subdirectories where research results can be stored.	D
R2.5.4	Perform actions on stored datasets and images (moving, copying, deleting, renaming, add new images,…).	D
R2.5.5	Search utility should be able to export and save searches for future use.	O
R2.5.6	Saved searches should be easily accessible via an interface.	O
R2.5.7	It should be possible to store a query that was used to generate a certain set of data as a research set. (this is the property set mentioned in 2.2.4)	O

U2.6 Monitor data quality and allow users to give feedback regarding research sets. E

User Requirements

R2.6.1	A viewer should be provided, together with information regarding the quality assessment that was made by the researcher that uploaded the image.	E
R2.6.2	A "Comment on this image" facility: other users' comments might be visible under a special link in the data list.	O

R2.6.3	It should be possible to share specific research sets with some predefined groups giving information about research methods, data type and other issues.	D
R2.6.4	The possibility to express a judgment about the quality of data could be useful. Then, this judgment (e.g.: 4- Excellent; 3-Good; 2-Sufficient; 1-Bad) could be taken into account during the creation of a research set.	D
R2.6.5	Provide tools to determine and monitor data set quality.	D
R2.6.6	Software managing saved searches and research sets, should have the functionality to allow permitted users to post comments and give feedback on research sets of other users.	D
R2.6.7	The interface for saved searches will allow users to add or remove users from commenting on research sets.	O

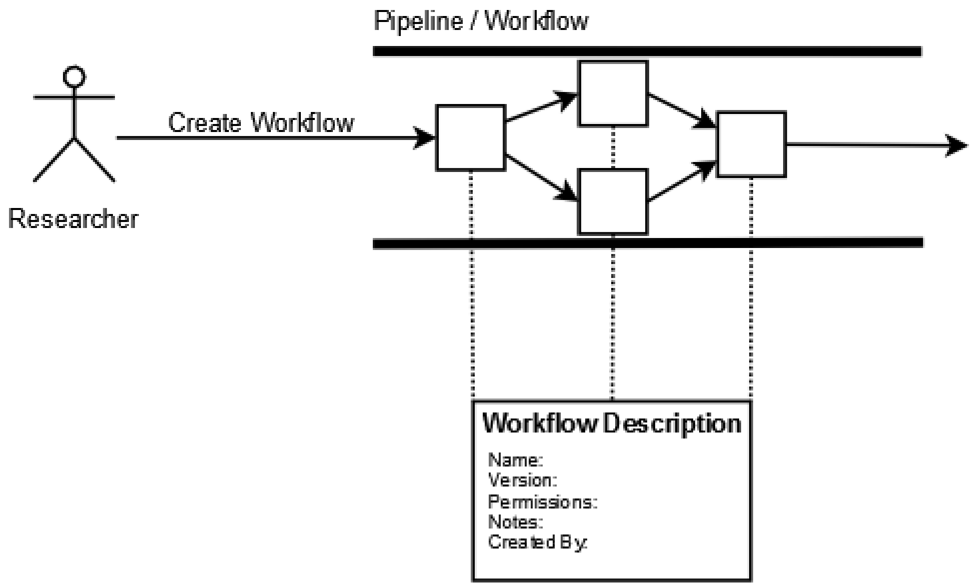
U2.7 Annotate a research set with useful information regarding the data that is contained within. O

User Requirements

R2.7.1	Comment the set lists in "my data sets" (comments seen when set lists viewed in 2.4.2)	O
R2.7.2	The information must be of a high-level, and will describe the type of a specific data user collection in an efficient way (for example: reporting the n° of patients, n° of AD, n° MCI and n° CTR, the Sequence type,…)	O
R2.7.3	Set "annotation" needs to be strictly controlled: users should have the possibility to submit annotations (e.g. comments on image quality, new measures, ...) but such annotations should be reviewed centrally and included only whenever they satisfy specific criteria. Finally, as measures are often protocol/scale-dependent the protocol/scale should be specified.	O
R2.7.4	An interface should be provided for the saving of searches and have the capability for users to provide annotations and metadata for saved research sets.	O

S3 Workflow Specification and Development:

A new image analysis methodology is developed and a researcher wishes to build a workflow to run it. Using an interactive creation tool the user constructs a workflow and specifies some initial settings. The user also creates a record which describes the workflow and gives other users information about its purpose and access controls. The system allows different versions of the workflow to be created, tested and released when they are ready for use by other researchers.



Indicative Use-cases:

U3.1 Construct, visualize, annotate and edit new workflows. E

User Requirements

R3.1.1	Select packages to use from categories of algorithms (e.g.: "statistical", "brain stripping").	D
R3.1.2	Construct a workflow by stringing together various algorithms and packages in a work area (drag and drop?), creating a series of connected boxes. Divisors, yes/no-alternatives for branching workflows may also be available in a graphical toolkit. This should be as simple as possible using a combination of arrows and nodes within a Graphical interface.	E
R3.1.3	Add comments next to each box in the workflow.	D
R3.1.4	The possibility to divide the workflow into logical units (the first three steps are brain stripping and have a pink background, next are five volumetric steps with a yellow background) with labels describing them.	O
R3.1.5	Visualize the workflow as a schematic boxed flow diagram (rough version can be seen in the work area, this should be printable as a PDF.)	E
R3.1.6	Edit the workflow by moving boxes around. A warning system saying "block A does not generate output that enables running block B directly after it" would be helpful.	D
R3.1.7	A possibility to edit input parameters in each algorithm (maybe an execution crashes because it requires a "4" instead of "2" in a given sub-process.)	E
R3.1.8	Save the workflow with a label under "My account"/"My workflows"/"Drafts".	E
R3.1.9	The provision of a command line scripting interface is necessary. It should be possible to upload a workflow as a Linux command script (e.g. bash) which calls a number of Linux executables residing on the grid or uploaded together with the script.	E
R3.1.10	The possibility to have a large range of pre-configured atomic modules from which new workflows can be created or to be able to integrate new functions efficiently.	D

R3.1.11	The opportunity to have a functional test-bed to validate efficiently workflows that are in construction (using trial appropriate reference data set already uploaded remotely and an efficient validating execution interface.)	D
R3.1.12	The ability to do a "debug error procedure" in order to show different actions that a final user can take in order to debug any validation or execution errors that could be encountered while using the Pipeline.	D
R3.1.13	The ability to preserve the order execution and the dependencies of the pipeline workflow.	D
R3.1.14	The ability to upload workflows generated within the major "workflow management systems" that are in use today (e.g.: the LONI pipeline, Scientific Kepler system and others.)	O
R3.1.15	The infrastructure should be platform-independent.	D
R3.1.16	The possibility to use images stored in the NeuGRID store to run a local analysis (e.g. in case a user wishes to run an analysis on NeuGRID images using software developed locally, which is not to be shared.)	D
R3.1.17	Provide a means of editing existing workflows.	E

U3.2 Work with draft workflows and use version control to manage them. D

User Requirements

R3.2.1	Open a workflow and edit it.	E
R3.2.2	When saving a previously existing draft workflow, automatically append version number and save under the workflow label under "My account"/"My workflows"/"Drafts" together with date edited. There should be a version control system for workflows that resides on neuGRID independent of their implementation (as a script file, program of graphical workflow.)	D
R3.2.3	The possibility to save the draft personal modules and workflow inside the neuGRID system.	D
R3.2.4	The possibility to open, drag and drop these draft modules quickly and easily.	D
R3.2.5	The possibility of creating pipelines by assembling existing workflows.	D
R3.2.6	Provide a repository for workflows with version control management.	D
R3.2.7	Provide user friendly interfaces, integrated with the workflow authoring software to upload/download/update workflows to the workflow repository.	D
R3.2.8	Changes between different versions of the software should be documented.	D

U3.3 Visualise, annotate and edit existing workflows. E

User Requirements

R3.3.1	Locate an existing workflow in the database of workflows that are accessible to all by selecting categories of algorithms that are desired to be included (this generates a list of workflows). The possibility to use all the features of the main programs in use today in the neuro-imaging field (e.g.: FSL, FREESURFER, SPM, MNI, ...)	D
R3.3.2	Select desired/interesting workflows and save under "My account"/"My workflows"/"Published".	D
R3.3.3	Provide a tool by which users can visualize existing workflows as in 3.1.5.	E
R3.3.4	Provide users the functionality to add annotations or comments to workflows	D

	as in 3.1.3	
R3.3.5	Provide users the capability to edit existing workflows as in 3.1.4, 3.1.6.	E
R3.3.6	Save as in 3.1.8 and 3.2.2 (to "Drafts").	D
R3.3.7	The opportunity to have a responsible person or group of people that maintain the main pipelines in use in the neuro-imaging field.	D
R3.3.8	The system should send email alerts to the final users when the workflow outputs are ready.	O
R3.3.9	There should be a way to assign a known bug list to a workflow.	D

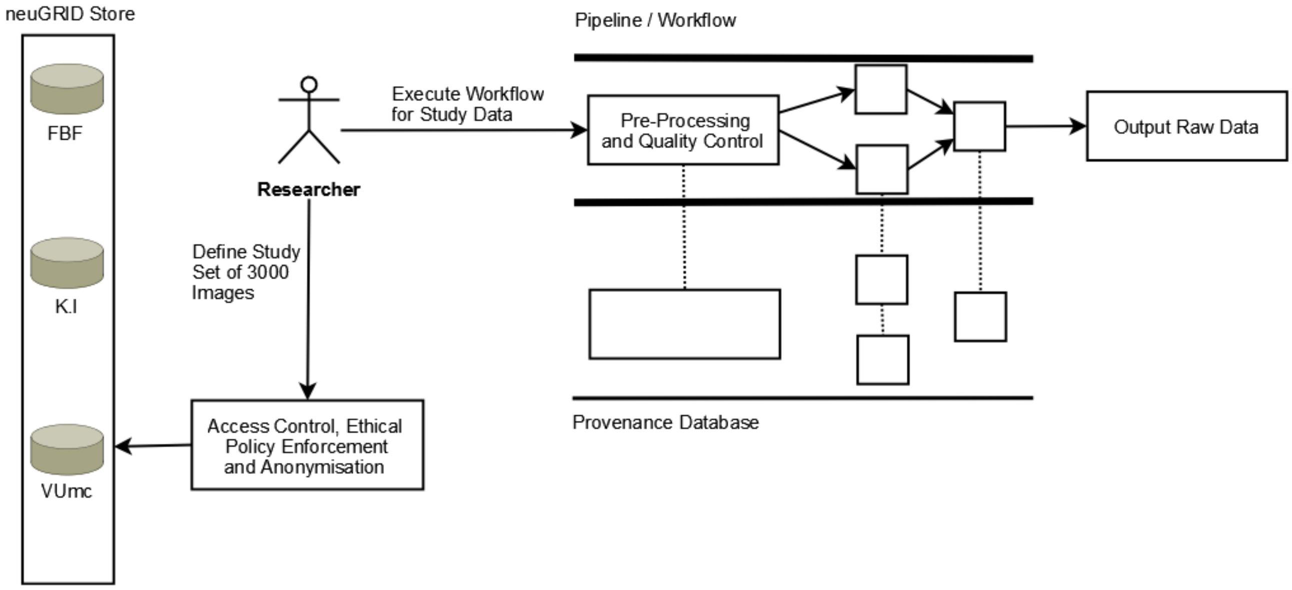
U3.4 Upload new packages, algorithms or analysis software to system for use in workflows. E

User Requirements

R3.4.1	Upload an algorithm or package (or draft) including source code; fill in what categories to store it under (3.1.1.)	E
R3.4.2	Make a workflow accessible and set access rights, fill in label name, builder name and institute, way to reference, terms of use (grant me a footnote, grant me authorship on any papers produced with the help of my flow) etc. See also use-case 7.	E
R3.4.3	The possibility to download an algorithm/package, to be able to tweak it oneself, by editing code or settings.	D
R3.4.4	Save the tweaked algorithms under My account/ My algorithms.	O
R3.4.5	If an algorithm is uploaded with the same name as an already existing one, automatically append version number (and ask the uploading researcher to enter a comment on what has changed.)	D
R3.4.6	If a package name changes, include source code dependencies (builds on package X by adding Y.)	D
R3.4.7	The upload of new packages/algorithms should be controlled centrally.	E
R3.4.8	The new tools to be uploaded should be rigorously tested and / or validated. Any new tool should be uploaded together with a specific documentation, including a user guide, algorithm explanations and appropriate references.	E
R3.4.9	The neuGRID "workflow management system" should be able to support and interface with many common languages classically used in the neuro-imaging field (like PERL, C++, Matlab, bash script and Python)	D
R3.4.10	Ensure and maintain architectural compatibility with the latest imaging software.	D
R3.4.11	Upload temporarily personal packages/software for specific studies. It should be able to upload a workflow as a Linux command script (e.g. bash) which calls a number of Linux executables residing on the grid or uploaded together with the script.	O
R3.4.12	Provide users with an interface for uploading new software packages, algorithms and analysis software subject to appropriate validation, which may then be used in future workflows.	D
R3.4.13	Provide users with a means of browsing existing uploaded algorithms, packages and analysis software to enable their use in workflows.	E

S4 Workflow Execution and Management

A researcher wishes to run a comparative analysis using a study set of 3000 MRI scans stored in geographically distributed medical centres. It is important that the results are generated in a timely fashion as the researcher has a number of different studies to do that week. The user interacts with the system to choose a study set of 3000 images, selects the pipeline or workflow through which the analysis will take place and starts the analytical process.



Indicative Use-cases:

U4.1 Search for existing research sets or define new groups of images and other information to be processed using the workflow. E

User Requirement

R4.1.1	Find a previously defined research set by selecting a data set under “My account”/”My data sets” (see 2.4.2, 2.2.5).	D
R4.1.2	Generate a new research set as in 2.5.1.	D
R4.1.3	A means to search publicly available research sets.	O
R4.1.4	The ability to edit research set access rights.	D
R4.1.5	To optimize performance, the images used for the analysis should also be present (if possible) locally in those nodes of the grid that don’t have a high level of bandwidth available. This is due to the fact that the transfer of a large number of images on the network will greatly increase the time to get the final results. Clearly, this is particularly true for a centre like FBF which is characterized by a connectivity of 10 Mbps.	D
R4.1.6	High redundancy and data availability is necessary.	D
R4.1.7	The possibility to integrate information provided by images and metadata with the definition of mathematical variables like vectors, list and structures. Define basic operations (like indexing, push, pop and length count) in order to perform command line operations on these objects containing images of interest.	D
R4.1.8	Provide a global search utility which searches distributed neuGRID data	D

	stores based on a user defined criteria.	
R4.1.9	Metadata should be present for each of the images in the system, this will identify images and allow them to be searched.	E
R4.1.10	User should be able to download data sets, if proper authentication has succeeded.	D
R4.1.11	Provide capability to the user to save a search and define it as a research set (see 2.5.1).	D
R4.1.12	Provide the capability of using saved data sets and research sets for input for workflows (see 4.2.1).	D

U4.2 Run, monitor and control the execution of a workflow. This would involve perhaps the ability to cancel, edit and restart an execution. E

User Requirements

R4.2.1	Apply a workflow to a data set, step by step or all at once.	D
R4.2.2	Output from the individual processes within the workflow is output to a progress window; also when a new process is started (process name_1: <output from 1 such as "calculating chi-2"> -- process name_2: <output> and so on).	O
R4.2.3	When the process stops (prematurely or not) the user can add comments at the bottom of the window.	O
R4.2.4	A GUI with buttons to stop, restart the workflow.	E
R4.2.5	The possibility to change the input parameters in a sub-process of the workflow (see 3.1.7.)	E
R4.2.6	The possibility to test a workflow on single images or subsets of the chosen data set (one could of course generate a new data set as in 2.2 but that is probably not as practical.)	D
R4.2.7	The ability to create, visualize and edit complex workflows in a convenient way.	E
R4.2.8	Simple way to monitor workflow execution.	D
R4.2.9	The user should have the possibility to check and perform quality control on each intermediate output.	E
R4.2.10	The ability to cancel, restart and debug workflows.	E
R4.2.11	The ability to share workflows with other researchers in the system.	D
R4.2.12	The possibility to provide the user with sample images for any kind of scan modality (MRI, fMRI, PET,…) in order to test his/her own workflow (or parts of it) using them and saving time uploading their own images.	D
R4.2.13	Extend workflow authoring environment to include basic execution functionality for:	D
R4.2.13.1	Starting the execution of a workflow.	D
R4.2.13.2	Providing an interface to monitor the status of a workflow.	D
R4.2.13.3	Provide ability to control the execution by cancelling or restarting the workflow.	D

