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VI-SEEM

VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean



Deliverable D4.1

Data sources and services deployment plan

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Abstract: Deliverable D4.1 describes the list of data sources to be integrated in the VRE as well as the deployment plan for the data-related services of the VRE.

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Preface

In the last decade, a number of initiatives were crucial for enabling high-quality research - by providing e-Infrastructure resources, application support and training - in both South East Europe (SEE) and Eastern Mediterranean (EM). They helped reduce the digital divide and brain drain in Europe, by ensuring access to regional e-Infrastructures to new member states, states on path to ascension, and states in European Neighborhood Policy area – in total 14 countries in SEE and 6 in EM.

This VI-SEEM project brings together these e-Infrastructures to build capacity and better utilize synergies, for an improved service provision within a unified Virtual Research Environment (VRE) for the inter-disciplinary scientific user communities in the combined SEE and EM regions (SEEM). The overall objective is to provide user-friendly integrated e-Infrastructure platform for regional cross-border Scientific Communities in Climatology, Life Sciences, and Cultural Heritage for the SEEM region; by linking compute, data, and visualization resources, as well as services, models, software and tools. This VRE aspires to provide the scientists and researchers with the support in full lifecycle of collaborative research: accessing and sharing relevant research data, using it with provided codes and tools to carry out new experiments and simulations on large-scale e-Infrastructures, and producing new knowledge and data - which can be stored and shared in the same VRE. Climatology and Life Science communities are directly relevant for Societal Challenges.

The driving ambition of this proposal is to maintain leadership in enabling e-Infrastructure based research and innovation in the region for the 3 strategic regional user communities: supporting multidisciplinary solutions, advancing their research, and bridging the development gap with the rest of Europe. The VI-SEEM consortium brings together e-Infrastructure operators and Scientific Communities in a common endeavor.

The overall objective is to provide user-friendly integrated e-Infrastructure platform for Scientific Communities in Climatology, Life Sciences, and Cultural Heritage for the SEEM region; by linking compute, data, and visualization resources, as well as services, software and tools.

The detailed objectives of the VI-SEEM project are:

1. Provide scientists with access to state of the art e-Infrastructure - computing, storage and connectivity resources - available in the region; and promote additional resources across the region.
2. Integrate the underlying e-Infrastructure layers with generic/standardised as well as domain-specific services for the region. The latter are leveraging on existing tools (including visualization) with additional features being co-developed and co-operated by the Scientific Communities and the e-Infrastructure providers, thus proving integrated VRE environments.
3. Promote capacity building in the region and foster interdisciplinary approaches.
4. Provide functions allowing for data management for the selected Scientific Communities, engage the full data management lifecycle, link data across the region, provide data interoperability across disciplines.
5. Provide adequate user support and training programmes for the user communities in the SEEM region.

6. Bring high level expertise in e-Infrastructure utilization to enable research activities of international standing in the selected fields of Climatology, Life Sciences and Cultural Heritage.

The VI-SEEM project kicked-off in October 2015 and is planned to be completed by September 2018. It is coordinated by GRNET with 15 contractors from Cyprus, Bulgaria, Serbia, Hungary, Romania, Albania, Bosnia-Herzegovina, FYR of Macedonia, Montenegro, Moldova (Republic of), Armenia, Georgia, Egypt, Israel, Jordan. The total budget is 3.300.000 €. The project is funded by the European Commission's Horizon 2020 Programme for Excellence in Science, e-Infrastructure.

The project plans to issue the following deliverables:

Del. no.	Deliverable name	Nature	Security	Planned Delivery
D1.1	Project management information system and "grant agreement" relationships	R	CO	M01
D1.2	3-Monthly progress report	R	CO	M03n *
D1.3a	First period progress reports	R	CO	M18
D1.3b	Final period progress reports	R	CO	M36
D2.1	Internal and external communication platform, docs repository and mailing lists	DEC	PU	M02
D2.2	Promotional package	DEC	PU	M04
D2.3	Dissemination and marketing plan	R	PU	M05
D2.4	Training plan	R	PU	M06
D2.5	Promotional package with updates	R	PU	M16
D2.6	1st Dissemination, training and marketing report	DEC	PU	M18
D2.7	2nd Dissemination, training and marketing report	R	PU	M35
D3.1	Infrastructure and services deployment plan	R	PU	M04
D3.2	Service registry, operational and service level monitoring	R	PU	M12
D3.3	Infrastructure overview, assessment and refinement plan	R	PU	M18
D3.4	VRE AAI Model and compatibility with other eInfrastructures	R	PU	M27
D3.5	Final infrastructure overview and assessment report	R	PU	M36
D4.1	Data sources and services deployment plan	R	PU	M06
D4.2	Description of the initial deployed data services	R	PU	M11
D4.3	Description of the final data platform available to VRE users	R	PU	M23
D4.4	Final report on data, services, availability and usage	R	PU	M35

D5.1	Detailed technical implementation plan for VRE services and tools	R	PU	M04
D5.2	Data management plans	R	PU	M06
D5.3	User-oriented documentation and training material for VRE services	R	PU	M13
D5.4	Report on integrated services and the VRE platform	R	PU	M14
D5.5	Final report on integrated services and the VRE platform	R	PU	M36
D6.1	Framework for VRE resource and service provision	R	PU	M09
D6.2	1st Report of open calls and integration support	R	PU	M20
D6.3	Sustainability and business model	R	PU	M24
D6.4	2nd Report of open calls and integration support	R	PU	M36

Legend: R = Document, report, DEC = Websites, patent fillings, videos, etc., PU = Public, CO = Confidential, only for members of the consortium (including the Commission Services).

* $n=1,2,3,\dots,12$

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Glossary

AAI	Authentication and Authorization Infrastructure
AARC	Authentication and Authorization for Research Collaboration
API	Application Programming Interface
CA	Certification Authority
CDI	Collaborative Data Infrastructure
CDMI	Cloud Data Management Interface
DSI	Data Storage Interface
DSS	Data Staging Script
EM	Eastern Mediterranean
EPIC	European Persistent Identifier Consortium
EUDAT	European Data Infrastructure
GB	Gigabyte
GPFS	General Parallel File System
GPU	Graphics Processing Unit
GRIB	GRIdded Binary
GridFTP	File Transfer Protocol for Grid computing
HDFS	Hadoop Distributed File System
HPC	High Performance Computing
HTTP	Hypertext Transfer Protocol
iRODS	integrated Rule-Oriented Data System
iCAT	iRODS metadata catalogue
MB	Megabyte
mmCIF	macromolecular CIF (Crystallographic Information File)
MPI	Message Passing Interface
netCDF	network Common Data Form
NFS	Network File System
OpenMP	Open Multi-Processing
OPeNDAP	Open-source Project for a Network Data Access Protocol
pbdR	Programming with Big Data in R
PBS	Parallel Batch System
PID	Persistent Identifiers
PEP	Policy Enforcement Point
PID	Persistent Identifier
PRACE	Partnership for Advanced Computing in Europe
REST	Representational State Transfer
SC	Scientific Community

SEE	South East European
SEEM	South East Europe and Eastern Mediterranean
SLA	Service Level Agreement
SLURM	Simple Linux Utility for Resource Management
SPMD	Simple program, Multiple data
SQL	Structured Query Language
TB	Terabyte
UI	User Interface
UUID	Universally Unique Identifier
VAS	VI-SEEM Archival Service
VI-SEEM	VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean
VRS	VI-SEEM Repository Service
VM	Virtual Machine
VRE	Virtual Research Environment
WP	Work Package

Executive summary

What is the focus of this Deliverable?

The Data Management Lifecycle Work-package aims to provide integrated data management solutions for the Scientific Communities (SC) allowing the management of the lifecycle of scientific data to be generated, stored, processed and re-used.

This deliverable, the "Data Sources and Services Deployment Plan" provides an overview of the work done in the context of the tasks defined in the DoA [1] of the VI-SEEM project regarding the design of generic services related to the management of data relevant to the three Scientific Communities of the project namely Life Sciences, Digital Cultural Heritage and Climate.

The deliverable assesses the needs of the three scientific communities identifying: data sources, generic and specific data management services, and their requirements.

The set of data services to be offered by VI-SEEM to satisfy the requirements defined by the communities is designed to offer a comprehensive data management solution.

The deployment of these operational data services is planned in detail and presented in this deliverable.

What is next in the process to deliver the VI-SEEM results?

The "Data Sources and Services Deployment Plan" will be used by WP4 to carry out the implementation of such services. Next, WP5 will use the results to design parts of the Virtual Research Environment (VRE) platform. WP4 will work in collaboration with WP5 to collect, pre-process, curate and make available these datasets through the VRE platform. WP3 will provide support for integrating Authentication and Authorization Infrastructure with candidate data services as well as all the necessary storage resources and infrastructure to run the storage services.

The results and conclusions from this deliverable will be used by the following activities:

- WP4.2 - Data access, preservation and re-use
- WP4.3 - Data collection and provisioning
- WP4.4 - Data analysis
- WP5.3 - Development of the VRE platform
- WP5.4 - Overall integration of services

What are the deliverable contents?

The deliverable contents include a detailed overview of the requirements of different Scientific Communities in terms of data management, including:

- Data sources and activity type
- Data format and metadata
- Data volumes and required services

Datasets used and produced are named and categorized by type (e.g. simulation, observational), format, and typical size. The name and description of each application related to the dataset (as described by the developers) is also given. It was important to

identify the required types of data services as well as amount of storage resources required for each application, thus making a concrete plan for the provision of services and the underlying storage to cover the needs of the three scientific communities.

The deliverable provides also information on the existing data services available among the infrastructure partners of the VI-SEEM consortium as well as the landscape of storage-related services in Europe.

Based on the careful analysis of each application's requirements, and identification of similar services used in the region and Europe, six data services were identified and are planned to be deployed by WP4. For each service, as description of several VI-SEEM specific use-cases is presented in the deliverable.

After identifying these data services, the next important task is the planning of deployment by assigning the responsible partners, and the detailed operational services to be offered by each partner.

Conclusions and recommendations

Since for the VI-SEEM scientific communities the input and output datasets vary in size, type, planned preservation lifetime, and workflow of use, it is crucial to provide support to all identified use cases by offering tailored data services. Various types of functionalities are needed. Data movement close to the processing facilities of the infrastructure requires high bandwidth, while metadata information is important to create a repository of scientific data. Data storage for longer periods needs archiving infrastructure. Switching between different types of data storage is a rather complex process that needs appropriate management tools.

To offer a comprehensive data management solution, capable of storing and serving different types of data for different timeframes, a set of different integrated services has to be deployed.

Generic data services available in the region have been assessed in this deliverable, and suitable services were chosen based on the user requirements. The following services were identified as types of services or capabilities to be deployed within the VI-SEEM project:

- Simple data sharing service
Service supporting storage of simple data objects (files) for each user
- Data repositories
A repository of data providing access to upload and identify datasets
- Data archiving
Long-term storage of data providing storage for large data sets and possibly offer slow access
- Work storage space / local storage
A short-term storage space with fast access to the computation resources
- Data search and catalogue
A catalogue of data sets that is easy to search by being associated with metadata and along with the assigned persistent identifier of each dataset
- Data analysis
Set of services to be provided for Big Data analytics (e.g. Hadoop service)

- Data access and security capabilities
A mechanism for users to authenticate and authorise themselves for accessing secure storage services and already existing data
- Persistent identifier capabilities
Methods to reference scientific data in order to name these data in a unique and timeless way

For these services and capabilities a specific implementation has been identified based on the experience of the VI-SEEM partners as well as the pan-European trends in data related services (mainly based on the flagship EUDAT2020 project).

The deployment of the data service portfolio needs to be carefully planned to offer a homogenous level of service to all users from all countries in the region. All geographic areas need to be covered by available services to provide fast connectivity and high transfer speeds close to the processing infrastructure, because of the big size of data in some cases.

This deliverable describes the plan for the deployment of each service component.

Integration is crucial and requires close collaboration with WP3 regarding AAI, and availability of the underlying data storage infrastructure, as well as providing technologies and interfaces relevant to the work of WP5 that will enable the creation of VRE platform using the deployed data services offered by WP4.

A total of 330 TB of disk and 510 TB of tape capacity have been offered from partners of the VI-SEEM project in order to support different services.

1. Introduction

WP4 aims to provide integrated data management solutions for Scientific Communities (SC) allowing the management of the lifecycle of scientific data to be generated, stored, processed and re-used. According to best practices a questionnaire was constructed and given to scientific communities to gather essential information about topics discussed in this document. This work was done in cooperation with WP5 and provided the baseline for the Data Management Plan [3] (D5.2) as well.

D5.1 of WP5 [4] has already presented the detailed structure of the survey therefore in this deliverable we only focus on parts closely related to data management. Sections "System requirements" and "Data services" and section "Application details" that have some additional relevant information.

The data-relevant parts of the questionnaire covered the following areas:

- Datasets
- Definition of datasets including existing data, data produced by the application, and output data
- System requirements with regards to storage space
- Definition of storage space and required preservation time
- Standards for data and metadata
- Definition of the data and metadata requirements
- Data management needs
- Definition of: technical, security and other data management requirements including the possibilities of using workflows; sharing methods required; possible duplication and backup requirements
- Data service needs
- Identifying use cases for data services provision; determining the data management needs of each application.

Detailed requirements as depicted from the results of the survey are being discussed in the following chapters, however the main result of the survey is the six types of generic data services identified:

a) Simple data sharing

There is a common need for sharing of simple scientific data files among scientists within a workgroup or with the whole community. This service needs to reach a wide audience therefore the usage has to be as simple as opening a webpage and uploading/downloading content. Simple Cloud Storage services are common and widely used solution to this problem.

b) Data repositories

To manage and share the data produced by communities in a standardized way, data repositories need to be operated. WP4 will have to deploy services for publishing scientific datasets through integrating persistent identifiers (PIDs) to each data set and making sure that the data can be accessible at any point using such PIDs.

c) Data archiving

Users of different applications indicated the requirement of storing data for longer periods of time (e.g. more than 12 months after the end of the data processing project). This requires reliable service able to store large amounts of data for multi-year timeframe. The data stored in this way is only accessed occasionally, and therefore fast access is not necessary.

d) Work storage space / Local storage

To make use of computational services, there is a need for storing data for limited amount of time, but on a system offering fast access to the compute resources to avoid situations when slow data access limits productivity - when computation capacity would be available. To tackle this challenge, computational facilities often offer work or scratch storage space with a fast connection to the compute resources (storage often available in the same data centre) offering temporary storage capacity to accommodate input data and to store output data produced throughout the scientific computational processes (e.g. Grid or HPC usage).

e) Data search and catalogue

Large numbers of data sets produced and stored by different scientific groups need sophisticated support mechanisms to be indexed and searched. A catalogue of scientific datasets is required to enable easy ways to locate data and their metadata. Application-specific data repositories along with community-specific external data repositories need to be indexed and VI-SEEM Data repository and VI-SEEM Archival service needs to be available to this service, offering browsing through data sets.

f) Data analysis

While data analysis is processing data, it is still interpreted as a data service, as this is one of the most important services related to Big Data challenges. VI-SEEM HPC, Grid or Cloud infrastructure is able to provide computational requirements for data analysis. Hadoop is a common example of data analytics, utilizing various compute resources.

Those services need to be accompanied by appropriate Authorization and Authentication mechanisms, while for some of those (data repositories and data archiving) it is important that data sets are assigned Persistent identifiers (PIDs).

An internal survey towards the VI-SEEM infrastructure providers was also conducted focusing on the identification of existing data service capabilities and resources in the VI-SEEM region. In this survey partners were asked to share their experience and data service solutions used for each of the generic data services identified.

Thus sections 2, 3 presents the VI-SEEM scientific community requirements as presented in the application's related survey, while Section 4 gives an overview of the data/storage related services in the region and in Europe. Section 5 provides information on the specific data services to be deployed by VI-SEEM and the related deployment plan. Finally, Section 6 provides the conclusions of the deliverable.

2. Scientific community requirements

In this chapter we present results of the application questionnaire. A total of 48 answers were provided:

- 17 for Climate Scientific Community
- 15 for Cultural Heritage Scientific Community
- 16 for Life Sciences Scientific Community

As not all applications groups had an exact estimation of their storage needs at the time of survey we expect that some estimations (e.g. required storage space for the application) might be inaccurate. This might mean more storage capacity will be requested at the later stage of the project. Hence the user requirements will be updated throughout the project when new details are revealed. Results are presented for each community in the subsections below. More information on the data sources described below can be found in the Data Management Plan [3].

2.1. *Climate scientific community*

2.1.1. Data sources and activity type

The climate modelling and weather forecasting communities use mainly two types of data: simulation and observational data. These kinds of data vary in terms of volume, terms of access and data management. In particular, the full output of simulation data cannot practically be transferred because of its size. The data are processed remotely, transferring only the final results and metadata, to enable reproduction of the simulation if needed. Simulation results are kept in internationally managed data repositories and are accessible to users. Observational data are diverse, such as weather station observations, satellite images and historical weather records. Access is scattered, as most data are hosted locally, and most data sources are freely accessible for non-commercial research and education.

2.1.2. Data format and metadata

Most applications (eleven out of seventeen) make use of netCDF. There are also three applications that work with the GRIB (GRIdded Binary) data format.

2.1.3. Data volumes and required services

Initial feedback from the users' survey demonstrates that:

- Most (10 out of 17) applications in this SC will require 10-100GB temporary space.
- For longer term storage (data repositories, archiving) most of them fall into two categories: 2-10TB (six applications) and 10-50TB (five applications).
- There also exists need for cloud related storage resources with 3-4 VMs and 100-500GB per VM.

The applications' needs regarding the required storage services are:

- Simple data sharing: 4 applications
- Data repositories: 8 applications
- Data archiving: 10 applications
- Data analysis: 10 applications

There are 3 applications for which no information on required services was given.

2.2. Digital cultural heritage scientific community

2.2.1. Data sources and activity type

Most output datasets from applications (nine out of fifteen) will be provided as results of image processing. One third of the applications will work with text files and there is one application that will handle observational data.

In the field of Digital Cultural Heritage the data produced and used is diverse, and applications will be developed to handle the diversity of the data. Examples include image search engines, trained classifiers, OCR for handwriting recognition. In addition, documentation of chemical and physical material properties of structures, works of art and artefacts, subsurface imaging and regional datasets with geo-referenced data will be used. Images of ancient coinage, inscriptions and digitized books necessitate tools such as ontology engineering and visualization viewers. Furthermore, 3D reconstruction tools, modelling and simulation are used for scientific visualization and geometric analysis of the data.

2.2.2. Data format and metadata

There is no widespread use of one format (like in Climate SC). There are some applications that use a variety of standards (CIDOC-CRM, Dublin Core, UNIMARC etc.) and also some others that use custom (domain specific) formats.

2.2.3. Data volumes and required services

Initial feedback from the users' survey demonstrates that:

- For temporary storage needs spread evenly in four categories: 1-5GB, 10-100GB, 100-500GB and 500GB-1TB.
- For longer term storage (data repositories, archiving) most require 1-2TB.
- Applications would also take advantage of cloud storage resources: ~9 VMs with 100GB per VM, ~16 VMs with 200GB per VM, ~4 VMs with 512GB per VM and one application that needs one VM with 1TB of storage space.