U4.3 Search for and select the desired analysis pipeline from a set of existing workflows, edit settings if required and execute. E

User Requirements

R4.3.1	New workflow sharing should be controlled (only functioning and validated workflows should be uploaded and shared.)	O
R4.3.2	All the pipelines should be organized in a clear and efficiency way in order to make clear their use.	D
R4.3.3	The presence of a facility that allows users to query for specific modules. The Search function should return results drawn from the module's name, author list, citations, tags, description, and parameter fields.	E
R4.3.4	Most modules could have 2-3 required metadata parameters on them and several more optional parameters. The possibility to switch on these additional options simply clicking on the modules could be useful.	O
R4.3.5	Provide a service for users to upload workflows.	D
R4.3.6	Provide an interface to allow users to select pre-authored workflows and execute them with a new/existing research set.	E
R4.3.7	Provide the capability of editing an existing workflow, and executing it.	E

U4.4 Search the history of a given workflow to find a particular version of it for use in a specific piece of research. D

User Requirements

R4.4.1	The possibility to compare different versions of the same workflow.	D
R4.4.2	Each workflow is described by its components (viewed as in 3.1.5) highlighting the differences of each version and by its provenance (who built it, uploaded when, changed when), their new applications or improvements.	D
R4.4.3	Select "Unfold history" to see older versions of the workflow, meaning also versions where no one has changed the workflow per se but one of the packages/algorithms making up the workflow.	D
R4.4.4	An old workflow can then be selected by clicking on it (perhaps one needs to rebuild it.)	D
R4.4.5	Provide a service for uploading workflows.	D
R4.4.6	Provide capability to annotate history of a workflow.	D
R4.4.7	Provide an interface to search existing workflows and their respective history.	D
R4.4.8	The possibility to use a workflow as it was on a given date by entering the date of interest.	O

U4.5 Store a history of each workflow execution, research set and settings. Allow user annotation of such information. D

User Requirements

R4.5.1	The progress window output from 4.2.2 could be saved as a file, with a header consisting of a description of the data set used and the settings made for each (named) algorithm in the workflow (this may also be saved	D

	separately as a “workflow setup”, which lists all the parameters that were given to the workflow’s algorithms.) It may end with some user generated comments as in 4.2.3.	
R4.5.2	The possibility to efficiently retrieve some standardized workflows that are used in daily routine tests and procedures by different labs.	D
R4.5.3	Provide capability to annotate history of a workflow.	D
R4.5.4	Provide an interface to search existing workflows and their respective history.	D

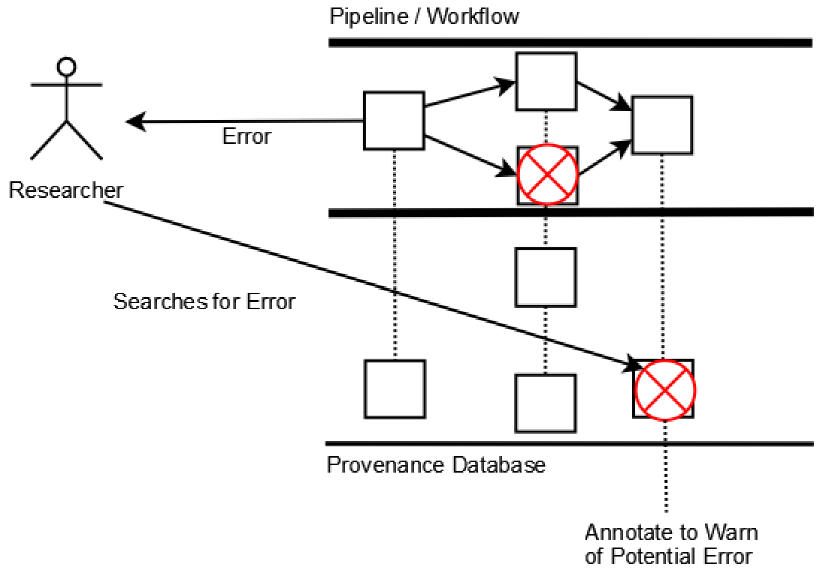
U4.6 Process raw output data by importing it into user specified analysis tools and toolkits. E

User Requirements

R4.6.1	Save the data set which has gone through the workflow with a label under “My account”/”My processed sets.”	D
R4.6.2	Allow transformation of data to suit the needs of some analysis tools. Provide conversion tools for toolkits compatibility	O
R4.6.3	Build a range of common analysis tools into the infrastructure (but licensing may prevent this).	O
R4.6.4	Save analyzed data under “My account”/”My analyzed sets” with links connecting each analyzed set to the corresponding processed set (by actual linking or by naming convention).	D
R4.6.5	Save the workflow setup and the progress window output under each processed set.	O
R4.6.6	Define a simple drag and drop interface in order to connect the raw data outputted to the next workflow as input.	D
R4.6.7	Define a simple click interface in order to add raw files.	D
R4.6.8	Allow user to use data in their desired format.	O
R4.6.9	Provide notifications to users on the status of a pipeline.	
R4.6.10	Upon completion of a workflow, allow users to download raw data output.	E
R4.6.11	Provide the necessary functionality to export the raw output into the desired data analysis software.	O
R4.6.12	Enable some basic analyses using inbuilt statistical tools such as those provided by FSL.	D

S5. Validation of Workflows:

A user creates a new workflow and runs a test data set using it. At each stage in the execution of the workflow, the intermediary images or data are stored and a full provenance track is kept. After results are produced, the user examines the provenance to check that each stage of the analysis was completed correctly. The raw results are then exported into the user’s preferred analysis tool and the whole process is added to the researcher’s history for future reference. Initially the new workflow produces some poor results during testing. The researcher therefore looks at the logs of the workflow execution and locates the problem. The user then interacts with the system to make changes to the relevant settings and re-runs the test study. This time the process runs correctly and meaningful results are produced.



Indicative Use-cases:

U5.1 Validate a workflow using provenance data to locate points of failure in it. E

User Requirements

R5.1.1	Load the workflow into a variant of the work area in 3.1.2. The order of the boxes and layout of the workflow cannot be changed, but by clicking on each box the appropriate set of provenance data can be viewed: lists of images that can be put into the viewer (possibility to compare images, from different provenance sets and within sets) and numerical output data (chi-2 etc). Also the workflow setup can be viewed.	D
R5.1.2	To check for errors try to execute the workflow.	E
R5.1.3	If any errors are found it could be useful that a dialog box will pop up listing all the errors found in the workflow.	D
R5.1.4	During the validation of the workflow the outputted data should be visualized.	D
R5.1.5	Provide user capability to browse provenance data collected from execution of workflows.	E
R5.1.5.1	he interface should be user friendly, and allow for browsing of process by process provenance data.	D
R5.1.5.2	Provenance data should link to the intermediary output produced during execution of the workflow.	E
R5.1.6	There should be a way to report outliers and to be able to check intermediate data for such indicators (this would be very useful!)	D

U5.2 Search for an appropriate reference data set to automatically verify the output from a workflow and create a test set for a newly developed analysis workflow. D

User Requirements

R5.2.1	When someone has developed a workflow, at upload they can be asked to specify a reference data set to be associated with the workflow. This	D

	reference set can then be found as a property of the workflow ("Test with reference data set?").	
R5.2.2	Generate a new data set for testing old or new workflows.	O
R5.2.3	The possibility to add a reference data set to the workflow's properties, even for those who have not constructed the original workflow.	O
R5.2.4	It could be useful to be able to choose from a number of predefined reference data sets (for example: one characterized by 3D volumetric images, fMRI images, DTI images, PET images,…) comprising 3-5 images of reference.	D
R5.2.5	Provide a tool to users to browse and select reference data sets for execution with a workflow.	O
R5.2.6	Provide the user with a comparative analysis of the output produced to output in the reference data set.	D

U5.3 Report errors in workflow execution. E

User Requirements

R5.3.1	The error report button in the 4.2.4 GUI sends an email to the appropriate place with information regarding workflow setup, workflow name and data set properties. It should also generate an error number for convenience and easy follow up.	D
R5.3.2	Inevitably, some of the instances of a module could fail sometimes and the execution of the module could be stopped denoting the failure. In this case, it could be useful to have a viewer box in which all the failed instances of the module could be shown. With this information neuGRID users could diagnose the problems encountered during the execution of a workflow and hopefully solve them.	D
R5.3.3	Provide notification for critical events during an execution of a workflow.	E

U5.4 Annotate workflows with version information and a full change history. D

User Requirements

R5.4.1	Add a comment to a workflow which can be seen under "Unfold history" in 4.4.3.	O
R5.4.2	The possibility to make a stratification of the different usage of each specific workflow.	O
R5.4.3	Useful to understand which are the most used values by the scientific community to analyze different type of acquisitions through different workflows.	O
R5.4.4	Provide a repository for workflows with version control management.	E
R5.4.5	Provide user friendly interfaces, integrated with the workflow authoring software to upload/download/update workflows to the workflow repository.	D
R5.4.6	The repository should have the functionality to add annotations from user about versions of the workflow. For a workflow that resides on neuGRID a versioning mechanism (version control system) should be present including a description of the differences between versions.	D
R5.4.7	The repository should log and document historical changes to a workflow.	D

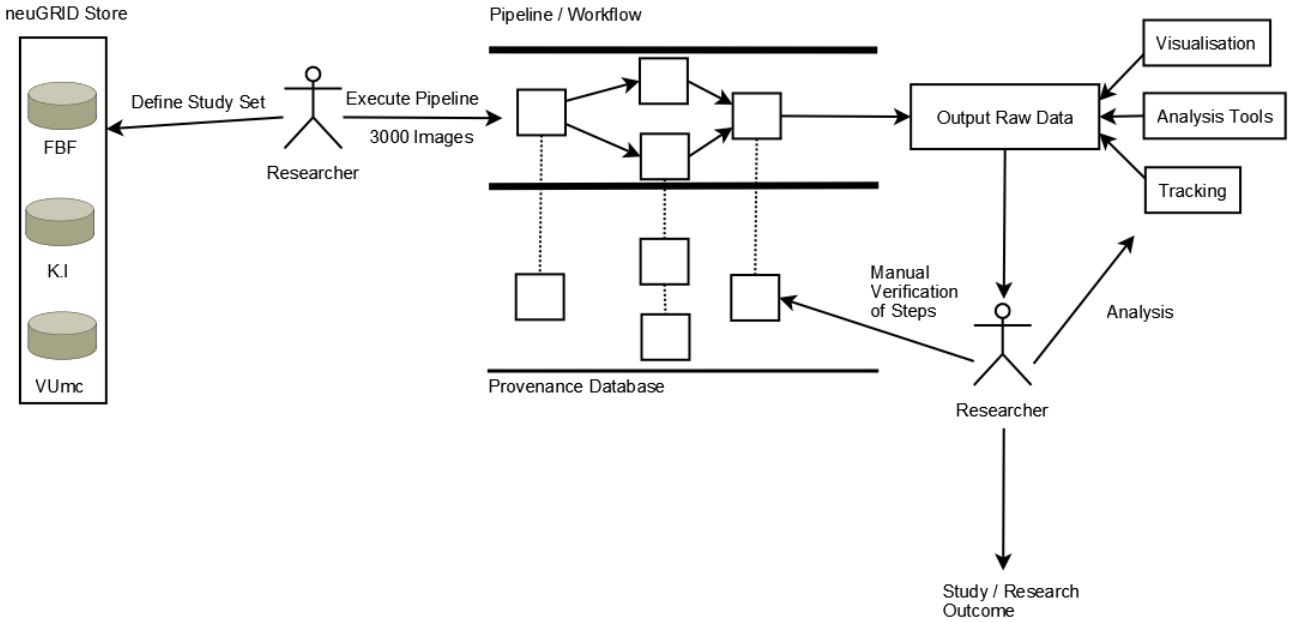
U5.5. Annotate a workflow with information regarding the settings that are appropriate in different situations. D

User Requirements

R5.5.1	As 5.4.	D
R5.5.2	The possibility to summarize the most useful and appropriate parameters used in the workflows through synoptic tables.	O
R5.5.3	Ease of reference parameters.	O
R5.5.4	Provide capability to users to annotate workflows, providing information about settings of the workflow in different execution contexts.	D

S6. Validation of Results using Provenance Data:

A workflow yields some surprising and possibly significant results. A researcher wishes to confirm that the results are accurate and identify any mistake that has been made. By analyzing all the intermediary image sets and workflow execution logs the user is able to manually verify that the results were incorrect. It is found that the error was due to a specific group of images interacting badly within the workflow. The user annotates the workflow so that other users are warned if they attempt a similar analysis.



Indicative Use-cases:

U6.1 Capture a complete provenance of workflow execution. E

User Requirements

R6.1.1	Store intermediary execution steps.	E
R6.1.1.1	The workflow processes and the workflow setup should be saved (see 4.5.1.)	D
R6.1.1.2	The intermediate, processed files (provenance data) are saved as well, according to the structure Run number/Process number/files, e.g.	D

	Run5/Process2 (Brain strip)/file_no5. It is useful to be able to save the output from more than one run at a time, for comparison. (upper limit could be 10 runs), and can be found under “My data sets”/”Provenance data.”	
R6.1.1.3	Provide explanation and details of any errors that occur and report possible causes.	E
R6.1.1.4	Send potential errors to the neuGRID administrators if the workflow resides on the neuGRID infrastructure.	D
R6.1.2	Keep a full record of all intermediary images and data.	E
R6.1.2.1	The tree structure in 6.1.1.2 should also include a summary of any numerical data that is produced (chi-2 etc).	D
R6.1.2.2	Store error messages and be able to navigate through them.	E
R6.1.2.3	Post problems on a neuGRID technical forum.	O
R6.1.2.4	All intermediary data and related logs should be stored during workflow execution.	E
R6.1.2.5	Provenance data should be presented in a user friendly fashion.	D

U6.2 Carry out a manual verification of all the stages that have been processed during workflow execution using the data stored in the provenance database. E

User Requirements

R6.2.1	The possibility to import selected files from 6.1.1.2 into the appropriate step in a given workflow using the GUI in 4.2.4 and analysis with toolkits.	D
R6.2.2	Taking the output from a single step in a workflow and looking at it in the viewer/seeing the full text output (see 5.1.1).	D
R6.2.3	The possibility to recall single workflow functions that were used at each processing step using a simple command line interface.	E
R6.2.4	Provide the user with an interface to browse a completely executed workflow, process by process, and enable user to view all relevant intermediary output and logging information.	E

U6.3 Search the provenance database for interesting information. D

User Requirements

R6.3.1	The possibility to check image anomalies through a specific link.	O
R6.3.2	Compare the outputted raw files with information from saved workflows (if any exists.)	O
R6.3.3	Provide a querying interface to the provenance store.	D

U6.4 Perform statistical analysis on the provenance data. O

User Requirements

R6.4.1	Check for additional abnormalities passed over in silence (weak field inhomogeneities, ringing artifacts etc.)	O
R6.4.2	Compare the results obtained with reference images.	D
R6.4.3	Allow user to export/download provenance data to their computer system	D

	and perform statistical analysis on it.	
R6.4.4	Results to be saved as a property of the provenance data set. Files go under Run number/Process number/User-selected analysis set name/files.	D
R6.4.5	Provide any necessary format conversion tools.	O

U6.5 Annotate a workflow with information regarding potential errors and incompatibilities. D

User Requirements

R6.5.1	As 5.4.1. The workflow comments should not be unstructured text inputs but sorted into categories (General, Errors, Inconsistencies, Comment made by <name>.)	O
R6.5.2	When an error occurs a red colour could be used to depict that the workflow has a problem.	D
R6.5.3	Provide a user with the capability to annotate an item in the provenance store.	O

U6.6 Search a list of common errors that are known to affect a given workflow. D

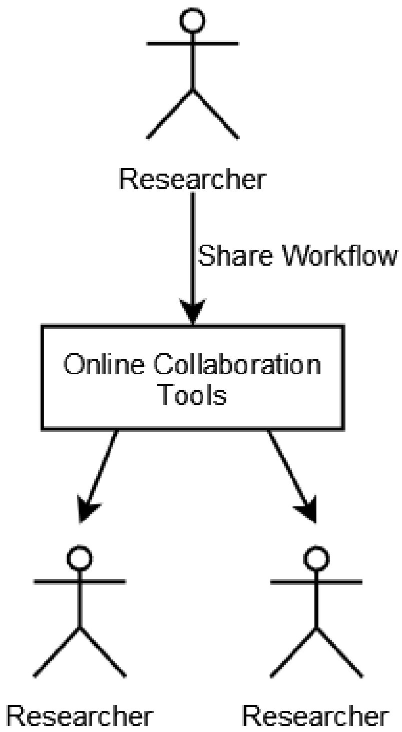
User Requirements

R6.6.1	Search and display workflow comments regarding errors. Also, automatically save and compile statistics on which errors crop up during the run of a certain workflow.	D
R6.6.2	See neuGRID technical on-line forum.	O
R6.6.3	Create a frequently asked question sections for each workflows.	O
R6.6.4	Provide the user with information about common errors that severely affect a workflow.	D

S7. Online Collaboration:

Sharing Workflows

A new workflow has been developed and verified. A user decides that it might be useful to share it with other researchers in the field. The user makes the workflow available to a team from a partner institution in a given project. The other team is delighted as it saves them some time and effort. The research that is produced acknowledges the contribution of the workflow it becomes an established research method more quickly than would have been possible otherwise.