The applications' needs regarding required services are:

- Simple data sharing: 7 applications
- Data repositories: 7 applications
- Data archiving: 9 applications
- Data analysis: 1 application

There are two applications for which no information on required services were given.

2.3. Life sciences scientific community

2.3.1. Data sources and activity type

Most output datasets from applications (ten out of sixteen) will be provided as results of simulations. There are five applications that will provide experimental data, and also four applications that will process images.

In life sciences section, the data will pertain to the six themes. These include: modelling and molecular dynamics study of drug targets, computer-aided drug design and analysis of next generation DNA sequencing data. Additional data sources comprise synchrotron data analysis of protein structures, image processing and computational DNA and RNA simulations.

2.3.2. Data format and metadata

Similar to Digital Cultural Heritage SC, there is no widespread use of one format. Some makes use of PDBx/mmCIF and there are also a couple of applications with custom (domain specific) formats.

2.3.3. Data volumes and required services

Initial feedback from the users' survey demonstrates that:

- Most (5 out of 16) applications in this SC will require 10-100GB temporary space. 3 applications require under 5GB and for another 3 applications between 300GB and 1TB. There is one application that requires extreme amounts of temporary storage (50TB).
- Regarding longer-term storage (data repositories, archiving), needs are spread quite evenly in four categories: under 100GB, 100GB-1TB, 1-2TB and above 10TB.
- Applications could also make use of cloud storage resources: 2 VMs with 50GB per VM, 1 VM with 100GB storage space, 3 VMs with 150GB per VM and 4 VMs with 300GB per VM.

Applications needs regarding required services are:

- Simple data sharing: seven applications
- Data repositories: five applications
- Data archiving: nine applications
- Data analysis: two applications

There are 3 applications for which no information on required services were given.

2.4. Summary of community requirements

Figure 1 shows the distribution of the number of applications requiring a specific type of storage service in total and for each scientific community. Overall, there is a roughly

equal demand for simple storage, data archiving system and data repositories, with less demand for in-situ interactive analysis of production data.

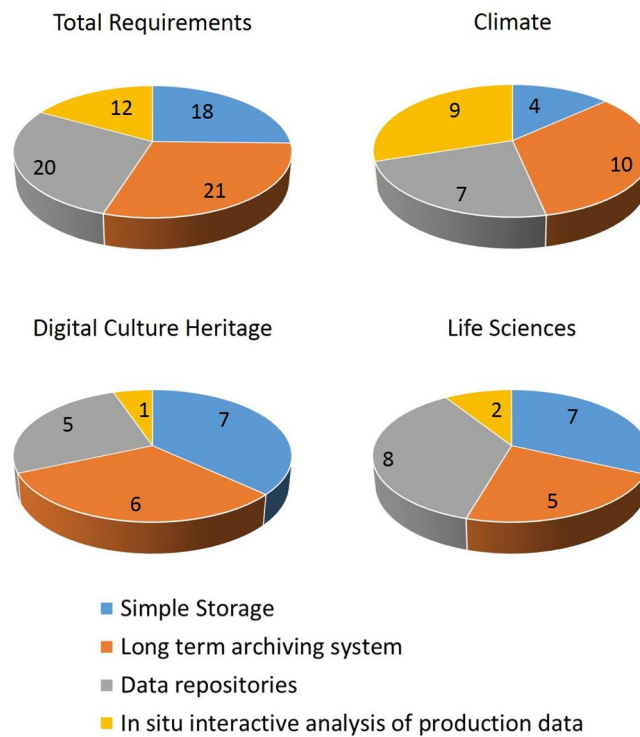


Figure 1 - Number of applications requesting a specific type of storage services overall and per scientific community

Figure 2 shows the distribution of the requested amount of storage per application in based on the responses of the questionnaire. The majority of the applications request between 0-5 TB of storage, while some applications request above 5 TB of storage.

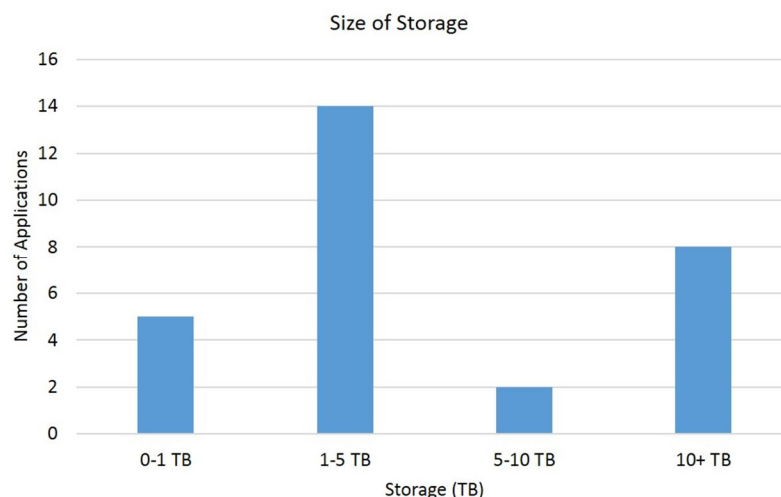


Figure 2 - Size of storage vs number of applications requesting it

3. Data sources

3.1. Data categorization

Data to be collected by the VI-SEEM scientific communities can be categorized as:

1. Simulation data: data as a result of modelling and simulation, such as climate projections
2. Experimental data: data as a result of experimental processes, such as biological data
3. Observational data: data as a result of observational surveys, such as climate data
4. Image data: data that consist mainly of images, such as medical and archaeological artefacts
5. Text data: data that consist mainly of text, such as books and archaeological artefacts

In conjunction with the above-mentioned types of data, metadata will be also generated and collected. Metadata are defined as data that provide information about the associated data. Such metadata are tags for better search and retrieval, context about data collection and data formats.

3.2. Community datasets

For each scientific community, we provide a table identifying the data sets to be produced and/or used by each application identified in the survey. For each data set, information about the data type is included alongside the data format, associated metadata and size. The types of generic data service required for managing each data set is also provided.

3.2.1. Climate scientific community

Application Acronym	Data source name	Data Type	Format / Associated metadata	Size	Required data Service
WRF-ARW	Daily model output (raw output data as well as post-processed output)	Simulation	NetCDF, Gif	7.5 GB	Simple, Analysis, Scratch
VINE	Observation dataset on dust particles in ambient air available from Georgian National Environmental Agency	Observational, Simulation	NetCDF, Grib	2 TB	Archive, Scratch
RCM MENA-CORDEX	Gridded datasets of temperature and rainfall for the MENA, via the CORDEX data portals	Simulation	NetCDF	43.5 TB	Archive, Repository, Analysis, Scratch
HIRECLIMS	ROCADA (Romanian Climatic Dataset)	Simulation	NetCDF	8.2 GB	Archive, Repository, Analysis Scratch
WRF-Chem (NOA)	WRF-Chem dust aerosol concentrations and various meteorological parameters	Simulation	NetCDF	200 TB	Archive, Analysis Scratch
DREAMCLIMATE	Downscaled atmospheric-dust DREAM covering wide North Africa, Southern Europe and Middle East regions.	Simulation	NetCDF, Grib	20 TB	Archive, Repository, Analysis Scratch
DRS-ACS	Characteristic constants describing the kinetics of atmospherically relevant processes and spectroscopic properties of the involved species.	Simulation	Text	1 TB	Scratch
ENB-RCM	Rainfall records at rain gauge stations in the Eastern Nile Basin	Observational, Simulation	NetCDF	N/A	Simple, Repository, Archive Scratch
OpenFOAM	Daily recorded meteorological parameters	Observational	ASCII, other	N/A	Simple Scratch

Table 1 - Data sets of Climate SC

3.2.2. Digital Cultural Heritage scientific community

Application Acronym	Data source name	Data Type	Format / Associated metadata	Size	Required data Service
Dioptra	RTi dataset of ancient Cypriot coinage	Image	RTi	N/A	Archive Scratch
CSAD	Hundreds of RTi files of Ptolemaic inscriptions	Image	RTi	N/A	N/A
3DINV	Existing and new datasets of geoelectrical tomographic data collected from field campaigns.	Observational	TEXT, PNG	Between 1Mb to 10Mb	Simple Scratch
AutoGR	A demo dataset will be used for demonstration purposes share with the VI-SEEM community for research purposes.	Image	JPG, TIF, GeoTIFF, PNG / georeferencing info	Between 10Mb and 200Mb	Simple, Archive Scratch
ELKA	Word, .pdf files of Karamanlidika texts	Text	Word, pdf	N/A	Archive Scratch
Manuscript	Datasets of digitized handwritten documents in Arabic or Hebrew	Text	/XML	N/A	Simple, Repository, Archive Scratch
PETRA	MEGA Jordan GPS/ geo-referenced data	Image		N/A	Simple, Archive Scratch
BVL	Banatica database: 1000 books and 200 digitized books	Text	JPEG, PDF, TEXT	Between 1Mb and 200Mb	Simple, Repository, Archive Scratch
VirMuf	3D models, CH Multimedia content and geo-spatial data	Image		N/A	Repository, Archive Scratch
CH-CBIR	Aerial images with annotated land cover types. Learned image representations for imagery in the areas of cultural heritage and remote sensing.	Image	JPEG, TIFF	Between 3GB and 10GB	Simple, Archive Scratch
IMC4CH	Digital material for archaeological monuments	Image	CIDOC-CRM	N/A	Repository, Archive Scratch