Indicative Use-cases:

U7.1 Control access to workflows and allow users to create and manage groups of collaborators with whom they wish to share workflows. E

U7.1.1 Publish a new stable workflow within a group or wider community. E

User Requirements

R7.1.1.1	A researcher on uploading / publishing a workflow, should be able to define access permissions for individuals or groups.	E
R7.1.1.2	Provide a service where users can upload and share workflows.	E
R7.1.1.3	Authorization should identify users uniquely.	E
R7.1.1.4	A specific group member should be able to share a workflow with other members of that group.	D

U7.1.2 Publish a developmental workflow for testing and evaluation within a group or wider community. D

User Requirements

R7.1.2.1	As in 7.1.1.1 but the uploading researcher can also tag the workflow as under development, which will show up clearly in connection to the workflow name, when searched for and viewed (as in 3.1.5).	D
R7.1.2.2	Allow users to create virtual groups within the service	O

U7.1.3 Leave feedback regarding the effectiveness of workflows. O

User Requirements

R7.1.3.1	See 6.5.1. Workflows under development may have more categories to comment under.	O
R7.1.3.2	Users should be able to provide feedback and comment on workflows that have been created by other users	O

U7.1.4 Provide information on the authors of a workflow and suitable references for referencing them in scholarly work. O

User Requirements

R7.1.4.1	See 3.4.2.	O
R7.1.4.2	Users should provide details about themselves in their accounts, this information should be associated with workflows they upload.	O

U7.1.5 Share an interesting workflow with a colleague. O

User Requirements

R7.1.5.1	See 3.4.2.	O
R7.1.5.2	Users should be allowed to share a workflow with another specific user of the service, irrespective of groups.	D

U7.1.6 Reproduce the results of another research team. D

User Requirements

R7.1.6.1	To reproduce results exactly, one needs the workflow and the data set it was applied to (i.e. the search property set). This could be accomplished by having research teams enter their publications into an article database in neuGRID. When entering the publication reference, the team could be asked to supply the names of the used workflows and a copy of the search property set. This could be a requirement, which if not signed denies access to the neuGRID project.	D
R7.1.6.2	Provide users the capability to download a workflow, import to their workflow execution environment and compare with results of previous executions.	D
R7.1.6.3	There should be a way to reuse a given dataset on a given workflow.	E

U7.1.7 Certification of workflows. D

User Requirements

R7.1.7.1	A policy is needed for who can certify workflows and the process by which certification takes place in neuGRID.	D
R7.1.7.2	Provide tools for certifying a workflow according to 7.1.7.1.	O
R7.1.7.3	An administrator should manage and control the certification process	D

	including requesting information regarding the data/software/workflows as needed.	

U7.2 Request a given research community to develop a new workflow for a particular task or add a feature to an existing method. O

User Requirements

R7.2.1	Supply contact details when uploading a flow as in 3.4.2.	D
R7.2.2	Provide a category of tags that can be added to a workflow and allow users to request new features.	O
R7.2.3	Share new workflow features with the research community according to the permissions of the various groups.	D
R7.2.4	After a certain period of exclusivity workflows of a given quality should be shared with the entire neuGRID community.	O
R7.2.5	Provide functionality within the service to enable users to request a workflow for a particular task from other users.	O

U7.3 Get assistance with the construction of a complex workflow from the wider research community. O

User Requirements

R7.3.1	Provide a category of tags that can be added to a workflow and allow users to request assistance from more experienced researchers.	O
R7.3.2	Possibly a discussion forum could be connected to workflows with different tags (this might ease the pressure on the comments section of the workflows.)	O
R7.3.3	Provide forum type functionality within the service, in order for users to discuss and solicit advice from other users about construction of workflows.	O
R7.3.4	A user guide is necessary.	D
R7.3.5	A technical glossary should be created.	D

U7.4 Request and interact with a consultant to construct a workflow. O

User Requirements

R7.4.1	NeuGRID-affiliated application specialists and consultants manning a built-in helpdesk would be helpful.	O
R7.4.2	Organize a mailing list for workflow constructors so that important messages can be circulated.	D
R7.4.3	Provide functionality to interact with volunteer specialist users to construct new workflows.	O
R7.4.4	Specialist users may be given a special account, and may at their choice be listed for easy discovery.	O

U7.5 Identify weaknesses in workflows and act as a community to resolve them quickly. O

User Requirements

R7.5.1	Provide a forum type capability to discuss specific workflows, in case problems arise, see 7.3.2.	O
R7.5.2	Create a neuGRID community in which users can see which modules are the most used, the statistic concerning the different workflows, the efficiency or malfunction of these workflows, and other various topics of interest for the users.	O

U7.6 Rapidly deploy advanced techniques and use online collaboration for training purposes. O

User Requirements

R7.6.1	Supplement 7.3.2 with a more general notice board.	D
R7.6.2	Organize some webinar meetings.	O
R7.6.3	Provide a modular service, so that new features can be added to enhance collaboration between users.	E

U7.7 Keep commercially or otherwise sensitive workflows private and secure. E

User Requirements

R7.7.1	See 1.5.	E
R7.7.2	Identify different levels of security and confidentiality within the grid.	E
R7.7.3	Access can be restricted to one person only. Provide users with the capability to restrict workflows from public access.	E

Sharing Results and Histories

A user interacts with the system to search existing studies and to compare, contrast and validate their results against research from other groups. This process helps the researcher to identify an error in their methodology and prevents them from making any embarrassing claims. The researcher did a similar study six months ago and is worried that it too, might have been influenced by a similar error. The user looks up their research history and identifies the appropriate study. The original process can be re-run on the original data set using the stored settings and pipeline configuration. This allows the researcher to confirm that the previous results were correct.

Indicative Use-cases:

U7.8 Create groups of researchers with similar / overlapping interests. O

User Requirements

R7.8.1	Ad “Research interests” to the profile data entered in 2.1.2.	O
R7.8.2	Similar interests could be assessed during user registration through a simple	O

	and fast questionnaire as checklists or free, searchable text.	
R7.8.3	Allow users to create virtual groups within the service.	O

U7.9 A user can search their and public histories for a specific workflow execution and allow it to be re-run on the original or new data. D

User Requirements

R7.9.1	The workflow setups from 4.5.1 can also be saved and searched under "My workflow setups". They should be coupled to the data set processed with these criteria (or the search property set used to generate the data eventually processed by the workflow in that specific setup).	O
R7.9.2	A tag can be set specifying that the workflow setup is public. Then a search for a specific workflow execution can also include all public workflow setups (and their connected processed data sets/search property sets).	O
R7.9.3	Provide a simple query interface through which past executions can be discovered.	D
R7.9.4	Functionality should be provided for the uploading and updating of specific workflow execution instances, and upload/link to relevant output data and workflow specification.	O
R7.9.5	A user should be able to download an archived workflow specification and select new/existing data set for processing.	D

U7.10 Allow records of common mistakes to be searched to improve the training of new researchers. O

User Requirements

R7.10.1	Create a FAQ like page for "Frequent errors", which might give tips on how to check that the output from block A is possible to use as input in block B in a workflow.	O
R7.10.2	Create a user comment database where researchers can note mistakes they made and how to avoid them.	O
R7.10.3	Log the error outputs and compile statistics on their frequency. The helpdesk (7.4.1) could help connect the error outputs to the mistakes creating them.	O
R7.10.4	Save a certain amount of bad workflows executions that should be useful as examples for the new users of the neuGRID platform.	D
R7.10.5	Make a validation test on the main tools that neuGRID provides.	D
R7.10.6	Provide/maintain a documentation of common workflow mistakes	O
R7.10.7	There should be a way to store non-standard patients, typical examples etc for a given workflow in a separate store.	O

The remainder of this Section considers in greater detail, the image processing and statistical analysis tools that are in frequent use by the research centres within the neuGRID project. The purpose of this is to provide an increased level of detail regarding individual software packages and tools. It was generally felt that including these within the earlier requirements specification might complicate what is presented and so this dedicated segment has been created. In D6.1 it was proposed that the brain imaging tools broadly fall into the following categories:

Image Processing

This includes a library of image processing algorithms focused on manipulating the source images so as to ultimately extract features of the images which can be used in a variety of statistical analyses. Examples of this include, the spatial normalization and blurring operations necessary to perform so-called Voxel-Based Morphometry (VBM); the registration and surface extraction algorithms used in the estimation of cortical thickness (e.g., the CLASP algorithm [8]); or the registration and voxel classification algorithms used in brain tissue identification. Some real-world examples include:

Example 1: FSL/TBSS

A recently released version of FSL, with the latest version of TBSS, was needed to be installed. TBSS was then run on 61 scans, each of which was under 1MB in size. TBSS required CPU intensive calculations to be run on each pair of scans. Therefore, 3,721 jobs, which took about 30 minutes each, needed to be run. Combining the output of the 3,721 jobs was easily performed on a single machine after the completion of all the jobs.

Example 2: FLUID

For an Alzheimer's study, 180 pairs of MRI scans needed to be compared to detect how the shape of the brain changed over time. The specialized software Fluid, which was available as a Linux executable, was used to compare the pairs of scans. The FSL routines BET and FLIRT were used to pre-process the scans before Fluid. Each pair of scans took about 6 hours of CPU time to process. Each individual scan was about 23MB in size.

Statistical Analysis

This includes any statistical analyses performed on data, be they “raw” (unprocessed) source data or more likely data processed using the library of methods covered under “Image processing.”

Statistical Analysis Example:

In order to locate structural changes within the hippocampal formation in AD patients of mild to moderate severity, several analysis steps are performed. First of all, the hippocampal formation has to be isolated by manually tracing on MRI coronal slices. Then 3D parametric surface mesh models are generated from the manually segmented hippocampal tracings. The models of each individual’s hippocampi are analyzed to estimate the regional specificity of hippocampal volume loss in AD compared to controls. To assess hippocampal morphology, a medial curve is automatically defined as the 3D curve traced out by the centroid of the hippocampal boundary in each image slice. The radial size of each hippocampus at each boundary point is assessed by automatically measuring the radial 3D distance from the surface points to the medial curve defined for individual’s hippocampal surface model. Shorter radial distances are typically used as an index of atrophy. Atrophy maps are visualized on 3D models of the hippocampal formation. The percent change relative to control and the associated P value describing the significance of group differences are plotted onto the model surface at each point of the hippocampus using a colour code to produce statistical maps. Overall P values are computed for the maps of the left and right hippocampal formation using a permutation testing approach. Permutation methods measure the distribution of features in statistical maps that would be observed by accident if the subjects were randomly assigned to groups and provide a P value for the observed effects that is corrected for multiple comparisons.

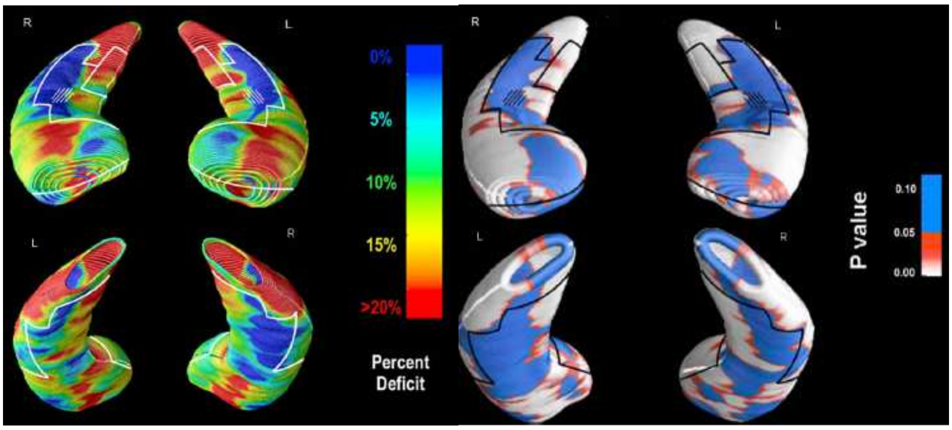


Figure 4: Topography distribution of atrophy in the hippocampal formation of AD compared to elderly controls. On the right is shown the hippocampal volume loss corresponded to a P value ranging from 0.10 to 0.00

The following table lists the pipeline tools that are in frequent use by the research centres within the neuGRID project.

Institute	PIPELINE TOOLS/ OPERATIONS	Analysis Tools
VUMC (See APPENDIX A)	• FSL Tools (FMRIB Software Library): Flirt, Fnirt, FDT, FAST, BET, FEAT, Melodic (visualization tool), Siena, XSiena. • MNI (BIC Tools & Software): N3. • BIRN (Gradiant Non-Linearity Distortion Correction): Gradient non-linearity. • DRG Fluid. • Generic:	SPM (Statistical Parametric Mapping)

	• Image calculations (adding subtracting, multiplying etc..) • Morphological operations on images • File format conversion	
KI (See APPENDIX B)	CIVET Pipeline (Pipeline 3) (CIVET Pipeline), FSL, Brainvoyager, Matlab, AFNI, E-prime and Statistica.	Hermes (Hermes Medical) (Pipeline 1 and Pipeline 2)
FBF (See APPENDIX C)	• FSL Tools: FMRIB's Diffusion Toolbox FDT 2.0, Melodic, BET Function, Flirt, Fnirt, Siena, Melodic • MNI Tools: Display, Register, • Brainsuite • LONI functions (LONI Software Tools): Dual_warpe_warpcurve, Decoder_blend_all, mk_seg16bit, mk_gray, add_gray_to_inflated_LEFT1, add_gray_to_inflated_RIGHT1, pmap_apeVSctrl, make_UVL_*; 1st_script_tracer_avg_DIAG; 2nd_script_core_test_L_DIAG; 2nd_script_core_test_R_DIAG; Pmap_DistCore_DIAG • MRIcro (MRIcron) (visualization) • Quanta 6.1 • IdeALab Tools (IdeALab) • Image Conversion software: MRIconverter; dcm2nii; nii2ana, fslchfiletype, … New Promising Tools FBF is evaluating: 3D Slicer, VTK, Freesurfer, MIPAV, NA-MIC Kit components, MED-INRIA, BrainVoyager, BrainMAP	SPSS, SPM, (Statistical Parametric Mapping) Matlab R2008a R

Common Pipeline Tools

Pipeline Tools	**INSTITUTE**
FSL Tools	VUMC, FBF
MNI tools	VUMC, KI, FBF
Generic Operations (Image conversion, calculations)	FBF, VUMC

Common Analysis tools

Analysis tool	**INSTITUTE**
SPM	VUMC, FBF

6. Non-Functional Requirements

Several non-functional requirements have been identified in the previous Section. These relate especially to user interface and certain performance requirements. This Section specifies the remaining non-functional requirements that have been collected.

NR1 The ability to manage restricted bandwidth by submitting processing intensive standalone computing jobs to the closest high-performance grid node.

NR2 Data should be archived and made available locally. In this way we will ensure that the time for image processing will be quick and avoid any problem during the sending of images from one node to another. Another important linked aspect could be to move queries from a centre to another, rather than large quantities of data.

NR3 The system should be designed so that it could be scaled up when new centres, in the future, will join the project.

NR4 The ability to add unspecified future functionalities and modules to the image analysis processing architecture. This is because neuGRID must be able to evolve and support new capabilities.

NR5 The system should be capable of c future analysis packages integration.

NR6 The neuGRID platform architecture should be accessible through and compatible with all major operating systems (Mac OS, Unix/Linux and Windows.)

NR7 An online help facility should be incorporated into the system.

NR8 The system should provide a significantly reduction in the execution response time of major workflows. The reduction factor should be x10, x100.

NR9 A service level agreement of at least 95% should be put in place and improved where possible.

NR10 Users should be equipped with the best possible space of storage and compute resources.

NR11 The system should be compatible with g-Lite middleware.

NR12 The system must be fully compatible with and be able to make use of grid resources that run a range of different middleware other than g-Lite.

NR13 Components must not be employed that couple the system to any particular middleware or software package.

NR14 The neuGRID infrastructure should have a sustainable post-project plan. Different access policies may be employed due to partner differences (Scientists should be guaranteed by an open source service while Pharmaceutical companies should pay a fee.)

NR15 The infrastructure must be fully compliant with Service Oriented Architecture principles and design methodologies.

NR16 The medical services that are produced are to be generic and fully reusable.

NR17 Users should "feel at home" recognizing all the functions and options usually used in the different tools of analysis. As a consequence, all the analysis functions used through the packages incorporated in neuGRID and, already in use inside the neuro-community, must be present. In this way the users should be able to install and operate inside the neuGRID platform with little or no training.

NR18 Where users construct new pipelines themselves, an appropriate disclaimer should be put in force regarding potential errors.

7. Mapping Requirements to Project Tasks

This Section has been created primarily for workpackage leaders and developers within the project and suggests an initial mapping of requirements to specific areas. Relevant tasks are also listed and described. This process will continue to evolve as the project progresses and it is difficult to be completely accurate that this stage. It will be a clear aim of the revision of the user requirements specification at the end of year two to update and finalise this information with input from clinical researchers and developers.

Work package number WP5 **Start date or starting event:** M1
Work package title *Brain Imaging Services Provision*
Activity Type SVC

User Requirements

R1.1.1	An interface is required for the upload of images and data sets into data stores. This should allow images to be imported into the "storage area" (drag and drop or lists of file names.)	D
R1.1.2	A basic QC viewer which allows comparison between different sets of images. It should be possible to show a DICOMDump of at least one image from each series to check for any information that has leaked through the anonymization steps.	E
R1.1.3	The ability to record the outcome of manual QC validation.	D
R1.1.4	A tool to delete images of inferior quality from a set.	E
R1.1.5	Provide software to enable the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and Anonymization.)	E
R1.1.6	The ability to adapt to new ethical policies is necessary.	D
R1.1.7	Logs should be kept outlining exactly what was uploaded and by whom. A tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	E
R1.1.8	A means of preventing duplicate data upload.	D
R1.1.9	The ability to visualize image(s) metadata (Acquisition Plane, Acquisition type and Field strength.)	D
R1.1.10	The ability to visualize image field inhomogeneities, subject position and artifacts.	D
R1.1.11	The possibility to perform corrective steps on images.	D
R1.1.12	Security and authentication of users should be enforced before images can be uploaded.	E
R1.1.13	Documentation should be provided that defines quality control and ethical compliance.	E
R1.1.14	The system should allow new anonymization methods to be applied as privacy standards evolve.	D
R1.1.15	Quality control should be done automatically where possible (number of images in series ranges of TE and TR values, pixel sizes, used coils etc.)	D
R1.1.16	It should be possible to do some manual quality control: visual inspection on snr, movement artifacts, inter-slice movement (for interleaved scanned series) etc. to assist the visual inspection process, an orthogonal view should be provided so that checks can be made for missing slices and artifacts between the slices.	E
R1.1.17	Something similar to the Linux/Unix strings command should be executed on at least one image in each series, to check for hidden patient information.	E
R1.1.18	If face scrambling is required, a surface rendering tool should be available	D

	and used to show the effect of the face scrambling.	
R1.1.19	It should be possible to trace back data on neuGRID to the original data (perhaps at the core labs)	D
R1.1.20	When data is uploaded into the neuGRID storage area access restrictions should be specified.	E
R1.2.1	An interface is required for the upload of images and data sets into data stores. This should allow images to be imported into the "storage area" (drag and drop or lists of file names.)	D
R1.2.2	A Basic QC viewer which allows comparison between different sets of images is necessary.	E
R1.2.3	A tool for deleting images of inferior quality from a set is required.	E
R1.2.4	Provide software to enable the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and anonymization.)	E
R1.2.5	Logs should be kept outlining exactly what was uploaded and by whom. A tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	E
R1.2.6	A means of preventing duplicate data upload.	D
R1.2.7	The ability to visualize image(s) metadata (Acquisition Plane, Acquisition type and Field strength.)	D
R1.2.8	The ability to visualize image field inhomogeneities, subject position, artifacts.	D
R1.2.9	The possibility to perform corrective steps on images. The possibility to perform specific correction steps for each kind of acquisition: Gradwarp and Non-uniformity correction for MRI images. Realigning, unwarping and slice timing correction for fMRI images. Pre-processing steps for PET images with particular attention to the ADNI protocols (http://www.loni.ucla.edu/ADNI/Data/ADNI_Data.shtml .)	D
R1.2.10	Security and authentication of users before images can be uploaded or managed. There should be a certificate-based system to identify users and to perform access control.	E
R1.2.11	Documentation should be provided for performing appropriate quality control and ethical compliance on data sets.	E
R1.2.12	Provide software for format conversion	D
R1.2.13	The system should allow new anonymization methods to be applied as privacy standard evolve.	D
R1.3.1	Define a set of image data rules for neuGRID. A checklist should be provided which itemizes the image parameters that need to be removed or added to the set to make it comply with the neuGRID standard data model (e.g. date of birth missing in images XX)	E
R1.3.2	A form/tool to allow complementary information to be written to the uploaded set, perhaps with a reporting mechanism.	D
R1.3.3	The ability to remove parameters not included in neuGRID standard	E
R1.3.4	The presence of an Image Data Archive web menu interface to establish the suitability of images before being uploaded/used in the neuGRID data store.	D
R1.3.5	Quality control needs to be done both locally (each centre should only	E

	upload high quality/usable images) and centrally (all uploaded images should undergo quality control with a unified criteria).	
R1.3.6	Provide software to check if uploaded data sets conform to the neuGRID data model, and provide tools for conversion if required. There should be tools to convert a given data set to the neuGRID data model. This could be supplied to the core labs, neuGRID users or both.	D
R1.4.4.1.	The ability to search for images based on subject and image-related criteria including (type of illness, date of birth etc.).	E
R1.4.4.2.	View images, form image collections (user collections) and download images in several file formats.	D
R1.4.4.3.	The possibility to use two different research modalities: BASIC (Subject_ID, Sex, Age, Modality, Series description) or ADVANCED (Diagnosis, MMSE Score, GD Scale Score, TE, TR, Slice thickness and more) with different fields / levels of search.	D
R1.4.4.4.	The ability to store and manage user defined data collections	D
R1.4.4.5.	The querying language should be user friendly and querying interface should be operable by both technical and non-technical users.	E
R1.4.5.1	Search QC records for images that pass a given set of QC parameters	D
R1.4.5.2.	View the QC records, sorted after parameter of choice (not just QC parameters.)	D
R1.4.5.3.	Search and view the record of format conversions that have been applied to an image/image set at upload.	D
R1.4.5.4.	The ability to display the QC results directly to the users with the subject image.	D
R1.4.5.5.	The anonymization process shouldn't be visible to the final user. This step could be done within the neuGRID consortium and should not be accessible (except for special privileges) by the end users of neuGRID.	E
R1.4.5.6.	neuGRID system images should be uploaded and stored as DICOM images. The image conversion process is something that has to be done during the different pipelines and, consequently, is something that could be checked by the final users as output. In the case there isn't a DICOM definition for a given type of image (e.g. MEG images), data can be uploaded in the original file format (but should be fully anonymized). But there is no promise that all the workflows will work on it.	D
R1.4.5.7.	Provide provenance information related to modifications made to a data set. Provenance information may include modifications made for quality control, ethical compliance, anonymization, any format conversions that were necessary and related information.	E
R1.4.6.1.	A copy of the initial data should be kept safely.	E
R1.4.6.2.	No seriously corrupted or unusable data should remain in the neuGRID data store.	E
R1.4.6.3.	Provide tools to detect corrupted data sets, and to recover them as required.	D
R.1.4.6.4.	Once data has been made available to users, ensure that it remains unaltered (with the exception of legal requirements) even if it has some degree of corruption. Any improvements to the data are handled by making a new version available to users while still keeping the old version available to users. It should be clear to users which is the most up to date version.	E
R1.4.6.5.	Delete corrupted data.	E

R1.4.6.6.	Locate origin of corrupted data and handle the possibility of systemic problems	D
R1.4.7.1.	Select data sets or groups (R1.4.8.3) to be removed as defined within authorization levels.	E
R1.4.7.2.	An automatic report of removal to be sent to the uploaded site contact email.	D
R1.4.7.3.	Provide functionality to delete data sets from the data store.	E
R1.4.7.4	Provide functionality to delete data sets from the user collections (R1.4.4.4.)	E
R1.4.8.1.	Select a data set that fits a certain criteria.	
R1.4.8.6.	The possibility to define the roles of specific data in the AD pathology.	D
R1.5.2.1.	Compose ethical agreements in writing which accompany a chosen data set/group.	E
R1.5.2.2.	Unless agreed to in writing, an ethically restricted set cannot be used.	E
R1.5.2.3.	Log the users who use such a set (see 1.4.8.2) with a flag that they have agreed to be bound by the ethical agreement.	E
R1.5.2.4.	Define different agreements and set different rules for public, academic, research, and industrial neuGRID users.	D
R1.5.2.5.	All users should accurately provide requested information regarding who will use neuGRID data and the analyses that are planned.	E
R1.5.2.7.	Provide tools to configure and define ethical rules applying on stored data sets.	D
R1.5.2.8.	There should be a description of the ethical rules (used informed consent for this data set etc.) for a given data set.	E
R1.5.3.1	A user may wish to check whether an existing workflow also works for a private dataset which holds a rare subset of patients MRI scans. A way of temporarily uploading the private dataset to neuGRID is therefore required.	E
R1.5.3.2	The dataset in R1.5.3.1 should be accessible to existing pipelines, uploaded batch scripts (e.g. bash) or Linux executables.	D
R1.5.3.3	A temporary dataset should be accessible for a given period of time and then be removed from the system.	D
R2.3.3.	Store the resulting data sets (lists) under a label under “My account”/”My data sets”.	D
R2.3.4.	Note prominently which property sets/meta-sets/data lists are bound by which ethical agreements.	D
R2.3.5.	Provide an interface which allows users to define groups of search results for research purposes.	E
R2.4.1.	The ability to basically visualize data which includes:	E
R2.4.1.1.	Clinical biological data (e.g.: Tau, Ab1-42, P-Tau 181P , Tau/Ab1-42 P-Tau181P/Ab1-42) regarding the group of patients considered in a specific study.	E
R2.4.1.2.	Imaging data (DTI, 3dT1, T2, PD, fMRI, PET) regarding the group of patients considered in a specific study.	E
R2.4.2.	The provision of a summary of a user’s research sets in list form under “My account”/”My data sets”.	D
R2.4.3.	View condensed lists of clinical biological data and the imaging data set properties (44 images with a 3 T camera, 1445 of different patients in 1943 etc.) under “My account”/My data sets”	D
R2.4.4.	The possibility to generate some descriptive statistics about the parameters	D

	that have been chosen using a basic statistical package that is integrated within the infrastructure.	
R2.4.4.1.	Provide appropriate visualization tools that are integrated in the search utility.	D
R2.4.4.2.	User should be able to visualize data sets with or without download.	D
R2.4.5.	An image viewer should be provided that provides a convenient browsing mechanism for users.	E
R2.5.1	A research set can be generated again using the saved property sets, or accessed from the saved data set lists.	O
R2.5.2	Each user has the possibility to view and download his/her own “User Collection” for local back up.	O
R2.5.4	Perform actions on stored datasets and images (moving, copying, deleting, renaming, add new images,…).	D
R2.5.5	Search utility should be able to export and save searches for future use.	O
R2.5.6	Saved searches should be easily accessible via an interface.	O
R2.5.7	It should be possible to store a query that was used to generate a certain set of data as a research set. (this is the property set mentioned in 2.2.4)	O
R2.6.1	A viewer should be provided, together with information regarding the quality assessment that was made by the researcher that uploaded the image.	E
R2.6.2	A “Comment on this image” facility: other users’ comments might be visible under a special link in the data list.	O
R2.6.3	It should be possible to share specific research sets with some predefined groups giving information about research methods, data type and other issues.	D
R2.6.4	The possibility to express a judgment about the quality of data could be useful. Then, this judgment (e.g.: 4- Excellent; 3-Good; 2-Sufficient; 1-Bad) could be taken into account during the creation of a research set.	D
R2.6.5	Provide tools to determine and monitor data set quality.	D
R2.6.6	Software managing saved searches and research sets, should have the functionality to allow permitted users to post comments and give feedback on research sets of other users.	D
R2.6.7	The interface for saved searches will allow users to add or remove users from commenting on research sets.	O
R2.7.1	Comment the set lists in “my data sets” (comments seen when set lists viewed in 2.4.2)	O
R2.7.2	The information must be of a high-level, and will describe the type of a specific data user collection in an efficient way (for example: reporting the n° of patients, n° of AD, n° MCI and n° CTR, the Sequence type,…)	O
R2.7.3	Set “annotation” needs to be strictly controlled: users should have the possibility to submit annotations (e.g. comments on image quality, new measures, ...) but such annotations should be reviewed centrally and included only whenever they satisfy specific criteria. Finally, as measures are often protocol/scale-dependent the protocol/scale should be specified.	O
R2.7.4	An interface should be provided for the saving of searches and have the capability for users to provide annotations and metadata for saved research sets.	O
R6.6.2	See neuGRID technical on-line forum.	O
R7.4.1	NeuGRID-affiliated application specialists and consultants manning a	O

	built-in helpdesk would be helpful.	
R7.4.2	Organize a mailing list for workflow constructors so that important messages can be circulated.	D
R7.4.3	Provide functionality to interact with volunteer specialist users to construct new workflows.	O
R7.4.4	Specialist users may be given a special account, and may at their choice be listed for easy discovery.	O

Tasks Identified

T5.3 Grid implementation (M6-18)

This task aims to demonstrate proof-of-principle that the LORIS database implementation and image analysis pipeline software operates transparently over the grid architecture. During the second half of Phase 1 and the first half of Phase 2, P2 NE and P4 MAAT will set up and conduct a series of tests which will evaluate and compare the results of the gridified LORIS system against the current, non-gridified implementation. P2 NE and P4 MAAT will develop a report describing these tests and their findings.

T5.4 Business Models (M24-32)

With input from CO1 FBF, P2 NE will assess existing business models that can be applied for the brain imaging services to be provided to each target community. As a first step, this implies that P2 NE and CO1 FBF will establish neuGRID operating costs for additional projects, in terms of incremental hardware and human resources, and train the selected model(s) through the user-communities. This task should lead to an appropriate model and its adoption for post-project industrial exploitation. The deliverable is a proposal which will include cost models to different end-user communities which will keep neuGRID viable.

T5.5 Services Provision (M6-36)

Implement the advanced community specific services which address the end-users requirements, including
but not restricted to:

- Brain imaging databasing with data security/redudancy
- Brain image processing (classification, volumetrics, cortical thickness)
- Clinical image databasing (test battery, clinical measures, genetics)
- Quality control of brain image or clinical data
- Statistical analysis of processed brain images, clinical data or joint data

The vast majority of this implementation work will be conducted by NE. NE will request input from MAAT and P3 UWE where needed; specifically relating to the interface between the end-user services and the underlying Grid infrastructure.