Table 2 - Data sets of Digital Cultural Heritage SC

3.2.3. Life Sciences scientific community

Application Acronym	Data source name	Data Type	Format / Associated metadata	Size	Level of Access
MD-Sim	MD trajectories of oncogenic proteins with mutations relevant to the SEEM area	Simulation		N/A	Simple, Archive Scratch
DICOMNetwork	Generalized statistical datasets. Patient dataset available after special permission or relevant anonymization of data.	Image	XML. JSON	2MB-1.5GB	Repository, Archive Scratch
CNCADD	Produce and share parameter sets relevant to the community	Simulation	Text	1TB	Scratch
PSOMI	Datasets with molecule synthesis results.	Experimental	.pdb, .gro, .namd, .psf, .pdf ...	up to 200 MB	Simple, Archive
SQP-IRS	Biological dataset. Computational vs. Experimental database for proteins secondary structures. Crystallographic vs. Spectroscopic database for selected targeted proteins	Simulation and experimental		N/A	Archive Scratch
THERMOGENOME	Datasets with data for thermodynamic stability of RNA/DNA and DNA/DNA duplexes for all transcripts, exons, introns, 5-UTRs, 3-UTRs for Homo sapiens (human), A. thaliana, C. elegans, D. melanogaster, D. rerio.	Experimental	txt file	400GB	Repository, Archive, Analysis Scratch
MDSMS	The molecular dynamics simulation of mixed systems	Simulation	pdb, trr, xtc, dcd	4TB	Archive Scratch

Table 3 - Data sets of Life Sciences SC

4. Data services

After analysing the requirements of the scientific communities six concrete types of generic data services to be deployed have been identified. These are:

a) Simple data sharing

Simple storage for file sharing is an easy-to-use data exchange service. It will allow scientific communities to store and synchronize their active data across different desktops, as well as to share these data with team members and other research communities.

Since the focus of the service is on active data (data under development, frequently changed), it will allow versioning of all ingested files. Considering that this service is intended for the volatile phase of data lifecycle, no persistent identifiers will be used for data objects within.

b) Data repositories

The main storage service that will allow the users of the VI-SEEM VRE to deposit and share data is the VI-SEEM Repository Service (VRS). Such a repository in VI-SEEM will be the main repository for hosting the "Regional Community Datasets" and therefore provide a component to host one of the main services of the VRE as specified in D5.1. It can also be used to host publications and their associated data as well as software or references to software and workflows, used to generate such data and publications.

The VRS will be also the service for storing simplified data formats such as images, videos or others suitable also for the general public. The VRS is therefore the platform to host all of the types of data specified in the VI-SEEM data management plan, D5.2, when users consider it suitable i.e. for sharing.

In general, the VRS will be hosting small to medium sized data. For very large datasets other services such a Data Staging or Data Archiving might be more suitable so that the data sets can be stored close to the processing power and in larger data stores available in the region i.e. Tape Libraries.

The VI-SEEM repository service is a generic repository service that can be used for data storage by any researcher associated with the VI-SEEM project or has gained access to the VI-SEEM services using the corresponding access policies that will be specified by WP6 of the project. Specific community or application-based repositories are also to be deployed in the VI-SEEM VRE.

Such repositories are the Clowder and Live Access Server repository described in sections 4.1.2 and 4.1.3. These applications will be harvested for metadata. Integration of these into VI-SEEM Data Discovery Service is required by VI-SEEM scientific communities.

The VI-SEEM repository service will also support the requirements for quality assurance, sharing, searching, provision of metadata, persistent identifiers, etc, of the VI-SEEM data management plan as specified in deliverable D5.2.

c) Data archiving

Users of VI-SEEM need a storage service that helps them store research data for longer periods of time, 6-12 months at least. The generic data service that will provide long-term data archival is the VI-SEEM Archival Service (VAS).

The VAS is a distributed service connecting multiple sites (at different partners) together. Such a system makes available different tiers of storage resources for reliable storage (with integrity check mechanisms in place) and handles other aspects of science communities' needs, e.g. off-site replication or data retention. A policy system will help to ensure such requests from users of VI-SEEM. Coupled with data staging capabilities the VAS will provide safe data replication across sites in accordance with the VI-SEEM data management plan as specified in D5.2.

While the VI-SEEM Repository Service (VRS) will be hosting small to medium sized data, the VAS is more intended for larger datasets therefore we will make use of tape libraries as they are cost-effective (better €/TB) and better suited for long-term preservation. VAS service will also support the requirements for quality assurance, sharing, searching, provision of metadata, persistent identifiers, etc, of the VI-SEEM data management plan as specified in deliverable D5.2.

d) Work storage space / Local storage

Efficient processing of research data at computing sites of the VI-SEEM VRE requires a data service that provides quasi-local storage spaces that are "close" to the computing resources and can be used for short-term storage while performing the computations.

It is expected to provide enough capacity for performing the required calculations while avoiding bottlenecks. For many applications the local hard drives of the compute nodes are not sufficient and thus additional techniques from the domains of HPC and Cloud are used, e.g., parallel filesystems, network-attached/virtualized storage, etc.

This type of service in VI-SEEM will exploit different solutions used at partner sites, so it is mandatory to couple it with a common data staging facility. For the efficient transfer of large datasets GridFTP will be used which is the de facto standard for high-performance, secure, reliable data-transfer in the HPC community.

e) Data search and catalogue

To facilitate discovery of data stored in different types of storage services, ranging from application specific data repositories to the generic services presented in this deliverable as well as data stored in external data repositories but still relevant to the VI-SEEM SCs, a specific Data Discovery Service for the VI-SEEM supported scientific communities is required.

The VI-SEEM Data Discovery Service will cover several of the researchers' needs for data discovery such as:

- Integration of data from:
 - o the VI-SEEM Data repository and VI-SEEM Archiving services
 - o application/domain-specific data service developed within WP5 activity
 - o data repositories external to the region
- Quick and easy search and identification of collections of scientific data from all the above types of repositories
- Allow for browsing and having a quick overview of the harvested data
- Browsing through data sets

The above functionality will be provided by means of harvesting specific metadata that the other data services make available to the Data Discovery Service. The

metadata that will be provided for the discovery service can be decided by each community or application based on their needs.

f) Data analysis

The analysis of research data can be done in various ways. It is expected that computationally intensive data analysis is done using the VI-SEEM HPC, Grid or, to lesser extent, Cloud infrastructure.

We also have to take into account the prevalence of Big Data so we consider some services and tools that were requested by substantial number of applications and are typically used for tackling this challenge.

Two main scenarios for provisioning data analysis capabilities of this type exist in the VI-SEEM environment. Some applications may create their own data analysis frameworks using the VI-SEEM Cloud infrastructure.

Due to the flexibility of the Cloud services that partners are offering and the substantial resources behind them application developers and users can establish services that deliver the desired data processing capability to the scientists that are end-users of the application. VI-SEEM may provide training and limited support but such a framework would be the sole responsibility of its designer.

The surveys that were performed by the project revealing certain commonalities among applications, especially within the same scientific domain, which speaks in favour of the second way of providing data analysis capabilities. Namely, we can provide access to sufficiently generic data analysis framework, built using industry standard open source components.

Those services need to be accompanied by appropriate Authorization and Authentication mechanisms, while for some of those (data repositories and data archiving) it is important that data sets are assigned Persistent identifiers (PIDs).

Beyond these generic services, following the user needs, specific services are also going to be identified, implemented and deployed in later phases of the project.

4.1. Existing data services in the region

VI-SEEM partners - who are registered as providing storage services - were asked to share details of their already existing services and experiences regarding the generic data services identified by the survey, or additional domain-specific services. A synopsis of their answers is presented for each category as follows.

4.1.1. Simple data sharing

4.1.1.1 Owncloud

Several partners have deployed or have experience with ownCloud. ownCloud describes itself as: "a self-hosted file sync and share server. It provides access to your data through a web interface, sync clients or WebDAV while providing a platform to view, sync and share across devices easily — all under your control. ownCloud's open architecture is extensible via a simple but powerful API for applications and plugins and it works with any storage." Some of the project partners are also interested in extending ownCloud, so it could support project-wide AAI, metadata, etc. It was also noted that B2DROP (developed by EUDAT) appears to be a custom skin on top of ownCloud so it would not be much harder to adopt it. Based on the fact that ownCloud is already present in the SEEM area and that no other service was mentioned in answers it is clear that ownCloud is a strong candidate for this type of service. [1]

4.1.1.2 Pithos+

Pithos+ is the Virtual Storage service of ~okeanos (<https://okeanos.grnet.gr>). Pithos+ enables users to store files online, share them with friends and colleagues and access them anytime, from anywhere in the world. It also allows access from inside the VMs hosted in the ~okeanos IaaS service. Pithos+ allows user to share files and content with other Pithos+ users or friends, provide a simple and intuitive Web UI to upload and organize user's files, allows the usage of Agkyra, the Pithos+ file syncing client to sync user's local folders with Pithos+.

Technically is an implementation of the OpenStack Object Storage API in Python and Django. At the backend, every file is stored as a collection of content-addressable blocks; Using content-based addressing for blocks brings deduplication (identical blocks of distinct files are stored only once) and efficient synchronization; a client may identify the parts of files which have changed either locally or remotely, and upload or download only the modified parts. Pithos+ comes with a full set of Web-based, command-line and native clients, all making calls to the same API.

Pithos+ is an integral part of ~okeanos: Both system Images and custom, user-provided Images are files on Pithos+ and are registered with Plankton to become available for VM creation.

4.1.2. Data repositories

There were not much details in answers regarding this type of service. For generic data services partners are willing to provide gridFTP support to enable access to data

repository. Apart from this some partners have experience providing domain-specific services with tools such as Clowder (see section 4.1.3.2) and Live Access Server. According to D2.3 of WP2 such features would be provided as domain-specific services to science communities so these tools will be candidates for adoption at a later phase of the project.