Work package number WP6 **Start date or starting event:** M9
Work package title *Distributed Medical Service Provision*
Activity Type SVC

User Requirements

R1.1.3	The ability to record the outcome of manual QC validation.	D
R1.1.5	Provide software to enable the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and anonymization.)	E
R1.1.6	The ability to adapt to new ethical policies is necessary.	D
R1.1.7	Logs should be kept outlining exactly what was uploaded and by whom. A tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	E
R1.1.14	The system should allow new anonymization methods to be applied as privacy standards evolve.	D
R1.1.19	It should be possible to trace back data on neuGRID to the original data (perhaps at the core labs)	D
R1.2.4	Provide software to enable the anonymization of data sets. The ability to easily anonymize the principal image fields defined by neuGRID ethical committee (if they are not already treated in some previous steps) ensuring that no identifiable patient information crosses the network (Images Scrambling and anonymization.)	E
R1.2.5	Logs should be kept outlining exactly what was uploaded and by whom. A tool to save the set (list of files) which will be uploaded (in case uploaded is delayed or interrupted for some reason.)	E
R1.2.13	The system should allow new anonymization methods to be applied as privacy standard evolve.	D
R1.4.1.1.	The ability to control and manage the system through a simple graphical interface.	D
R1.4.4.1.	The ability to search for images based on subject and image-related criteria including (type of illness, date of birth etc.).	E
R1.4.4.3.	The possibility to use two different research modalities: BASIC (Subject_ID, Sex, Age, Modality, Series description) or ADVANCED (Diagnosis, MMSE Score, GD Scale Score, TE, TR, Slice thickness and more) with different fields / levels of search.	D
R1.4.4.5.	The querying language should be user friendly and querying interface should be operable by both technical and non-technical users.	E
R1.4.5.1.	Search QC records for images that pass a given set of QC parameters.	D
R1.4.5.2.	View the QC records, sorted after parameter of choice (not just QC parameters.)	D
R1.4.5.3.	Search and view the record of format conversions that have been applied to an image/image set at upload	D
R1.4.5.4.	The ability to display the QC results directly to the users with the subject image.	D
R1.4.5.5.	The anonymization process shouldn't be visible to the final user. This step could be done within the neuGRID consortium and should not be accessible (except for special privileges) by the end users of neuGRID.	E

R1.4.5.7.	Provide provenance information related to modifications made to a data set. Provenance information may include modifications made for quality control, ethical compliance, anonymization, any format conversions that were necessary and related information.	E
R2.1.1.	Download neuGRID interaction tool bundle (unless web-based?). A signed usage agreement could be put in place.	E
R2.1.2.	Fill in requested neuGRID user data (institute, name etc) and store as “My profile” under “My account”.	E
R2.1.3.	The possibility to become part of a group of researchers (start a new group, be invited to an existing one).	D
R2.1.4.	Sensitive individual data sets will generate specific access agreements to be signed (1.5.2.2), which will be stored under “My account”	E
R2.1.5.	All the neuGRID users must be registered. They will fill an on-line form in which neuGRID staff will provide both a specific user_ID and a password.	E
R2.2.1.	Select a set of properties with which to generate data subsets from the database.	E
R2.2.2.	Generate feedback about the data sets (lists), which can be sorted after for instance QC parameters, type of camera etc.	D
R2.2.3.	Fine-tune the property set interactively.	D
R2.2.4.	Store the final property set under a label under “My account”/”My search property sets”.	D
R2.2.5.	Store the resulting data sets (lists of data generated by applying the property set on the data base) under “My account”/”My data sets”.	D
R2.2.6.	Provide a global search utility which searches distributed neuGRID data stores based on user defined criteria. Researchers should be able to search for a certain type of patients based on medical information as well on imaging information. For instance patients with Mild Cognitive Impairment with a given range of MMSE values which have had a T1 MPR sequence with a pixel size smaller equal 1.5 mm in each direction. The range of fields that can be used for searching should include:	E
R2.2.6.1.	Subject information: Subject Id, Sex, Research Group, Age, Weight.	E
R2.2.6.2.	Project specific information.	D
R2.2.6.3.	Clinical assessment information: MMSE Total Score, GDScale Total Score, Global CDR, Modified Hachinski Total Score, NPI-Q Total Score, Functional Assessment Questionnaire Total Score.	D
R2.2.6.4.	Study information: Study date, Visit.	E
R2.2.6.5.	Image information: Original (Choose Modality, Series Description, Acquisition type, Weighting, Slice Thickness, TE, TR, Acquisition Plane, Manufacturer, Field Strength) – Pre-processed (Series Description, Image File Type, Anatomic Structure, Tissue Type, Laterality, Registration/Space) – Post Processed (Series Description, Image File Type, Anatomic Structure, Tissue Type, Laterality, Registration/Space.)	E
R2.2.7.	Metadata will need to be stored for images to enable search functionality, this will identify images and the search will be performed on the metadata.	E
R2.6.1	A viewer should be provided, together with information regarding the quality assessment that was made by the researcher that uploaded the image.	E
R2.6.2	A “Comment on this image” facility: other users’ comments might be visible under a special link in the data list.	O

R2.6.4	The possibility to express a judgment about the quality of data could be useful. Then, this judgment (e.g.: 4- Excellent; 3-Good; 2-Sufficient; 1-Bad) could be taken into account during the creation of a research set.	D
R2.6.6	Software managing saved searches and research sets, should have the functionality to allow permitted users to post comments and give feedback on research sets of other users.	D
R2.6.7	The interface for saved searches will allow users to add or remove users from commenting on research sets.	O
R3.1.1	Select packages to use from categories of algorithms (e.g.: "statistical", "brain stripping").	D
R3.1.2	Construct a workflow by stringing together various algorithms and packages in a work area (drag and drop?), creating a series of connected boxes. Divisors, yes/no-alternatives for branching workflows may also be available in a graphical toolkit. This should be as simple as possible using a combination of arrows and nodes within a Graphical interface.	E
R3.1.3	Add comments next to each box in the workflow.	D
R3.1.4	The possibility to divide the workflow into logical units (the first three steps are brain stripping and have a pink background, next are five volumetric steps with a yellow background) with labels describing them.	O
R3.1.5	Visualize the workflow as a schematic boxed flow diagram (rough version can be seen in the work area, this should be printable as a PDF.)	E
R3.1.6	Edit the workflow by moving boxes around. A warning system saying "block A does not generate output that enables running block B directly after it" would be helpful.	D
R3.1.7	A possibility to edit input parameters in each algorithm (maybe an execution crashes because it requires a "4" instead of "2" in a given sub-process.)	E
R3.1.8	Save the workflow with a label under "My account"/"My workflows"/"Drafts".	E
R3.1.9	The provision of a command line scripting interface is necessary. It should be possible to upload a workflow as a Linux command script (e.g. bash) which calls a number of Linux executables residing on the grid or uploaded together with the script.	E
R3.1.10	The possibility to have a large range of pre-configured atomic modules from which new workflows can be created or to be able to integrate new functions efficiently.	D
R3.1.11	The opportunity to have a functional test-bed to validate efficiently workflows that are in construction (using trial appropriate reference data set already uploaded remotely and an efficient validating execution interface.)	D
R3.1.12	The ability to do a "debug error procedure" in order to show different actions that a final user can take in order to debug any validation or execution errors that could be encountered while using the Pipeline.	D
R3.1.13	The ability to preserve the order execution and the dependencies of the pipeline workflow.	D
R3.1.14	The ability to upload workflows generated within the major "workflow management systems" that are in use today (e.g.: the LONI pipeline, Scientific Kepler system and others.)	O
R3.1.15	The infrastructure should be platform-independent.	D
R3.1.16	The possibility to use images stored in the NeuGRID store to run a local	D

	analysis (e.g. in case a user wishes to run an analysis on NeuGRID images using software developed locally, which is not to be shared.)	
R3.1.17	Provide a means of editing existing workflows.	E
R3.2.1	Open a workflow and edit it.	E
R3.2.2	When saving a previously existing draft workflow, automatically append version number and save under the workflow label under “My account”/”My workflows”/”Drafts” together with date edited. There should be a version control system for workflows that resides on neuGRID independent of their implementation (as a script file, program of graphical workflow.)	D
R3.2.3	The possibility to save the draft personal modules and workflow inside the neuGRID system.	D
R3.2.4	The possibility to open, drag and drop these draft modules quickly and easily.	D
R3.2.5	he possibility of creating pipelines by assembling existing workflows.	D
R3.2.6	Provide a repository for workflows with version control management.	D
R3.2.7	Provide user friendly interfaces, integrated with the workflow authoring software to upload/download/update workflows to the workflow repository.	D
R3.2.8	Changes between different versions of the software should be documented.	D
R3.3.1	Locate an existing workflow in the database of workflows that are accessible to all by selecting categories of algorithms that are desired to be included (this generates a list of workflows). The possibility to use all the features of the main programs in use today in the neuro-imaging field (e.g.: FSL, FREESURFER, SPM, MNI, ...)	d
R3.3.2	Select desired/interesting workflows and save under “My account”/”My workflows”/”Published”.	D
R3.3.3	Provide users to visualize existing workflows as in 3.1.5.	E
R3.3.4	Provide users the functionality to add annotations or comments to workflows as in 3.1.3	D
R3.3.5	Provide users the capability to edit existing workflows as in 3.1.4, 3.1.6.	E
R3.3.6	Save as in 3.1.8 and 3.2.2 (to “Drafts”).	D
R3.3.7	The opportunity to have a responsible person or group of people that maintain the main pipelines in use in the neuro-imaging field.	D
R3.3.8	The system should send email alerts to the final users when the workflow outputs are ready.	O
R3.3.9	There should be a way to assign a known bug list to a workflow.	D
R3.4.2	Make a workflow accessible and set access rights, fill in label name, builder name and institute, way to reference, terms of use (grant me a footnote, grant me authorship on any papers produced with the help of my flow) etc. See also use-case 7.	E
R3.4.3	The possibility to download an algorithm/package, to be able to tweak it oneself, by editing code or settings.	D
R3.4.9	The neuGRID “workflow management system” should be able to support and interface with many common languages classically used in the neuro-imaging field (like PERL, C++, Matlab, bash script and Python)	D
R3.4.10	Ensure and maintain architectural compatibility with the latest imaging software.	D
R3.4.11	Upload temporarily personal packages/software for specific studies. It should be able to upload a workflow as a Linux command script (e.g. bash)	O

	which calls a number of Linux executables residing on the grid or uploaded together with the script.	
R3.4.13	Provide users with a means of browsing existing uploaded algorithms, packages and analysis software to enable their use in workflows.	E
R4.1.1	Find a previously defined research set by selecting a data set under “My account”/”My data sets” (see 2.4.2, 2.2.5).	D
R4.1.3	A means to search publicly available research sets.	O
R4.1.4	The ability to edit research set access rights.	D
R4.1.5	To optimize performance, the images used for the analysis should also be present (if possible) locally in those nodes of the grid that don’t have a high level of bandwidth available. This is due to the fact that the transfer of a large number of images on the network will greatly increase the time to get the final results. Clearly, this is particularly true for a centre like FBF which is characterized by a connectivity of 10 Mbps.	D
R4.1.6	High redundancy and data availability is necessary.	D
R4.1.7	The possibility to integrate information provided by images and metadata with the definition of mathematical variables like vectors, list and structures. Define basic operations (like indexing, push, pop and length count) in order to perform command line operations on these objects containing images of interest.	D
R4.1.8	Provide a global search utility which searches distributed neuGRID data stores based on a user defined criteria.	D
R4.1.10	User should be able to download data sets, if proper authentication has succeeded.	D
R4.1.11	Provide capability to the user to save a search and define it as a research set (see 2.5.1).	D
R4.1.12	Provide the capability of using saved data sets and research sets for input for workflows (see 4.2.1).	D
R4.2.1	Apply a workflow to a data set, step by step or all at once.	D
R4.2.2	Output from the individual processes within the workflow is output to a progress window; also when a new process is started (process name_1: <output from 1 such as “calculating chi-2”> -- process name_2: <output> and so on).	O
R4.2.3	When the process stops (prematurely or not) the user can add comments at the bottom of the window.	O
R4.2.4	A GUI with buttons to stop, restart the workflow.	E
R4.2.5	The possibility to change the input parameters in a sub-process of the workflow (see 3.1.7.)	E
R4.2.6	The possibility to test a workflow on single images or subsets of the chosen data set (one could of course generate a new data set as in 2.2 but that is probably clumsier.)	D
R4.2.7	The ability to create, visualize and edit complex workflows in a convenient way.	E
R4.2.8	Simple way to monitor workflow execution.	D
R4.2.9	The user should have the possibility to check and perform quality control on each intermediate output.	E
R4.2.10	The ability to cancel, restart and debug workflows.	E
R4.2.11	The ability to share workflows with other researchers in the system.	D
R4.2.12	The possibility to provide the user with sample images for any kind of scan	D

	modality (MRI, fMRI, PET,…) in order to test his/her own workflow (or parts of it) using them and saving time uploading their own images.	
R4.2.13	Extend workflow authoring environment to include basic execution functionality for:	D
R4.2.13.1	Starting the execution of a workflow.	D
R4.2.13.2	Providing an interface to monitor the status of a workflow.	D
R4.2.13.3	Provide ability to control the execution by cancelling or restarting the workflow.	D
R4.3.1	New workflow sharing should be controlled (only functioning and validated workflows should be uploaded and shared.)	O
R4.3.2	All the pipelines should be organized in a clear and efficiency way in order to make clear their use.	D
R4.3.3	The presence of a facility that allows users to query for specific modules. The Search function should return results drawn from the module's name, author list, citations, tags, description, and parameter fields.	E
R4.3.4	Most modules could have 2-3 required metadata parameters on them and several more optional parameters. The possibility to switch on these additional options simply clicking on the modules could be useful.	O
R4.3.5	Provide a service for users to upload workflows.	D
R4.3.6	Provide an interface to allow users to select pre-authored workflows and execute them with a new/existing research set.	E
R4.3.7	Provide the capability of editing an existing workflow, and executing it.	E
R4.4.1	The possibility to compare different versions of the same workflow.	D
R4.4.2	Each workflow is described by its components (viewed as in 3.1.5) highlighting the differences of each version and by its provenance (who built it, uploaded when, changed when), their new applications or improvements.	D
R4.4.3	Select "Unfold history" to see older versions of the workflow, meaning also versions where no one has changed the workflow per se but one of the packages/algorithms making up the workflow.	D
R4.4.4	An old workflow can then be selected by clicking on it (perhaps one needs to rebuild it.)	D
R4.4.5	Provide a service for uploading workflows	D
R4.4.6	Provide capability to annotate history of a workflow.	D
R4.4.7	Provide an interface to search existing workflows and their respective history.	D
R4.4.8	The possibility to use a workflow as it was on a given date by entering the date of interest.	O
R4.5.1	The progress window output from 4.2.2 could be saved as a file, with a header consisting of a description of the data set used and the settings made for each (named) algorithm in the workflow (this may also be saved separately as a "workflow setup", which lists all the parameters that were given to the workflow's algorithms.) It may end with some user generated comments as in 4.2.3.	D
R4.5.2	The possibility to efficiently retrieve some standardized workflows that are used in daily routine tests and procedures by different labs.	D
R4.5.3	Provide capability to annotate history of a workflow.	D
R4.5.4	Provide an interface to search existing workflows and their respective history.	D

R4.6.1	Save the data set which has gone through the workflow with a label under "My account"/"My processed sets."	D
R4.6.4	Save analyzed data under "My account"/"My analyzed sets" with links connecting each analyzed set to the corresponding processed set (by actual linking or by naming convention).	D
R4.6.5	Save the workflow setup and the progress window output under each processed set	O
R4.6.6	Define a simple drag and drop interface in order to connect the raw data outputted to the next workflow as input.	D
R4.6.7	Define a simple click interface in order to add raw files	D
R4.6.8	Allow user to use data in their desired format	O
R4.6.9	Provide notifications to users on the status of a pipeline.	D
R4.6.10	Upon completion of a workflow, allow users to download raw data output.	E
R4.6.11	Provide the necessary functionality to export the raw output into the desired data analysis software.	O
R4.6.12	Enable some basic analyses using inbuilt statistical tools such as those provided by FSL.	D
R5.1.1	Load the workflow into a variant of the work area in 3.1.2. The order of the boxes and layout of the workflow cannot be changed, but by clicking on each box the appropriate set of provenance data can be viewed: lists of images that can be put into the viewer (possibility to compare images, from different provenance sets and within sets) and numerical output data (chi-2 etc). Also the workflow setup can be viewed.	D
R5.1.2	To check for errors try to execute the workflow.	E
R5.1.3	If any errors are found it could be useful that a dialog box will pop up listing all the errors found in the workflow.	D
R5.1.4	During the validation of the workflow the outputted data should be visualized.	D
R5.1.5	Provide user capability to browse provenance data collected from execution of workflows.	E
R5.1.5.1	The interface should be user friendly, and allow for browsing of process by process provenance data.	D
R5.1.5.2	Provenance data should link to the intermediary output produced during execution of the workflow.	E
R5.1.6	There should be a way to report outliers and to be able to check intermediate data for such indicators (this would be very useful!)	D
R5.2.1	When someone has developed a workflow, at upload they can be asked to specify a reference data set to be associated with the workflow. This reference set can then be found as a property of the workflow ("Test with reference data set?").	D
R5.2.2	Generate a new data set for testing old or new workflows	O
R5.2.3	The possibility to add a reference data set to the workflow's properties, even for those who have not constructed the original workflow.	O
R5.2.4	It could be useful to be able to choose from a number of predefined reference data sets (for example: one characterized by 3D volumetric images, fMRI images, DTI images, PET images,…) comprising 3-5 images of reference.	D
R5.2.5	Provide a tool to users to browse and select reference data sets for execution with a workflow.	O