4.1.2.1 Live Access Server

The Live Access Server (LAS) is a highly configurable web server designed to provide flexible access to geo-referenced scientific data. It can present distributed data sets as a unified virtual data base through the use of networking. [16]

LAS enables the data provider to:

- unify access to multiple types of data in a single interface
- create thematic data servers from distributed data sources
- offer derived products on the fly
- remedy metadata inadequacies (poorly self-describing data)
- offer unique products (e.g. visualization styles specialized for the data)

LAS enables the user to:

- visualize data with on-the-fly graphics
- request custom subsets of variables in a choice of file formats
- access background reference material about the data (metadata)
- compare (difference) variables from distributed locations

4.1.3. Data archiving

Two partners mentioned this type of service. One of them has a long time experience with OpenAFS while the other has Clowder in place for Data archiving.

4.1.3.1 OpenAFS

The Bibliotheca Alexandrina has been operating an OpenAFS cell for approximately 6 years. OpenAFS is the open-source implementation of the Andrew File System (AFS), initially conceived at Carnegie Mellon University as part of the Andrew Project. Quoting the Wikipedia page, AFS is "a distributed file system which uses a set of trusted servers to present a homogeneous, location-transparent file name space to all the client workstations." AFS was developed as a way to promote the sharing of data across universities and other types of institutions under one global space. From within this global space, given sufficient permissions, each institution's "cell" may be accessed as a subdirectory.

OpenAFS depends on the Kerberos protocol for authenticating users. Under the hood, operating an OpenAFS cell involves running a set of servers that work together to manage storage, replication of data, authentication of access, and other aspects of the distributed file system implementation. BA's OpenAFS cell is hosted on the large-scale

storage cluster where 100 TB of storage are to be provided to VRE users as part of the VI-SEEM project.

4.1.3.2 Clowder

A web-based data management system that allows users to share, annotate, organize and analyze large collections of datasets. [7]

Digitizing large collections of Cultural Heritage resources and providing tools for their management, analysis and visualization is critical to DCH research. A key element in achieving the above goal is to provide user-friendly software offering an abstract interface for interaction with a variety of digital content types. To address these needs, the Clowder content management system has been developed as a Web 2.0 environment integrating analysis tools for the auto-curation of un-curated digital data, allowing automatic processing of input datasets, and visualization of both data and collections. It offers a simple user interface for dataset preprocessing, previewing, automatic metadata extraction, user input of metadata and provenance support, storage, archiving and management, representation and reproduction. It is a scalable, flexible, robust distributed framework with wide data format support (including 3D models, GigaPan images and Reflectance Transformation Imaging-RTI) and metadata functionality.

Clowder can accept, persist and process two kinds of metadata for each dataset or file:

1. automatically-generated; and,
2. community-generated (CIDOC-CRM).

In terms of database operation, the NoSQL MongoDB is used as the system's database management system (DBMS).

4.1.4. Work storage space / local storage

4.1.4.1 Attachable/detachable VM volumes for ~okeanos

A volume provides storage to a guest VM. The volume can provide for a boot disk or an additional data disk. ~okeanos defines a volume as a unit of storage available to a guest VM. Volumes are either root or data disks. Data disks provide for additional storage, for example: "/opt" or "D:". Every guest VM has a root disk, and VMs can also optionally have a data disk. End users can mount multiple data disks to guest VMs. The user can create snapshots of volumes. Volumes that can be snapshotted can even belong to other users. New images can be created from snapshotted volumes.

4.1.4.2 Fast-access storage near compute resources

Several other partners indicated they are providing scratch or work storage space. Usage of such storage is very common when offering HPC or Grid resources, as large amount of data needs to be stored to offer fast input or output transfer speeds between the compute system, and the work storage space.

4.1.5. Data search and catalogue

There are no readily available services of this type. Though partners have no more than some testing experience they seem to be interested in solutions like iRODS and EUDAT's B2FIND.

4.1.6. Data analysis

Several partners have experience with Hadoop and related tools. It was also noted that Hadoop - if adopted - should be deployed on cloud resources. The project will analyse other trends in Data Analysis as well.

4.1.6.1 Orka

eScience is a cloud-based integrated service platform for big data analytics offered by GRNET and the associated ~okeanos IaaS. Currently the codenamed orka CLI and Web interfaces enable ~okeanos users to create and manage Hadoop 2.x (YARN) multi-node clusters in order to run, save and replay their big data algorithms. Furthermore, a number of other pre-cooked images with Hadoop-centered software is available for faster, easier and friendlier development: Ecosystem (Pig, Hive, HBase, Oozie, Flume, Spark), Cloudera, Hue.

Researchers, university students and teachers can fully exploit the MapReduce (as well as others) programming paradigm without wasting time and resources in hardware, software setup, etc. In order to aid them in everyday research work, VM images with a range of installed software (wiki, project management, portal setup, teleconference and digital repositories) can also be deployed through the orka VRE (Virtual Research Environment) options.

4.1.6.2 Hadoop

Surveys showed that Hadoop is already widely used at VI-SEEM partners and the Science Communities. Hadoop is a distributed processing system for large data sets spread across data nodes, which also execute computations on data blocks local to them. Usually Hadoop is deployed on a cluster of real or virtual machines, with similar configuration, with some of the machines providing interfaces for submitting computational and data jobs to it.

There are two major versions of Hadoop. In version 1 Hadoop is based on the distributed file system HDFS and MapReduce batch execution engine that supports executions of mapper and reducer functions on datasets in HDFS. The HDFS provides two services - namespace and block storage services. The namespace service is provided by a single Namenode and it handles file operations, such as creation of files and directories, and their modification. Block storage service is implemented on multiple data nodes that store data divided into blocks of fixed size and distributed across multiple nodes and with multiple block copies to enable resistance to failures. This approach gives better throughput for faster file access and in case any data nodes fail, the computation continues without data loss and with performance hit proportional to the number of failed data nodes. MapReduce implements a programming model for distributed processing of

large data sets, described in the paper by Jeffrey Dean et al. from Google (<http://research.google.com/archive/mapreduce.html>). The main idea is that a map function is executed in parallel on each data element, which outputs the intermediate result consisting of key-value pairs, which are then sorted and redistributed between nodes running reduce function on them to get the final result, again consisting of key-value pairs. MapReduce is especially useful for scientific applications that process huge volumes of sensor data, performing substantial amount of filtering. It is less suitable for applications that need real-time or soft-real time guarantees.

The version 2 of Hadoop keeps the HDFS but adds support for federating multiple Namenodes for better horizontal scaling and support for multiple namespaces. Also in this version, MapReduce is still supported, but it is replaced by YARN resource manager that supports more general processing and enables more flexible execution of data analysis tasks that don't fit well into the map-reduce model.

Due to the flexibility of Hadoop, one can plug-in other platform for real-time processing. One popular choice for this case is Storm. Apache Storm operates on continuous streams of data. Essentially the data is flowing through a set of queries. Another option is Apache Spark, which is gaining traction in the last years. It offers the possibility for faster batch processing than MapReduce and is suitable for iterative processing, interactive processing and even for stream processing. Spark is compatible with Hadoop and can run alongside other tools in the Hadoop ecosystem like Hive, which we describe later.

Typically business data was stored in SQL databases and SQL queries were used to process and analyse it. However, with the exponential growth of available data the scalability limits of typical SQL databases became a problem (see, e.g., the so-called CAP theorem). The NoSQL model for storing data where some of the guarantees of SQL databases are relaxed has become basis for operation of the world's biggest commercially delivered services. The scientific users of VI-SEEM have also expressed interest in such technologies like Cassandra (<http://cassandra.apache.org/>), MongoDB (<https://www.mongodb.org/>) or OrientDB (<http://orientdb.com/>).

On top of Hadoop one can use the Apache HBase to provide random, realtime read/write access to the research data. Apache HBase is a non-relational database built on top of Hadoop and HDFS. To actually execute SQL-type queries over this database, one needs to use something like Hive.

Hive can convert SQL statements into MapReduce jobs. It can make use of Tez (<https://tez.apache.org/>), which is much faster than MapReduce for these tasks. The Hadoop clusters need some tools for managing the underlying physical or virtual infrastructure. Usually ZooKeeper (<https://zookeeper.apache.org/>) would monitor the health of the system and YARN or Mesos (<http://mesos.apache.org/>) would manage the scheduling of tasks across the Hadoop cluster.

The programming model of Hadoop is usually simpler than traditional message passing architectures because the communication and parallelism is implicitly managed with map-reduce. However, in the Hadoop ecosystem there are powerful higher-level tools that further simplify the use, such as PIG data flow language, or Hbase and Hive, which are SQL-like databases on top of Hadoop. There are also other modules, not based on map-reduce, like Spark which provide tools for machine learning (MLib), graph processing (GraphX) and more, which leverages memory to improve the speed of data analysis. All these can be installed on top of Hadoop, as needs arise.

4.1.6.3 Other trends in data analysis

Many of the scientific users, especially in the life science community, use the R language and its many packages for statistical data processing. Recently the package named "Programming with Big Data in R" (pbdR) has become popular because it allows statistical computing on Big Data by using high-performance statistical computation. The pbdR uses the same programming language as R but it mainly focuses on distributed memory systems (clusters), where data are distributed across the computational nodes and analyzed in a batch mode, while communications between processors are based on the well established in the HPC community MPI standard. The two main implementations that allow use of MPI in R are Rmpi and pbdMPI. The pbdMPI is able to use both SPMD and task parallelisms. The SPMD (single program, multiple data) programming model is important for efficient use of accelerators like GPUs or Xeon Phi, which are available in VI-SEEM. Thus a properly tested installation of R and such popular packages would preferably be provided at the VI-SEEM resources.

One data format that is used mainly by the Climate and Forecast communities is the netCDF (network Common Data Form), which is a machine-independent, self-describing, binary data format standard for exchanging scientific data. It is the data format, and the conventions define metadata that provide a definitive description of what the data in each variable represents, and the spatial and temporal properties of the data.

The NetCDF package is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. The libraries are also used for creating and distributing climate data sets, based on the OPeNDAP servers and clients. The parallel NetCDF and the HDF5 libraries are also used in relation to netCDF data. These libraries have to be installed in the HPC infrastructure in a way that is optimized for the particular hardware for each cluster. Some of the filtering and analysis of netCDF data can be performed in the Hadoop ecosystem, since it is more of a data intensive task rather than the compute-intensive simulation and moving these types of analysis to a Hadoop cluster may save computational resources for the other applications.

4.2. Pan-European trends in data services

Within the last 5 years EUDAT [10] is developing a data services platform, using a set of services integrated into one solution, and several communities are already using the services for a longer period of time, trusting the knowledge and reliability they offer.

EUDAT's vision is to enable European researchers and practitioners from any research discipline to preserve, find, access, and process data in a trusted environment, which fits the requirements of VI-SEEM communities.

The EUDAT project has implemented the so-called Collaborative Data Infrastructure (CDI). It consists of five core services (explained with EUDAT descriptions): [8]

- B2SAFE (Replicate Research Data Safely)
"Core data management service allowing for the automatic, rule and policy-driven replication of data across a federation of EUDAT CDI datacenters (either community or non-specific)" [9]
- B2STAGE (Get Data to Computation)
"High-performance data movement service which allows data to be staged into and out of the CDI to, for instance, external HPC services" [10]
- B2SHARE (Store, Share and Publish Research Data)
"User-facing service which provides an easy way to upload, tag and share research data. Furthermore, uploaded data are made citable via PIDs." [11]
- B2FIND (Find Research Data)
"Service exposing metadata catalogue harvested across EUDAT, through a user-friendly, web-based search portal and a standard API." [12]
- B2DROP (Sync and Exchange Research Data)
"A service for storing, synchronizing and exchanging dynamic research data with colleagues and team members" [13]

These are depicted in Figure 3 - EUDAT's Collaborative Data Infrastructure. In terms of technology, the core services make use of several tools that project members have experience with or have shown interest towards.

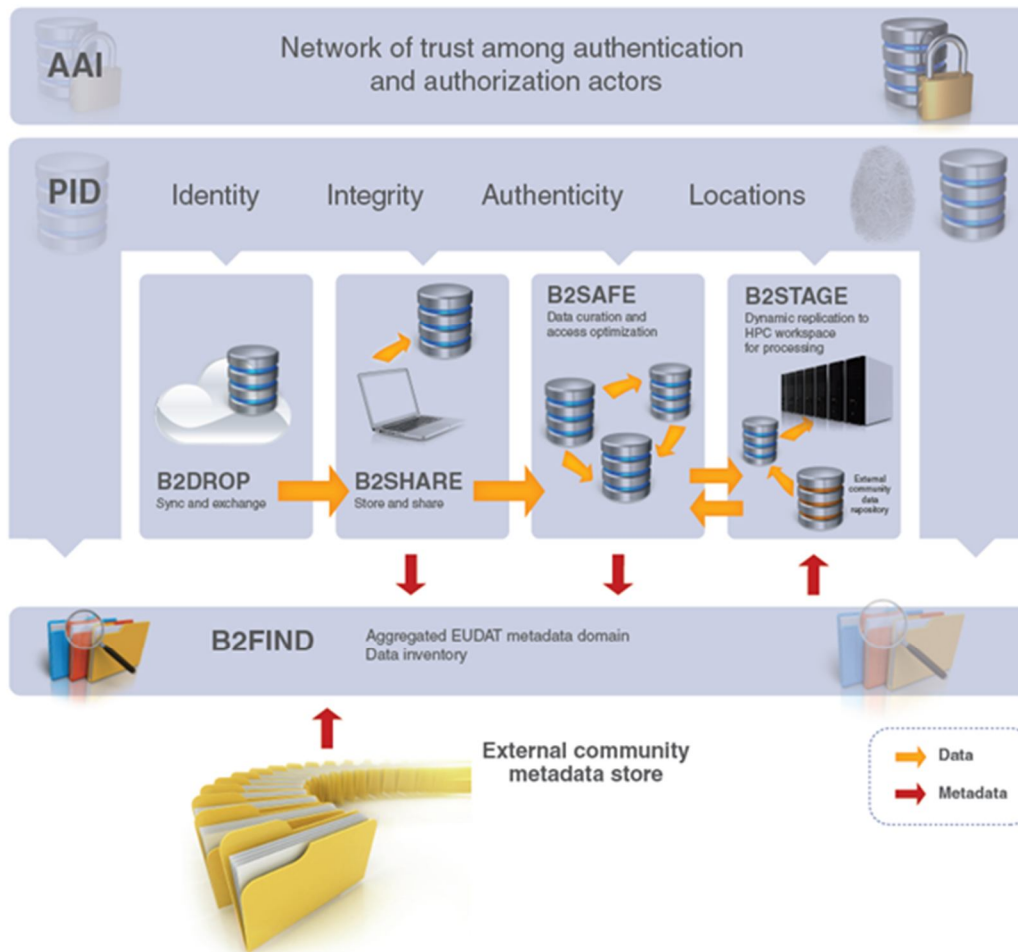


Figure 3 - EUDAT's Collaborative Data Infrastructure

4.2.1. B2DROP

B2DROP is a simple storage service for file sharing based on top of ownCloud (<https://owncloud.org/>) technology, and therefore it inherits all features of ownCloud:

- user-friendly web interface that allows connection from any web browser;
- desktop clients for popular Operation System;
- selective synchronization and version control;
- access and management of deleted and encrypted files;
- video, PDF, ODF viewer.

It enables to store and exchange data with colleagues and team members, synchronise multiple versions of data and ensure automatic desktop synchronisation of large files. An online version of EUDAT sync and share solution for data can be found at <https://b2drop.eudat.eu> website.

4.2.2. B2SHARE

B2SHARE is EUDAT's service for storing, sharing and publishing so called "long tail" data, i.e. small and medium scale research data in various formats, which is usually not covered by institutional data preservation policies.

B2SHARE has a web-based graphical user interface and is primarily intended for the individual researchers to upload their data directly using a standard web browser. However, B2SHARE can also be integrated with other software or external web sites, e.g. research community portals via application programming interfaces (APIs).

Persistent Identifiers (PIDs) are also supported in B2SHARE, based on the European Persistent Identifier Consortium (EPIC) technology. PIDs in B2SHARE point to the landing page in the repository which presents the metadata and a link to download the uploaded data file(s). All deposits made in B2SHARE can be traced and linked via PIDs.

4.2.3. B2SAFE

B2SAFE services provide an integrated solution for robust, long-term data preservation, designed and implemented by the EUDAT project.

The core part of the B2SAFE service relies on iRODS and includes rule sets based on iRODS syntax and grammar, but at the same time the service extends the iRODS capabilities with external scripts and libraries. (See: <https://github.com/EUDAT-B2SAFE/B2SAFE-core>)

The core package architecture has a modular design to minimize software lock-in. Therefore, the rules are grouped in six sets representing six different functional areas. Any function which is not strictly dependent on iRODS capabilities is implemented in an external component.

The core package includes the following components:

- The EUDAT commons provides a rule set containing the low-level functions and utilities for enabling all the other tasks from replication to integrity checks. All other components are connected to the EUDAT commons and make use of the basic rules.
- The Replication Management functions to transfer a single data object or a whole data collection (which can consist of data directories), together with integrity check mechanisms. The module calls on rules defined in the EUDAT commons.
- The Authorization mechanism is based on a JSON file, which contains triplets (subject, action, target) that represent who is allowed to do what. These triplets are called assertions and match the requirements of the iCAT catalogue, a component of iRODS to store metadata about data objects. The existing JSON file is just a placeholder which can be replaced by a connector to an external authorization system in the future.
- The PID management contains rules to perform the main operations related to the PID service. It is based on a python script, which acts as a client to the PID system, i.e. the HTTP REST interface of the EPIC PID service.
- The Logging component is built on two different data structures, "queue" and "log", and based on a python script to perform different operations on them. This logging mechanism is used for retrieving information to monitor data transfers

and the PID management operations. It works as a replication tracking system, which manages the failed transfers in an asynchronous way and propagates this information to an external logging system, currently a python module which can be replaced by other libraries at a later stage.

- The Error Management includes functions to process errors during data transfers. It can detect errors about checksum and size inconsistencies, PID processing and data object ownership.

4.2.4. B2STAGE

B2STAGE is a service designed to facilitate transfers of large data sets between the EUDAT infrastructure and external computing facilities in a reliable, efficient, and light-weight manner. The service comprises three different packages (described below) which support the following functionalities:

- Transfer of large data collections from EUDAT storage facilities to external HPC/HTC facilities for further processing
- In conjunction with B2SAFE, replicate community data sets, ingesting them onto EUDAT storage resources for long-term preservation
- Improved data accessibility by providing standard protocols and interfaces, such as the RESTful HTTP based on the CDMI specification (in progress).

The packages, part of B2STAGE:

- The GridFTP DSI (Data Storage Interface) to enable fast data transfer through the GridFTP protocol
- The Data Staging Script to instrument data transfers via a command-line tool
- The HTTP CDMI to permit access and management of data via a programmatic interface

4.2.5. B2FIND

The aim of B2FIND is to offer an interdisciplinary EUDAT metadata catalogue which allows users to easily find collections of scientific data that:

- Are managed by EUDAT services like B2SHARE
- Are described by metadata made available from external community center archives and repositories, both from EUDAT and non-EUDAT communities via OAI-PMH

B2FIND also acts as a discovery service for cross-disciplinary research.