R5.2.6	Provide the user with a comparative analysis of the output produced to output in the reference data set.	D
R5.4.1	Add a comment to a workflow which can be seen under “Unfold history” in 4.4.3.	O
R5.4.2	The possibility to make a stratification of the different usage of each specific workflow.	O
R5.4.3	Useful to understand which are the most used values by the scientific community to analyze different type of acquisitions through different workflows.	O
R5.4.4	Provide a repository for workflows with version control management.	E
R5.4.5	Provide user friendly interfaces, integrated with the workflow authoring software to upload/download/update workflows to the workflow repository.	D
R5.4.6	The repository should have the functionality to add annotations from user about versions of the workflow. For a workflow that resides on neuGRID a versioning mechanism (version control system) should be present including a description of the differences between versions.	D
R5.4.7	The repository should log and document historical changes to a workflow.	D
R5.5.1	As 5.4.	D
R5.5.2	The possibility to summarize the most useful and appropriate parameters used in the workflows through synoptic tables.	O
R5.5.3	Ease of reference parameters.	O
R5.5.4	Provide capability to users to annotate workflows, providing information about settings of the workflow in different execution contexts.	D
R6.1.1	Store intermediary execution steps.	E
R6.1.1.1	The workflow processes and the workflow setup should be saved (see 4.5.1.)	D
R6.1.1.2	The intermediate, processed files (provenance data) are saved as well, according to the structure Run number/Process number/files, e.g. Run5/Process2 (Brain strip)/file_no5. It is useful to be able to save the output from more than one run at a time, for comparison. (upper limit could be 10 runs), and can be found under “My data sets”/”Provenance data.”	D
R6.1.1.3	Provide explanation and details of any errors that occur and report possible causes.	E
R6.1.2	Keep a full record of all intermediary images and data.	E
R6.1.2.1	The tree structure in 6.1.1.2 should also include a summary of any numerical data that is produced (chi-2 etc).	D
R6.1.2.2	Store error messages and be able to navigate through them.	E
R6.1.2.3	Post problems on a neuGRID technical forum.	O
R6.1.2.4	All intermediary data and related logs should be stored during workflow execution.	E
R6.1.2.5	Provenance data should be presented in a user friendly fashion.	D
R6.2.1	The possibility to import selected files from 6.1.1.2 into the appropriate step in a given workflow using the GUI in 4.2.4 and analysis with toolkits.	D
R6.2.2	Taking the output from a single step in a workflow and looking at it in the viewer/seeing the full text output (see 5.1.1).	D
R6.2.3	The possibility to recall single workflow functions that were used at each processing step using a simple command line interface.	E
R6.2.4	Provide the user with an interface to browse a completely executed workflow, process by process, and enable user to view all relevant	E

	intermediary output and logging information.	
R6.3.2	Compare the outputted raw files with information from saved workflows (if any exists.)	O
R6.3.3	Provide a querying interface to the provenance store.	D
R6.4.1	Check for additional abnormalities passed over in silence (weak field inhomogeneities, ringing artifacts etc.)	O
R6.4.2	Compare the results obtained with reference images.	D
R6.4.3	Allow user to export/download provenance data to their computer system and perform statistical analysis on it.	D
R6.4.4	Results to be saved as a property of the provenance data set. Files go under Run number/Process number/User-selected analysis set name/files.	D
R6.5.1	As 5.4.1. The workflow comments should not be unstructured text inputs but sorted into categories (General, Errors, Inconsistencies, Comment made by <name>.)	O
R6.5.2	When an error occurs a red colour could be used to depict that the workflow has a problem.	D
R6.5.3	Provide a user with the capability to annotate an item in the provenance store.	O
R6.6.1	Search and display workflow comments regarding errors. Also, automatically save and compile statistics on which errors crop up during the run of a certain workflow.	D
R6.6.2	See neuGRID technical on-line forum.	O
R6.6.3	Create a frequently asked question sections for each workflows.	O
R6.6.4	Provide the user with information about common errors that severely affect a workflow	D
R7.1.1.1	A researcher on uploading / publishing a workflow, should be able to define access permissions for individuals or groups.	E
R7.1.1.2	Provide a service where users can upload and share workflows.	E
R7.1.1.4	A specific group member should be able to share a workflow with other members of that group.	D
R7.1.2.1	As in 7.1.1.1 but the uploading researcher can also tag the workflow as under development, which will show up clearly in connection to the workflow name, when searched for and viewed (as in 3.1.5).	D
R7.1.2.2	Allow users to create virtual groups within the service.	O
R7.1.3.1	See 6.5.1. Workflows under development may have more categories to comment under.	O
R7.1.3.2	Users should be able to provide feedback and comment on workflows that have been created by other users	O
R7.1.4.1	See 3.4.2.	O
R7.1.4.2	Users should provide details about themselves in their accounts, this information should be associated with workflows they upload.	O
R7.1.5.1	See 3.4.2.	O
R7.1.5.2	Users should be allowed to share a workflow with another specific user of the service, irrespective of groups.	D
R7.1.6.1	To reproduce results exactly, one needs the workflow and the data set it was applied to (i.e. the search property set). This could be accomplished by having research teams enter their publications into an article database in neuGRID. When entering the publication reference, the team could be asked to supply the names of the used workflows and a copy of the search	D

	property set. This could be a requirement, which if not signed denies access to the neuGRID project.	
R7.1.6.2	Provide users the capability to download a workflow, import to their workflow execution environment and compare with results of previous executions.	D
R7.1.6.3	There should be a way to reuse a given dataset on a given workflow.	E
R7.1.7.1	A policy is needed for who can certify workflows and the process by which certification takes place in neuGRID.	D
R7.1.7.2	Provide tools for certifying a workflow according to 7.1.7.1.	O
R7.1.7.3	An administrator should manage and control the certification process including requesting information regarding the data/software/workflows as needed.	D
R7.2.1	Supply contact details when uploading a flow as in 3.4.2.	D
R7.2.2	Provide a category of tags that can be added to a workflow and allow users to request new features.	O
R7.2.3	Share new workflow features with the research community according to the permissions of the various groups.	D
R7.2.4	After a certain period of exclusivity workflows of a given quality should be shared with the entire neuGRID community.	O
R7.2.5	Provide functionality within the service to enable users to request a workflow for a particular task from other users.	O
R7.3.1	Provide a category of tags that can be added to a workflow and allow users to request assistance from more experienced researchers.	O
R7.3.2	Possibly a discussion forum could be connected to workflows with different tags (this might ease the pressure on the comments section of the workflows.)	O
R7.3.3	Provide forum type functionality within the service, in order for users to discuss and solicit advice from other users about construction of workflows.	O
R7.3.4	A user guide is necessary.	D
R7.3.5	A technical glossary should be created.	D
R7.4.2	Organize a mailing list for workflow constructors so that important messages can be circulated.	D
R7.4.3	Provide functionality to interact with volunteer specialist users to construct new workflows.	O
R7.4.4	Specialist users may be given a special account, and may at their choice be listed for easy discovery.	O
R7.5.1	Provide a forum type capability to discuss specific workflows, in case problems arise, see 7.3.2.	O
R7.5.2	Create a neuGRID community in which users can see which modules are the most used, the statistic concerning the different workflows, the efficiency or malfunction of these workflows, and other various topics of interest for the users.	O
R7.6.1	Supplement 7.3.2 with a more general notice board.	D
R7.6.3	Provide a modular service, so that new features can be added to enhance collaboration between users.	e
R7.7.1	See 1.5	E
R7.8.1	Add “Research interests” to the profile data entered in 2.1.2.	O
R7.8.2	Similar interests could be assessed during user registration through a	O

	simple and fast questionnaire as checklists or free, searchable text.	
R7.8.3	Allow users to create virtual groups within the service.	O
R7.9.1	The workflow setups from 4.5.1 can also be saved and searched under “My workflow setups”. They should be coupled to the data set processed with these criteria (or the search property set used to generate the data eventually processed by the workflow in that specific setup).	O
R7.9.2	A tag can be set specifying that the workflow setup is public. Then a search for a specific workflow execution can also include all public workflow setups (and their connected processed data sets/search property sets).	O
R7.9.3	Provide a simple query interface through which past executions can be discovered.	D
R7.9.4	Functionality should be provided for the uploading and updating of specific workflow execution instances, and upload/link to relevant output data and workflow specification.	O
R7.9.5	A user should be able to download an archived workflow specification and select new/existing data set for processing.	D
R7.10.1	Create a FAQ like page for “Frequent errors”, which might give tips on how to check that the output from block A is possible to use as input in block B in a workflow.	O
R7.10.2	Create a user comment database where researchers can note mistakes they made and how to avoid them.	O
R7.10.3	Log the error outputs and compile statistics on their frequency. The helpdesk (7.4.1) could help connect the error outputs to the mistakes creating them.	O
R7.10.4	Save a certain amount of bad workflows executions that should be useful as examples for the new users of the neuGRID platform.	D
R7.10.5	Make a validation test on the main tools that neuGRID provides.	D
R7.10.6	Provide/maintain a documentation of common workflow mistakes.	O
R7.10.7	There should be a way to store non-standard patients, typical examples etc for a given workflow in a separate store.	O

Tasks Identified

T6.2. Design Interface with user-facing services (M13-M24)
In this stage, P2 NE assisted by P3 UWE will design the interfaces which either append or factor out LORIS services into the generic layer, based on the work done in WP5. The resulting interfaces should be suitable for use by other medical applications desiring distributive capability.

T6.3. Design Interface with grid-facing services (M13-M24)
P4 MAAT and P3 UWE will create the interfaces to interact with the Grid services. They should be distribution aware, but not Grid specific. All platform specific services should be wrapped up below.

T6.4. Design & implementation of reusable medical service layer (M13-M36)
P3 UWE will address the overall design, architecture and implementation of the distributed medical services. They will work with P7 HEALTHGRID to ensure adherence to emerging standards in health Grids. The output will be a package of services which can be used by any medical application, and able to be deployed on top of different distributed computing

solutions. This will be specifically tuned for LORIS requirements and will be optimized to run on the gLite enabled Grid Services. A report will be produced on the prototype implementation of the service on M24 (D6.2).

T6.5 Service testing and evaluation (M25-M36)
P3 UWE in collaboration with P2 NE and P4 MAAT will carry out a comprehensive testing and evaluation of the medical services and their interfaces with the grid and user services. Any architectural and coding problems will be debugged in this stage and will be handled appropriately. This will act as quality assurance stage for the whole work package deliverables and will feed into the workpackage on overall system integration, (WP10). User and programmer manuals, release and distribution issues will also be managed in this phase.

Work package number WP7 **Start date or starting event:** M7
Work package title *Grid Services Provision*
Activity Type SVC

User Requirements

R1.5.1.1.	Sort data sets into groups to which a certain access control is set.	E
R1.5.1.2.	Edit the access control of a group of data (see 1.5.2.2.)	E
R1.5.1.3.	Sort and edit access control for a named individual/ or group of researchers. Provide tools to administrators to define user specific access control policies (at the project and individual levels.)	E
R1.5.1.4.	A supervisor or responsible person should define both the access level and the policies that pertain to gaining access to the data stored inside neuGRID.	E
R1.5.1.5.	Provide secure access to data storage resources.	E
R1.5.1.6.	There should be a possibility to give individual users special access to a certain data set.	D
R2.1.1.	Download neuGRID interaction tool bundle (unless web-based?). A signed usage agreement could be put in place.	E
R2.1.2.	Fill in requested neuGRID user data (institute, name etc) and store as “My profile” under “My account”	E
R2.1.3.	The possibility to become part of a group of researchers (start a new group, be invited to an existing one).	D
R2.1.4.	Sensitive individual data sets will generate specific access agreements to be signed (1.5.2.2), which will be stored under “My account”	E
R2.1.5.	All the neuGRID users must be registered. They will fill an on-line form in which neuGRID staff will provide both a specific user_ID and a password.	E
R2.1.6.	Provide a global security model, which enables individual researchers from collaborating institutes to access other institutes’ data sets. There should be a certificate-based system to identify users and to perform access control.	E
R2.1.7.	Allow institutes to define local access control policies.	D
R2.1.8.	It is necessary to have access controls at the Project and Individual data set levels.	E
R3.4.1	Upload an algorithm or package (or draft) including source code; fill in what categories to store it under (3.1.1.)	E
R3.4.2	Make a workflow accessible and set access rights, fill in label name, builder name and institute, way to reference, terms of use (grant me a footnote,	E

	grant me authorship on any papers produced with the help of my flow) etc. See also use-case 7.	
R3.4.3	The possibility to download an algorithm/package, to be able to tweak it oneself, by editing code or settings.	D
R3.4.4	Save the tweaked algorithms under My account/ My algorithms.	O
R3.4.5	If an algorithm is uploaded with the same name as an already existing one, automatically append version number (and ask the uploading researcher to enter a comment on what has changed.)	D
R3.4.6	If a package name changes, include source code dependencies (builds on package X by adding Y.)	D
R3.4.7	The upload of new packages/algorithms should be controlled centrally.	E
R3.4.8	The new tools to be uploaded should be rigorously tested and / or validated. Any new tool should be uploaded together with a specific documentation, including a user guide, algorithm explanations and appropriate references.	E
R3.4.9	The neuGRID "workflow management system" should be able to support and interface with many common languages classically used in the neuro-imaging field (like PERL, C++, Matlab, bash script and Python)	D
R3.4.10	Ensure and maintain architectural compatibility with the latest imaging software.	D
R3.4.11	Upload temporarily personal packages/software for specific studies. It should be able to upload a workflow as a Linux command script (e.g. bash) which calls a number of Linux executables residing on the grid or uploaded together with the script.	O
R3.4.12	Provide users with an interface for uploading new software packages, algorithms and analysis software subject to appropriate validation, which may then be used in future workflows.	D
R3.4.13	Provide users with a means of browsing existing uploaded algorithms, packages and analysis software to enable their use in workflows.	E
R4.2.1	Apply a workflow to a data set, step by step or all at once.	D
R4.2.2	Output from the individual processes within the workflow is output to a progress window; also when a new process is started (process name_1: <output from 1 such as "calculating chi-2"> -- process name_2: <output> and so on)	O
R4.2.4	A GUI with buttons to stop, restart the workflow.	E
R4.2.5	The possibility to change the input parameters in a sub-process of the workflow (see 3.1.7.)	E
R4.2.8	Simple way to monitor workflow execution.	D
R4.2.9	The user should have the possibility to check and perform quality control on each intermediate output.	E
R4.2.10	The ability to cancel, restart and debug workflows.	E
R4.2.11	The ability to share workflows with other researchers in the system.	D
R4.2.12	The possibility to provide the user with sample images for any kind of scan modality (MRI, fMRI, PET,…) in order to test his/her own workflow (or parts of it) using them and saving time uploading their own images.	D
R4.2.13	Extend workflow authoring environment to include basic execution functionality for:	D
R4.2.13.1	Starting the execution of a workflow.	D
R4.2.13.2	Providing an interface to monitor the status of a workflow.	D
R4.2.13.3	Provide ability to control the execution by cancelling or restarting the	D

	workflow.	
R4.3.1	New workflow sharing should be controlled (only functioning and validated workflows should be uploaded and shared.)	O
R4.3.2	All the pipelines should be organized in a clear and efficiency way in order to make clear their use.	D
R4.3.5	Provide a service for users to upload workflows.	D
R4.3.6	Provide an interface to allow users to select pre-authored workflows and execute them with a new/existing research set.	E
R4.3.7	Provide the capability of editing an existing workflow, and executing it.	E
R4.5.1	The progress window output from 4.2.2 could be saved as a file, with a header consisting of a description of the data set used and the settings made for each (named) algorithm in the workflow (this may also be saved separately as a "workflow setup", which lists all the parameters that were given to the workflow's algorithms.) It may end with some user generated comments as in 4.2.3.	D
R4.5.2	The possibility to efficiently retrieve some standardized workflows that are used in daily routine tests and procedures by different labs.	D
R4.5.3	Provide capability to annotate history of a workflow.	D
R4.5.4	Provide an interface to search existing workflows and their respective history.	D
R5.3.1	The error report button in the 4.2.4 GUI sends an email to the appropriate place with information regarding workflow setup, workflow name and data set properties. It should also generate an error number for convenience and easy follow up	D
R5.3.2	Inevitably, some of the instances of a module could fail sometimes and the execution of the module could be stopped denoting the failure. In this case, it could be useful to have a viewer box in which all the failed instances of the module could be shown. With this information neuGRID users could diagnose the problems encountered during the execution of a workflow and hopefully solve them.	D
R5.3.3	Provide notification for critical events during an execution of a workflow.	E
R6.1.1	Store intermediary execution steps	E
R6.1.1.1	The workflow processes and the workflow setup should be saved (see 4.5.1.)	D
R6.1.1.2	The intermediate, processed files (provenance data) are saved as well, according to the structure Run number/Process number/files, e.g. Run5/Process2 (Brain strip)/file_no5. It is useful to be able to save the output from more than one run at a time, for comparison. (upper limit could be 10 runs), and can be found under "My data sets"/"Provenance data."	D
R6.1.1.3	Provide explanation and details of any errors that occur and report possible causes.	E
R6.1.1.4	Send potential errors to the neuGRID administrators if the workflow resides on the neuGRID infrastructure.	D
R6.1.2	Keep a full record of all intermediary images and data.	E
R6.1.2.1	The tree structure in 6.1.1.2 should also include a summary of any numerical data that is produced (chi-2 etc).	D
R6.1.2.2	Store error messages and be able to navigate through them.	E
R6.1.2.3	Post problems on a neuGRID technical forum.	O
R6.1.2.4	All intermediary data and related logs should be stored during workflow	E

	execution.	
R6.1.2.5	Provenance data should be presented in a user friendly fashion.	D
R7.1.1.1	A researcher on uploading / publishing a workflow, should be able to define access permissions for individuals or groups.	E
R7.1.1.2	Provide a service where users can upload and share workflows.	E
R7.1.1.3	Authorization should identify users uniquely.	E
R7.1.1.4	A specific group member should be able to share a workflow with other members of that group	D
R7.1.2.1	As in 7.1.1.1 but the uploading researcher can also tag the workflow as under development, which will show up clearly in connection to the workflow name, when searched for and viewed (as in 3.1.5).	D
R7.1.2.2	Allow users to create virtual groups within the service.	O
R7.1.5.1	See 3.4.2.	O
R7.1.5.2	Users should be allowed to share a workflow with another specific user of the service, irrespective of groups.	D
R7.7.1	See 1.5.	E
R7.7.2	Identify different levels of security and confidentiality within the grid.	E
R7.7.3	Access can be restricted to one person only. Provide users with the capability to restrict workflows from public access.	E

Tasks Identified

***T7.1. Grid Middleware Education & Feedback** (M7-36)*

P4 MAAT and P5 UWE will undertake education related to gLite services functionality and gLite interfaces. Evaluate, select and test existing application programming interfaces to gLite services. Coordinate the interaction between neuGRID and EGEE, and ensure relevant middleware requirements from neuGRID are forwarded to EGEE.

T7.2. Grid Middleware Migrations (M7-36)

P4 MAAT will evaluate and test gLite releases (new services, upgrade of existing services) in the test-bed prior to migration in production. P7 HEALTHGRID will assist in the definition of compliance of the services with data protection issues. All migrations in Production will be accompanied with internal reports circulated to relevant partners. An interim grid middleware migrations test report will be issued on M24 (D7.2) and a final report on M36 (D7.3).

Work package number WP8 **Start date or starting event:** M1
Work package title *Deployment Services Provision*
Activity Type SVC

User Requirements

R1.4.2.1.	Manage backup data	E
R1.4.2.2.	Provide a means to backup data storage resources	E
R1.4.2.3.	The ability to ask to users to save data not yet backed up, in an iterative way	D
R1.4.3.1.	The possibility to follow a step-by-step predefined GUI-based wizard for the performance of system maintenance.	D
R1.4.3.2.	Provide a manual for performing system maintenance.	D
R1.4.3.3.	A means of communicating periods of service downtime to users.	D
R1.4.3.4.	Mechanisms for recovering from system failure should be provided.	D

R1.4.3.5.	A maintenance mode with the ability to take the system off-line for a period.	D
R1.4.3.6.	A system dashboard could be provided to give an overall picture of status of the infrastructure at any given point in time.	D
R1.4.6.1.	A copy of the initial data should be kept safely.	E
R1.4.6.2.	No seriously corrupted or unusable data should remain in the neuGRID data store.	E
R1.4.6.3.	Provide tools to detect corrupted data sets, and to recover them as required.	D
R.1.4.6.4.	Once data has been made available to users, ensure that it remains unaltered (with the exception of legal requirements) even if it has some degree of corruption. Any improvements to the data are handled by making a new version available to users while still keeping the old version available to users. It should be clear to users which is the most up to date version.	E
R1.4.6.5.	Delete corrupted data.	E
R1.4.6.6.	Locate origin of corrupted data and handle the possibility of systemic problems.	D
R1.4.7.1.	Select data sets or groups (R1.4.8.3) to be removed as defined within authorization levels.	E
R1.4.7.2.	An automatic report of removal to be sent to the uploaded site contact email.	D
R1.4.7.3.	Provide functionality to delete data sets from the data store.	E
R1.4.7.4.	Provide functionality to delete data sets from the user collections (R1.4.4.4.)	E
R5.3.1	The error report button in the 4.2.4 GUI sends an email to the appropriate place with information regarding workflow setup, workflow name and data set properties. It should also generate an error number for convenience and easy follow up.	D
R5.3.2	Inevitably, some of the instances of a module could fail sometimes and the execution of the module could be stopped denoting the failure. In this case, it could be useful to have a viewer box in which all the failed instances of the module could be shown. With this information neuGRID users could diagnose the problems encountered during the execution of a workflow and hopefully solve them.	D
R5.3.3	Provide notification for critical events during an execution of a workflow.	E
R7.1.7.1	A policy is needed for who can certify workflows and the process by which certification takes place in neuGRID.	D
R7.1.7.2	Provide tools for certifying a workflow according to 7.1.7.1.	O
R7.1.7.3	An administrator should manage and control the certification process including requesting information regarding the data/software/workflows as needed.	D

Tasks Identified

T8.6. Platform & Infrastructure Maintenance (M7-36)

P4 MAAT and P2 NE will put in place the necessary mechanisms to monitor and detect any hardware/software bad performing in the infrastructure. To take corrective actions in case of infrastructure issues. To guaranty a minimal quality of services on the infrastructure hardware/software performing and uptime.

T8.7. Deployment Support & Consultancy (M7-36)

P4 MAAT and P2 NE will provide expert advises to additional sites willing to join in the infrastructure. To provide/receive education on software deployment to support the WP11 team and any addition support site/infrastructure to be attached to the neuGRID virtual organisation. This task will in particular support the inclusion of external facilities at P6 KI, P5 VUmc and CO1 FBF, where there are pre-existing supercomputing/clusters/grid sites facilities.

Work package number WP10 **Start date or starting event:** M7
Work package title *Algorithms and Pipeline Gridification*
Activity Type RTD

User Requirements

R2.2.5.	Store the resulting data sets (lists of data generated by applying the property set on the data base) under "My account"/"My data sets".	D
R3.4.1	Upload an algorithm or package (or draft) including source code; fill in what categories to store it under (3.1.1.)	E
R3.4.2	Make a workflow accessible and set access rights, fill in label name, builder name and institute, way to reference, terms of use (grant me a footnote, grant me authorship on any papers produced with the help of my flow) etc. See also use-case 7.	E
R3.4.3	The possibility to download an algorithm/package, to be able to tweak it oneself, by editing code or settings.	D
R3.4.4	Save the tweaked algorithms under My account/ My algorithms.	O
R3.4.5	If an algorithm is uploaded with the same name as an already existing one, automatically append version number (and ask the uploading researcher to enter a comment on what has changed.)	D
R3.4.6	If a package name changes, include source code dependencies (builds on package X by adding Y.)	D
R3.4.7	The upload of new packages/algorithms should be controlled centrally.	E
R3.4.8	The new tools to be uploaded should be rigorously tested and / or validated. Any new tool should be uploaded together with a specific documentation, including a user guide, algorithm explanations and appropriate references.	E
R3.4.9	The neuGRID "workflow management system" should be able to support and interface with many common languages classically used in the neuro-imaging field (like PERL, C++, Matlab, bash script and Python)	D
R3.4.10	Ensure and maintain architectural compatibility with the latest imaging software.	D
R3.4.11	Upload temporarily personal packages/software for specific studies. It should be able to upload a workflow as a Linux command script (e.g. bash) which calls a number of Linux executables residing on the grid or uploaded together with the script.	O
R3.4.12	Provide users with an interface for uploading new software packages, algorithms and analysis software subject to appropriate validation, which may then be used in future workflows.	D
R3.4.13	Provide users with a means of browsing existing uploaded algorithms, packages and analysis software to enable their use in workflows.	E
R4.1.1	Find a previously defined research set by selecting a data set under "My account"/"My data sets" (see 2.4.2, 2.2.5).	D
R4.1.2	Generate a new research set as in 2.5.1.	D

R4.1.3	A means to search publicly available research sets.	O
R4.1.4	The ability to edit research set access rights.	D
R4.1.5	To optimize performance, the images used for the analysis should also be present (if possible) locally in those nodes of the grid that don't have a high level of bandwidth available. This is due to the fact that the transfer of a large number of images on the network will greatly increase the time to get the final results. Clearly, this is particularly true for a centre like FBF which is characterized by a connectivity of 10 Mbps.	D
R4.1.6	High redundancy and data availability is necessary.	D
R4.1.7	The possibility to integrate information provided by images and metadata with the definition of mathematical variables like vectors, list and structures. Define basic operations (like indexing, push, pop and length count) in order to perform command line operations on these objects containing images of interest.	D
R4.1.12	Provide the capability of using saved data sets and research sets for input for workflows (see 4.2.1).	D
R4.2.1	Apply a workflow to a data set, step by step or all at once.	D
R4.2.2	Output from the individual processes within the workflow is output to a progress window; also when a new process is started (process name_1: <output from 1 such as "calculating chi-2"> -- process name_2: <output> and so on).	O
R4.2.3	When the process stops (prematurely or not) the user can add comments at the bottom of the window.	O
R4.2.4	A GUI with buttons to stop, restart the workflow.	E
R4.2.5	The possibility to change the input parameters in a sub-process of the workflow (see 3.1.7.)	E
R4.2.6	The possibility to test a workflow on single images or subsets of the chosen data set (one could of course generate a new data set as in 2.2 but that is probably clumsier.)	D
R4.2.7	The ability to create, visualize and edit complex workflows in a convenient way.	E
R4.2.8	Simple way to monitor workflow execution.	D
R4.2.9	The user should have the possibility to check and perform quality control on each intermediate output.	E
R4.2.10	The ability to cancel, restart and debug workflows.	E
R4.2.11	The ability to share workflows with other researchers in the system.	D
R4.2.12	The possibility to provide the user with sample images for any kind of scan modality (MRI, fMRI, PET,…) in order to test his/her own workflow (or parts of it) using them and saving time uploading their own images.	D
R4.2.13	Extend workflow authoring environment to include basic execution functionality for:	D
R4.2.13.1	Starting the execution of a workflow.	D
R4.2.13.2	Providing an interface to monitor the status of a workflow.	D
R4.2.13.3	Provide ability to control the execution by cancelling or restarting the workflow.	D
R4.3.1	New workflow sharing should be controlled (only functioning and validated workflows should be uploaded and shared.)	O
R4.3.2	All the pipelines should be organized in a clear and efficiency way in order to make clear their use.	D

R4.3.3	The presence of a facility that allows users to query for specific modules. The Search function should return results drawn from the module's name, author list, citations, tags, description, and parameter fields.	E
R4.3.4	Most modules could have 2-3 required metadata parameters on them and several more optional parameters. The possibility to switch on these additional options simply clicking on the modules could be useful.	O
R4.3.5	Provide a service for users to upload workflows.	D
R4.3.6	Provide an interface to allow users to select pre-authored workflows and execute them with a new/existing research set.	E
R4.3.7	Provide the capability of editing an existing workflow, and executing it.	E
R4.5.1	The progress window output from 4.2.2 could be saved as a file, with a header consisting of a description of the data set used and the settings made for each (named) algorithm in the workflow (this may also be saved separately as a "workflow setup", which lists all the parameters that were given to the workflow's algorithms.) It may end with some user generated comments as in 4.2.3.	D
R4.5.2	The possibility to efficiently retrieve some standardized workflows that are used in daily routine tests and procedures by different labs.	D
R4.5.3	Provide capability to annotate history of a workflow.	D
R4.5.4	Provide an interface to search existing workflows and their respective history.	D
R4.6.1	Save the data set which has gone through the workflow with a label under "My account"/"My processed sets."	D
R4.6.2	Allow transformation of data to suit the needs of some analysis tools. Provide conversion tools for toolkits compatibility	O
R4.6.3	Build a range of common analysis tools into the infrastructure (but licensing may prevent this).	O
R4.6.4	Save analyzed data under "My account"/"My analyzed sets" with links connecting each analyzed set to the corresponding processed set (by actual linking or by naming convention).	D
R4.6.5	Save the workflow setup and the progress window output under each processed set.	O
R4.6.6	Define a simple drag and drop interface in order to connect the raw data outputted to the next workflow as input.	D
R4.6.7	Define a simple click interface in order to add raw files.	D
R4.6.8	Allow user to use data in their desired format.	O
R4.6.9	Provide notifications to users on the status of a pipeline.	D
R4.6.10	Upon completion of a workflow, allow users to download raw data output.	E
R4.6.11	Provide the necessary functionality to export the raw output into the desired data analysis software.	O
R4.6.12	Enable some basic analyses using inbuilt statistical tools such as those provided by FSL.	D
R5.2.1	When someone has developed a workflow, at upload they can be asked to specify a reference data set to be associated with the workflow. This reference set can then be found as a property of the workflow ("Test with reference data set?").	D
R5.2.2	Generate a new data set for testing old or new workflows.	O
R5.2.3	The possibility to add a reference data set to the workflow's properties, even for those who have not constructed the original workflow.	O
R5.2.4	It could be useful to be able to choose from a number of predefined reference	D

	data sets (for example: one characterized by 3D volumetric images, fMRI images, DTI images, PET images,…) comprising 3-5 images of reference.	
R5.2.5	Provide a tool to users to browse and select reference data sets for execution with a workflow.	O
R5.2.6	Provide the user with a comparative analysis of the output produced to output in the reference data set.	D
R5.3.1	The error report button in the 4.2.4 GUI sends an email to the appropriate place with information regarding workflow setup, workflow name and data set properties. It should also generate an error number for convenience and easy follow up.	D
R5.3.2	Inevitably, some of the instances of a module could fail sometimes and the execution of the module could be stopped denoting the failure. In this case, it could be useful to have a viewer box in which all the failed instances of the module could be shown. With this information neuGRID users could diagnose the problems encountered during the execution of a workflow and hopefully solve them.	D
R5.3.3	Provide notification for critical events during an execution of a workflow.	E
R6.1.1	Store intermediary execution steps.	E
R6.1.1.1	The workflow processes and the workflow setup should be saved (see 4.5.1.)	D
R6.1.1.2	The intermediate, processed files (provenance data) are saved as well, according to the structure Run number/Process number/files, e.g. Run5/Process2 (Brain strip)/file_no5. It is useful to be able to save the output from more than one run at a time, for comparison. (upper limit could be 10 runs), and can be found under "My data sets"/"Provenance data."	D
R6.1.1.3	Provide explanation and details of any errors that occur and report possible causes.	E
R6.1.1.4	Send potential errors to the neuGRID administrators if the workflow resides on the neuGRID infrastructure.	D
R6.1.2	Keep a full record of all intermediary images and data.	E
R6.1.2.1	The tree structure in 6.1.1.2 should also include a summary of any numerical data that is produced (chi-2 etc).	D
R6.1.2.2	Store error messages and be able to navigate through them	E
R6.1.2.3	Post problems on a neuGRID technical forum.	O
R6.1.2.4	All intermediary data and related logs should be stored during workflow execution.	E
R6.1.2.5	Provenance data should be presented in a user friendly fashion.	D
R6.2.1	The possibility to import selected files from 6.1.1.2 into the appropriate step in a given workflow using the GUI in 4.2.4 and analysis with toolkits.	D
R6.2.2	Taking the output from a single step in a workflow and looking at it in the viewer/seeing the full text output (see 5.1.1).	D
R6.2.3	The possibility to recall single workflow functions that were used at each processing step using a simple command line interface.	E
R6.2.4	Provide the user with an interface to browse a completely executed workflow, process by process, and enable user to view all relevant intermediary output and logging information.	E
R7.7.2	Identify different levels of security and confidentiality within the grid.	E
R7.7.3	Access can be restricted to one person only. Provide users with the capability to restrict workflows from public access.	E
R7.9.1	The workflow setups from 4.5.1 can also be saved and searched under "My	O

	workflow setups”. They should be coupled to the data set processed with these criteria (or the search property set used to generate the data eventually processed by the workflow in that specific setup).	
R7.9.2	A tag can be set specifying that the workflow setup is public. Then a search for a specific workflow execution can also include all public workflow setups (and their connected processed data sets/search property sets).	O
R7.9.3	Provide a simple query interface through which past executions can be discovered.	D
R7.9.4	Functionality should be provided for the uploading and updating of specific workflow execution instances, and upload/link to relevant output data and workflow specification.	O
R7.9.5	A user should be able to download an archived workflow specification and select new/existing data set for processing.	D

Tasks Identified

T10.2 Algorithms Gridification (M7-36)
Develop the necessary ‘glue’ to tie together the gridification components, the distributed medical and brain image processing services, in a comprehensive, self-contained, secure and deployable package. Gridify and test the existing algorithms within the infrastructure, based on the gridification model defined in T10.1. Propose optimised/refined gridification models based on the test driven by WP11 in the infrastructure. Release the prototype software following the guidelines expressed in T11.1.The outcome of this task will be a gridified Toolbox, which will be refined/optimized until the end of the project (P4 MAAT, P2 NE, and P3UWE). A document will be produced by P4 MAAT, P2 NE and P3 UWE detailing the portfolio of gridifed algorithms . The portfolio description will be amended to include new algorithms as those are made available in the system .