Key element for enabling this cross-community approach is the semantic mapping of selected metadata elements to a limited number of broadly used metadata facets in B2FIND.

The initial design decision was to keep the architecture of the service as modular as possible in order to avoid technology lock-in and, if required, to be able to change components at a later stage. After some evaluation it was decided to use the CKAN20 data management software as a basis for the B2FIND service. CKAN is a widely used open-source software from the Open Knowledge Foundation for publishing, sharing and finding data.

Three major modules were developed in order to load data into the B2FIND repository:

- Harvester
- Mapper
- Uploader

The harvester collects metadata records from provider-named endpoints (typically using OAI-PMH). The mapper transforms harvested metadata from XML to JSON format and performs semantic mapping (according to the specific mapping definitions for the relevant metadata scheme) and some intelligent processing to combat sparse metadata and increase usability. The uploader imports the converted and mapped records to the B2FIND repository using the CKAN API.

5. VI-SEEM generic data services portfolio

5.1. Services to be deployed

The VI-SEEM project aims to cover the full data lifecycle of scientific research. To efficiently handle this, we need an integrated environment rather than a set of standalone services that have little or no connection to each other. Therefore, the generic data services described beforehand should be selected so that they could - as a whole - reflect all aspects of the data lifecycle.

As developing a comprehensive system of data management services would not fit into the timeframe of the project, the project decided to build its service portfolio on existing solutions which are proven to satisfy the requirements.

5.1.1. VI-SEEM simple storage service

Simple storage for file sharing will be based on B2SHARE (described in section 4.2.1) and will be deployed on top of ownCloud (<https://owncloud.org/>) technology, and therefore it will inherit all the mentioned features of ownCloud:

- user-friendly web interface that allows connection from any web browser;
- desktop clients for popular Operation System;
- selective synchronization and version control;
- access and management of deleted and encrypted files;
- video, PDF, ODF viewer.

However, in order to harmonize this service with VI-SEEM environment, it will be extended with a module responsible for AAI integration. The module will allow users to be authenticated using a single identity, and enable uniform managing of access to the service. EUDAT (<https://eudat.eu/>) B2DROP service and development standing behind it will be of great help here.

5.1.2. VI-SEEM repository service

For the implementation of the VI-SEEM repository service (VRS) the main component to be used is the Invenio Digital Library Framework (<http://invenio.readthedocs.org/>).

Invenio is a free software suite enabling users to run their own digital library or document repository on the web. The technology offered by the software covers all aspects of digital library management, from document ingestion through classification, indexing, and curation up to document dissemination.

Invenio complies with standards such as the Open Archives Initiative and uses MARC 21 as its underlying bibliographic format. The flexibility and performance of Invenio make it a comprehensive solution for management of document repositories of moderate to large sizes.

Some of the main features offered by Invenio which correspond to the VI-SEEM requirements are the following:

- Provide a navigable directory of data sets.

- Provide search functionality among the contents of the data sets.
- Ability to assign flexible metadata to data collections. In VI-SEEM it is envisaged that different metadata templates might be needed for each SC, in some cases per application domain, or per data file type.
- Sharing functionalities based on customizable access policies, and user groupings.

Further to the above-mentioned main functional requirements the VRS should also support the assignment and management of persistent identifiers (PID) for each data set that is deposited in the repository as well as support for the AAI solution that has been adopted by the project and is described in D3.1 [14].

For this purpose, the developments that have taken place in the context of the EUDAT and EUDAT2020 projects will be used in VI-SEEM as well. The EUDAT Collaborative Data Infrastructure has developed the B2SHARE service (see section 4.2.2) on top of Invenio to serve similar use cases as the ones specified by the VI-SEEM users. The VI-SEEM Repository deployment will use the code developed within EUDAT and available at <https://github.com/EUDAT-B2SHARE/b2share> to enable the above-mentioned required features.

5.1.3. VI-SEEM archival service

For the implementation of the VI-SEEM Archival Service (VAS) iRODS [<http://irods.org>] will be utilised. iRODS is open source data grid middleware for:

- Data discovery
- Workflow automation
- Secure collaboration
- Data virtualization

Data discovery is supported by its metadata catalogue (iCAT). It is used to locate data, manage metadata, access control etc.

Workflow automation could be achieved by the means of customized policies. That is, administrative actions could be enforced on a variety of events in the system (so called Policy Enforcement Points - PEPs). Such policy could be e.g. validating checksums on data ingestion, harvesting basic metadata for image files or asserting that a Persistent Identifier (PID) is generated for a data object (using an external PID provider).

An administrative domain in iRODS is called a zone. Collaboration in iRODS could be managed both in the local zone and across separate (remote) zones the latter being called a federation. Federations allow controlled access where the remote partner is subject to the constraints of the local zone's policies.

Data virtualization means that heterogeneous storage systems could be presented in a homogeneous way. There are plenty of drivers in iRODS and there is the possibility to add new ones. Data virtualization could help us to integrate several types of storage resources available at VI-SEEM members in a transparent way for the benefit of our science communities.

Regarding the VI-SEEM VRE, it is envisaged that multiple data centers will join together in a federation, and safe data replication amongst them will be implemented with a set of iRODS policies.

The EUDAT Collaborative Data Infrastructure (CDI) has developed the B2SAFE service to address user requirements for safe data replication. The VI-SEEM Archival Service deployment will use the code developed within EUDAT (available at <https://github.com/EUDAT-B2SAFE>) to satisfy similar needs of the VI-SEEM community (see B2SAFE description in section 4.2.3 for further details about the service).

5.1.4. VI-SEEM work storage space / local storage and data staging

Available computing resources (HPC and Grid clusters) within the project have independent local organization of available storage spaces. Such organization aims to improve the performance of running applications and services.

Usually, it includes a file system that is shared between nodes within the cluster (accessible from all nodes), file systems that could only be used on a particular node (local hard drive on a node), and file system(s) for storage purposes (independent local storage system).

The size of these file systems increases from local hard drives (up to 1 TB) and shared partitions (up to 100 TB) to local storage systems (up to 1 PB).

In the same order, this increase of available storage space is coupled with decreasing bandwidth.

Most shared file systems within the VI-SEEM project are implemented over Infiniband interconnect technology using Lustre or GPFS parallel file systems.

In some cases, it is implemented with IBRIX, while the Network File System (NFS) is commonly used on Grid clusters.

Typically, these file systems hold home directories, which keep job submission scripts, binaries, source files, input files, relatively small outputs of applications, etc.

Compute nodes have local hard drives that could be utilized to store intermediate results created during the execution of an application. This storage space is commonly used by serial applications, and parallel applications that are executed only on one node (shared memory paradigm, e.g., OpenMP). In some cases, it is also useful for parallel applications executed on multiple nodes (distributed memory paradigm, e.g., MPI). For example, a parallel MPI application can be designed in a way that MPI processes executed on one node create and access intermediate files only on that node's local hard disk. In this case, produced results at the end of the application execution should be transferred back to home directory. This storage space is commonly referred to as temporary or scratch directory.

Work storage space / local storage service in the VI-SEEM VRE will utilise already existing home and scratch directories of partner sites. Although they are implemented in various ways, a common data transfer capability will be introduced to provide a standard way of access to those resources.

Data needed for the computation or analysis is often not available on local storage spaces of clusters and it needs to be transferred from remote location to the local file system in order to be processed. In the same way, when the computation is over, results usually need to be transferred to the remote storage location.

Both the VI-SEEM archival service and the Work storage space / local storage service described above should be coupled with a facility that supports data staging, i.e. to move large datasets between:

- users of VI-SEEM and the VI-SEEM VRE
- VI-SEEM data centers and HPC resources

The EUDAT Collaborative Data Infrastructure has developed the B2STAGE service to provide such capabilities for users. B2STAGE is based on EUDAT Data Storage Interface (DSI) component that provides interface between GridFTP and iRODS servers. To use this service within VI-SEEM, target iRODS servers would need to have B2STAGE GridFTP DSI component installed together with a GridFTP server. In addition, there is also EUDAT File Manager with support for various transfer protocols (native iRODS, FTP, GridFTP) as well as Data Staging Script (DSS) developed by EUDAT that also takes care of all generated PIDs.

DSS is implemented in Python and easily deployable on any server that can be found in VI-SEEM computing part of the e-Infrastructures.

B2STAGE service allows transfer of datasets between client computer and iRODS server (installed together with GridFTP DSI component and GridFTP server) or third party transfer between two servers. A typical use case for third party transfer for a user would be to initiate a data transfer from an HPC GridFTP server, deployed on cluster (where some computation needs to be done), to an iRODS server, or vice versa using his laptop or personal computer. In the case of B2STAGE client-server usage, key application for the user would be to initiate data transfer from iRODS server to local file system on HPC login or compute node before the computation, and then to return results back to iRODS server after the computation is finished. In this case, in order to initiate data staging, the user would have to log in to cluster's login node via SSH or it could also be done on compute node during the execution of submitted job (if it is part of the job execution script).

Another benefit of usage of this service is the possibility of interaction between iRODS servers and already deployed Grid Storage Elements that are also utilizing GridFTP protocol. Also, on all Grid sites available in VI-SEEM, Globus client commands (e.g. `globus-url-copy`) are already installed on User Interface and Worker Nodes so that interaction with iRODS server becomes simple.

Currently in development, there is also a RESTful HTTP interface that will allow interaction with the iRODS server and management of data using HTTP protocol. It is based on the CDMI (Cloud Data Management Interface) specifications.