T10.3. Algorithm Pipeline Gridification (M7-36)
Design and implement the necessary framework of services on top of the grid infrastructure, including metascheduler, high-availability and optimisation services adapted to the project requirements, capable of triggering algorithms executions across centres from the grid to local clusters. Implement the neuGRID Workflow Engine for managing the execution of different combinations of algorithms.

8. Revision Framework and Conclusion

The requirements gathering process in neuGRID has had excellent support from the clinical researcher community. The first series of requirements elicitation sessions were completed and were most productive in bridging the gap between system developers and clinical researchers. Meetings focused initially on the description of high-level stories and usage patterns. As these were produced a range of use-cases were created and then prioritised. This provided a clear framework on which more detailed individual requirements could be based. It has been of benefit in terms of describing the project and ensuring that important components are not overlooked. This also led to a clear hierarchical conceptual framework being identified that linked high-level stories to more finely grained use-cases and to individual users requirements. The primary focus of this document has been on the production of easily understandable models that are meaningful to both clinical researchers and software developers. The verification, prioritization and refinement of the constructed models has greatly benefited from the identified stakeholders at FBF, VUmc and KI.

Through this work an important prioritization of the services that the neuGRID platform will offer to the final users has been collected, agreed and documented. A list of pipelines and capabilities coming directly from the neuroimaging community, represented by three of the major neuroimaging centres in the world VUMC, Karolinska and IRCCS-FBF, has been studied and evaluated. This survey makes it possible to draw a safe path to ensure an effective development of the neuGRID platform. The initial mapping of requirements to workpackages that has been produced will assist workpackage leaders in making informed design decisions and ensuring that the needs of end users are not overlooked. WP9 has responded to all requests for information during year one and will continue to do so as the project develops.

It is planned that the final revision of this document will take place between months 22 and 26 of the project. The revision will take into account feedback from developers / WP leaders and will address any information that was not contained in D9.1. This process will include a second round of visits being made to each of the clinical partners (FBF, VUmc and KI.) It will allow the requirements team to benefit from the information and questions that developers gather during the analysis and prototyping of system components. Where prototypes have been produced, they can be used to validate the requirements that have been gathered thus far and provide useful feedback to developers. This will further enrich the requirements specification and finalise it.

Next Steps

Following the release of this document the next stage is for system designers, developers and workpackage leaders to analyse the requirements that have been mapped to their particular tasks. This should lead to a technical evaluation of the designs that have been produced thus far and how they address the essential requirements that have been identified. In doing this the project should verify that important components have not been overlooked. This process will enrich Section 7 of this document and lead to a set of verifiable and measurable indicators being finalised which show that development and deliverables are in line with the project scope and the description of dependencies between these indicators and project deliverables. The project should use the requirements specification to measure and verify that the users' requirements are being fully addressed. To this end, it is recommended that a thorough evaluation is made with respect to each technical workpackage at Month 24.

Bibliographical References

[1] Systems Engineering Fundamentals. Defense Acquisition University Press, 2001 , ISBN: 0160732905 .
[2] Clegg, Dai; Barker, Richard (2004-11-09). Case Method Fast-Track: A RAD Approach. Addison-Wesley. ISBN 978-0201624328.

APPENDIX A: VUMC Pipelines and Capabilities

VUmc can contribute to neuGRID in three main ways:

1. As a **data acquisition centre** Over the years, the VU university medical center has built up a wealth of images, including MRI, CT, PET and MEG data, from a wide patient populations including Alzheimer's, other types of dementia, and multiple sclerosis. Supplemental data, such as medical history, MMSE, EDSS, and CSF samples etc., were also acquired. This data may be available neuGRID depending on the patients informed consent and other considerations. The VUmc also participated as an acquisition centre in the EADNI pilot project.

2. As a **core lab** the Image Analysis Center (IAC) within the VUmc performs core lab functions for various clinical trials, including pharmaceutical trials. As part of its core lab functions, the IAC co-ordinates and collects data from acquisition centres, quality controls the collected data, and can fully anonimize (including defacing) of the collected data.

3. As an **image processing lab** VUmc has an ongoing research line assessing existing software for analysing MRI scans of the human brain. Assessments include (1) which software package is the best for performing a particular segmentation or calculating a measure or biomarker, (2) the reliability of the software, (3) whether the software works correctly on data that was acquired under different circumstances than it was original designed for, such as different patients populations and/or other MRI sequences. It also develops/test combinations of existing software to perform extended measurement. For example, VUmc recently evaluated the "fluid" software (Dementia Research Group of London) for atrophy measures of the hippocampi instead of its routine use on the whole brain.

A summary of the pipelines in use at VUmc. While they do use other packages, (more detail is provided below) FSL appears to be the primary tool.

Researcher's Comments:

The most important packages for in the near future in FSL are TBSS,
maybe FIRST (for segmentation) and FDT (other DTI stuff) too.

Building blocks that can be combined into pipelines (this is how we usually work!):

- Image intensity homogenisation e.g. MNI N3.

- Geometric corrections e.g. BIRN Gradient non-linearity distortion correction.

- Registration:
- Linear e.g. FSL Flirt.

- Nonlinear e.g. DRG Fluid, FSL Fnirt.

- VBM e.g. SPM.
- DTI Tracing e.g. FSL FDT.
- Segmentation:
- Brain e.g. FSL BET.
- Grey / white matter e.g. FSL FAST.
- fMRI analysis e.g. FSL Melodic, FSL FEAT.
- Brain volume measurements e.g. FSL Siena, FSL SienaX.
- File format conversions.
- Image calculations (adding, subtracting, multiplying etc.)
- Morphological operations on images.

Examples of pipelines we currently use (identically applied for multiple subjects):

* Brain volume measurements :
- [needs fileconversions dicom/nifti]
- Bet
- Sienax + siena

* Non linear registration of brains :

- [needs fileconversions dicom/nifti/mgh/minc]
- Gradient distortion correction
- N3
- Bet
- Linear registration
- Fluid

* Non linear registration of hippocampi :

- [needs fileconversions dicom/nifti]
- [needs filconversions for manually drawn ROI files]
- Extraction of subimages within ROIs
- Fluid

* VBM

- [needs fileconversions dicom/nifti]
- Linear registration
- Nonlinear registration

- Segmentation (e.g. grey/white matter)
- Voxelwise calculations w.r.t. template/atlas/average

APPENDIX B: KI Pipelines

Examples of pipelines in use at KI SMILE:

Volumetric pipeline 1:

1. Data is moved into SMILE by
2. Downloading DICOM files from the internet
3. Making an import of DICOM images to the Hermes DICOM server (see below)
4. Sending data from the hospital's PACS system (patient database) to the Hermes DICOM server

Hermes is a commercial system (see www.hermesmedical.com) with their own software solutions and file format (InterFile). A DICOM server forms the image database and applications can be launched within the "GOLD" milieu. It is possible to develop lab-specific programs (in C) and turn them into local Gold applications.

5. The MR-data is subjected to structural analysis via the following steps:
6. Preprocessing with in-house Hermes application which reorients the brain and re-slices it
7. Registering the brain using 9 parameters in Hermes multimodality application
8. Performing brain extraction… (i.e. skull stripping)
9. Performing inhomogeneity correction…
10. Segmentating tissues…
11. Performing regional analysis…
12. …all with the help of in-house Hermes applications.

Note that all systems are inside the hospital's firewall. There is a special telerad connection between different hospitals in the Stockholm area which is used to transfer images between the hospitals' PACS systems.

Volumetric pipeline 2:

1. Images are continuously scanned and transferred in DICOM format via SCP from the camera (at another hospital) to an account in a Linux machine at SMILE.
2. The images are imported into Hermes
3. Register the brain in Hermes in cubic voxels
4. Start the program cutout and zoom in to make the brain bigger
5. Make new mean slices in multimodality (Process->Add slices) to average four slices into one
6. Use (Process->View) to show nine averaged slices at a time
7. Print out the views (with nine slices on each page)
8. Export the images in DICOM format from Hermes to a Linux machine
9. Use avwswapdim to change the axes (Hermes swaps axes around)
10. Use the freeware MRIcro to rescale the images (lessens "granularity")
11. Run BET in MRIcro to extract the brain
12. Use MRIcro to show the brain surface in 3D and compare it with the slice printouts to identify landmarks such as the frontal gyrus and the frontal/orbital cortex

13. Mark these landmarks by hand on the printout
14. Return to the Hermes system and use the in-house application Display MR from scaled to perform greyscale normalization
15. Step through the slices and draw ROI:s (region of interest) on the various gyri
16. Collect the ROI:s into a VOI (volume of interest) and save it
17. Run multimodality on both brain and VOI, using a personalized protocol with initial values
18. The VOI is displayed on the 3D image of the brain, check for consistency.

INNOMED project (SMILE part):

1. DICOM-data arrives on CD
2. The data is read into a Linux Ubuntu machine using rsync
3. The data is sorted through using various perl scripts to see that all parameters (date of birth etc) exist and that the images have been anonymized. A cross-check that all parameters are the same between visits is also made.
4. If everything is OK the data is uploaded to the DICOM archive database on the server outside KI's firewall (otherwise the responsible site is contacted).
5. The data is converted to MINC format.
6. A manual QC is made on the MINC images in the database, looking for among other things homogeneity, coverage and artifacts such as ringing and movement. If the images do not pass QC a rescan of the patient is requested.
7. The data is run through the CIVET pipeline, which uses perl scripts developed at McGill to do inhomogeneity correction, skull stripping etc.
8. After the processing is done, the server outside the firewall contains images, processed images and clinical data (also memory test results etc) for each scan.

At the moment we use the following programs sparingly, but have and will use them again:

- FSL.
- Brainvoyager.
- Matlab.
- AFNI.
- E-prime.
- Statistica.

APPENDIX C: FBF Pipelines

PIPELINES IN USE AT IRCCS - FBF			
PIPELINE NAME	MODULES USED	PRIORITY	NOTES
IMAGE CONVERTION	MRIconverter (freeware: http://lcni.uoregon.edu/~jolinda/MRIConvert/) / dcm2nii (freeware: http://www.sph.sc.edu/comd/rorden/mricron/dcm2nii.html)./ MNI ad hoc functions (mnc2dcm, dcm2mnc, ana2mnc, mnc2ana, minc2nii, nii2minc, ana2dcm, dcm2ana) (GNU: http://packages.bic.mni.mcgill.ca/) / FSL tools (fslchfiletype) (GNU: http://www.fmrib.ox.ac.uk/fsl/).	Low	
PET-FDG IMAGE PROCESSING PIPELINE	SPM2 (Matlab) & home made scripts (ppvspm.m; ppv_template.m; ppv_priors.m; ppv_complete.m; ppv_TPC; ppv_defaults.m, mask.m, normalize.m) (GNU: http://www.fil.ion.ucl.ac.uk/spm/software/)	High	
MRI IMAGE PROCESSING PIPELINE	SPM2 (Matlab) & home made scripts (ppvspm.m; ppv_template.m; ppv_priors.m; ppv_complete.m; ppv_TPC; ppv_defaults.m, normalize.m)	High	Changing from SPM2 to SPM5 (DARTEL)
DARTEL	SPM5 (Matlab)	High	
VOXEL BASED MORPHOMETRY (VBM)	SPM2 (Matlab) (GNU: http://www.fil.ion.ucl.ac.uk/spm/software/)	High	

INDIPENDENT COMPONENT ANALYSIS (ICA)	FSL-MELODIC (GNU: http://www.fmrib.ox.ac.uk/fsl/) / GIFT (Matlab) (GNU:http://icatb.sourceforge.net/)	Medium	
CORTICAL PATTERN MATCHING (CPM)	MRICro (freeware:http://www.sph.sc.edu/comd/rorden/mricro.html), SPM99/SPM2/home made scripts (MatLab), DISPLAY 1.4.2 (freeware: http://packages.bic.mni.mcgill.ca/), MNI functions (mni2ana, register, classify, ana2mnc, myana2mnc, crop_mnc, crop_back.sh, mincmask, mincresemple) (GNU: http://packages.bic.mni.mcgill.ca/), BrainSuite (freeware: http://brainsuite.usc.edu/), LONI analysis tools (Dual_warpe_warpcurve, Decoder_blend_all, mk_seg16bit, mk_gray, add_gray_to_inflated_LEFT1, add_gray_to_inflated_RIGHT1, pmap_apeVSctrl) (Private-Licence)	High	
WMHs MAPPING (WHITE MAPPING HYPERINTENSITIES)	Quanta 6.1 & other IDeALab Tools (svcleanup, 1.2.chg_parityFL, chg_nameFL_ima, ima2img, chg_data-matchParity, LinCoreg3, wmt_replace, sv) (GNU & Private PV-WAVE Licence: http://neuroscience.ucdavis.edu/idealab/software/index.php), BET function (freeware: http://www.fmrib.ox.ac.uk/fsl/bet2/index.html)	Medium	
DTI (TRACTOGRAPHY AND DIFFUSION TENSOR)	FMRIB's Diffusion Toolbox - FDT v2.0 (FSL), MRIconverter	High	
RADIAL ATROPHY MAPPING (RAM)	MRICro, SPM2 & home made scripts (MatLab), Dx (freeware: http://www.opendx.org/download.html), Seg3D, MNI functions (mni2ana, register, classify, ana2mnc), LONI analysis tools (make_UVL_*; 1st_script_tracer_avg_DIAG; 2nd_script_core_test_L_DIAG; 2nd_script_core_test_R_DIAG; Pmap_DistCore_DIAG) (Private-Licence)	High	

HIPPOCAMPUS VOLUME	MNI functions (dcm2mnc, preproc, mincresample, mincinfo, mincreshape, autocrop, volume_extraction, manualfit, linfit), REGISTER 1.3.6 (GNU: http://packages.bic.mni.mcgill.ca/), DISPLAY 1.4.2 (GNU: http://packages.bic.mni.mcgill.ca/), SPSS 12.0 (Private Licence).	Medium	
TOTAL INTRACRANIAL VOLUME (TIV)	MNI functions (dcm2mnc; autocrop; mincinfo; mincreshape; mincresample), DISPLAY 1.4.2.	Low	