The VI-SEEM VRE will use the codes developed within EUDAT (available at <https://github.com/EUDAT-B2STAGE>) to provide data staging for the VI-SEEM community.

5.1.5. VI-SEEM data discovery service

VI-SEEM will follow the developments undertaken by the EUDAT and EUDAT2020 projects and will base the data discovery service on CKAN [15].

CKAN provides a rich search experience, which allows for quick "Google-style" keyword search as well as faceting by tags and browsing between related datasets. Users can quickly see what datasets are available, in which formats and with which license, straight

from the search results. All dataset fields are searchable (see below for the metadata we bring out into the interface).

CKAN allows for four main functional characteristics.

- Publish & find datasets. Publishing is achieved via import or through a web interface. Users can search by keywords or apply some filters based on tags.
- Store and manage data. CKAN allows for storing actual raw scientific data.
- However, since the VI-SEEM Repository service will be built using the Invenio software this feature of CKAN might not be exploited to a full extent.
- Allows engagement with users, by offering customizable interfaces as well as user interaction and commenting of the data.
- Finally, CKAN provides flexible APIs in order to allow customizations and it is an open source software.

5.1.6. VI-SEEM data analysis service

The basis of the data analysis framework in VI-SEEM - as identified by the storage service survey (part of WP5 user survey conducted in December 2015) among the project partners - should be Hadoop.

Considering that the participating HPC infrastructures already have some resource management in place (such as PBS, SLURM), Hadoop would impose changes to the systems, if it were to be installed natively. While it would be possible to run Hadoop on demand on an HPC machine, it would beat the purpose of it because the big data that is to be analysed would need to be stored on a shared storage and frequently moved across the network to the compute nodes, which is the slow operation Hadoop was designed to avoid. The HPC resources with high speed interconnect would also be underutilized, as map-reduce applications on Hadoop do not require that much inter-process communication over the network once the data is stored in its HDFS. For these reasons, it would be more optimal to deploy Hadoop on VI-SEEM Cloud infrastructure.

It would be preferable to build custom Hadoop ecosystems for each SC so that community specific trends of data analysis (as described before) could be exploited as well.

5.2. Additional required common services

5.2.1. VI-SEEM persistent identifier service

To facilitate the development of a strategy for the long term preservation of scientific resources, in order to ensure its long-lasting accessibility, it is necessary that the resources are registered in well-kept repositories with a content that is never changing and which can be referenced and cited. Since repositories are not permanent and data sets might be moved from one repository to another, one needs to assign to data Persistent Identifiers (PIDs) as a method to reference the primary and secondary scientific data in order to name these data in a unique and timeless way. A PID is an identifier pointing to a resource with no knowledge of the resource. It is the combination of the prefix/suffix. The prefix is the provider's API Prefix. As a suffix we use a dynamically created UUID. To provide for PIDs in all VI-SEEM data sets the project will

rely on the GRNET Handle service. The Handle service is a service dedicated to provide, resolve and mint persistent identifiers (PID). The handle RESTful API supports the following functions:

- GET for getting the data of a selected PID
- POST for creating a new PID with automatic generation of suffix name.
- PUT for creating/updating a new PID with manual generation of suffix name
- DELETE for deleting a selected PID

PID EPIC is fully compatible with the DOI (Digital Object Identifier) and a PID (including the prefix) can also be interpreted from any server DOI.

5.2.2. VI-SEEM AAI

The AAI activity in VI-SEEM followed the developments in the AARC project (flagship cross-eInfrastructure AAI EC project) in order to identify the requirements of the scientific communities. This work resulted in a set of guiding principles:

- Users should be able to access the VI-SEEM Services using the credentials they have from their Home Organizations using eduGAIN when possible, but alternate methods should be available
- Within the VI-SEEM environment, a user should have one persistent non-reassignable non-targeted unique identifier.
- There should be a distinction (LoA) between self-asserted attributes and the attributes provided by the Home Organization/VO
- Access to the various services should be granted based on the VO/VI-SEEM roles the user have.
- Users should be able to access all VI-SEEM services, regardless of the technologies and protocols used by each service.
- VI-SEEM Services should not have to deal with the complexity of multiple IdPs/Federations/Attribute Authorities/technologies. This complexity should be handled centrally and should be hidden from the VI-SEEM Services.

Based on these principles we chose to adopt the architecture that has been proposed by the AARC project.

In the AAI Proxy Model, all internal Services (SPs) trust only one Identity Provider, the AAI Proxy. The connected SPs get consistent/harmonised user identifiers and accompanying attribute sets that can be interpreted in a uniform way for authorization purposes, while the harmonization is handled centrally by the AAI proxy. In a nutshell, internal services do not have to deal with the complexity of multiple IdPs/Federations/Attribute Authorities/technologies. This complexity is handled centrally by the AAI proxy. From the point of view of the external IdPs, there is only one SP they have to establish trust with, the AAI proxy. This simplifies the trust model significantly and it allows the maximum flexibility for the development of internal services with the minimum possible overhead.

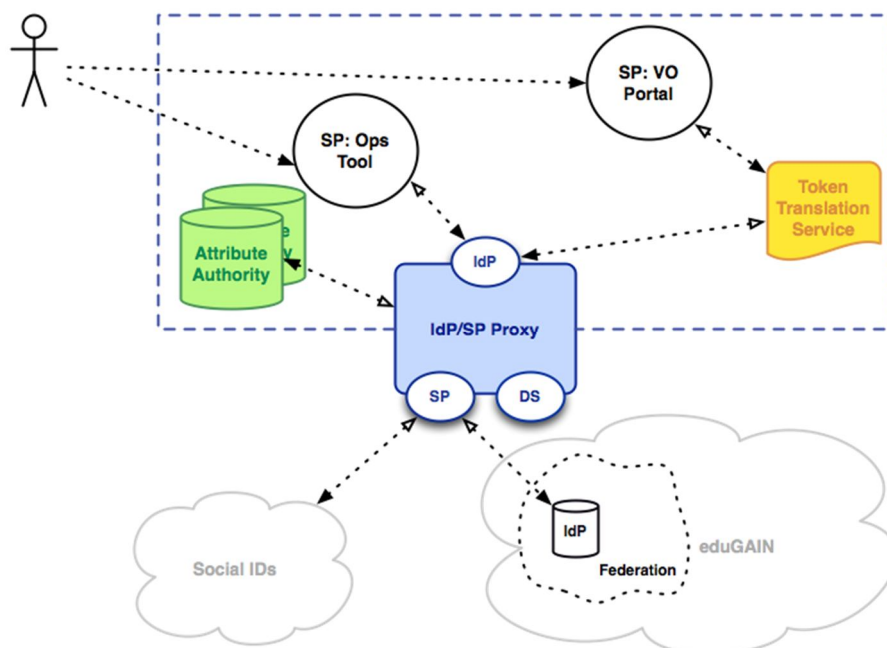


Figure 4 - AAI Proxy model, AARC

The VI-SEEM AAI proxy will be based on SimpleSamlPhp and will be the authentication gateway between the VI-SEEM platform of services and external Identity Providers, with multi-protocol capabilities (SAML2, OpenID Connect, OAUTH2). The proxy will provide the IdP Discovery functionality, User Enrollment, a mechanism for requesting User Consent and it will support Levels of Assurance for different authentication sources and Attribute Aggregation. Internally, the Attribute and Group Management is going to be provided by the HEXAA tool and it is going to be connected directly to the VI-SEEM AAI proxy. The Token Translation Service is going to be introduced later on in the VI-SEEM AAI. Currently we are following the relevant work in the AARC project and we are investigating CILogon, Moonshot and LDAP Facade as possible candidates.

5.3. Available storage in the region

To analyze and plan the underlying storage infrastructure supporting each of the services described above, we present in Table 4 the storage resources offered by VI-SEEM partners. The table contains disk and tape storage separately.

Disk is suitable for the following storage services:

- Simple storage
- Data repository
- Work storage space / local storage

Tape is primarily suitable for data archive storage service.

Partner	Country	Disk	Tape
GRNET	Greece	50	210
CYI	Cyprus	20	-
IICT-BAS	Bulgaria	5	-
IPB	Serbia	10	-
NIIF	Hungary	53	272
UVT	Romania	5	-
UNI BL	Bosnia	1	-
UKIM	FYR of Macedonia	2	-
RENAM	Moldova	1	-
IIAP-NAS-RA	Armenia	3	-
BA	Egypt	100	-
IUCC	Israel	5	-

Table 4 - Storage offered by VI-SEEM partners

5.4. Data services & data sources deployment plan

Service deployment is envisaged as a three-step process. First, a proof of concept deployment should be done at select partner site(s). Next, all sites that would provide that specific capability would set up the service according to the deployment scenario. Third and final step would be to enable service for use by scientific communities and to provide support. The current plan of services deployment is as follows.

5.4.1. VI-SEEM simple storage service

Simple storage for file sharing will be deployed at the Institute of Physics Belgrade. Beta version will be available in M07, and each user will be provided with 50 GB of storage space.

5.4.2. VI-SEEM repository service

Initially we will deploy one instance of the VI-SEEM repository service (VRS). The deployment will be done at GRNET. Depending on the actual storage needs and the resources availability a second instance of the service might be deployed at another infrastructure provider of the project, the main candidate being NIIF in Hungary. It is expected that the initial version of the service will be deployed by M08 of the project and the associated storage space will be 10TB.

5.4.3. VI-SEEM archival service

Initially we will deploy the VI-SEEM archival service (VAS) at four sites: GRNET, IPB, CYI and NIIF. Each partner will have its own iRODS zone and these zones will be federated together. Other partners should decide whether they:

- want to use the service provided as is
- join an already existing zone and provide additional storage resources which would require installing iRODS resource server(s) but not an iCAT server
- create their own iRODS zone and join the federation

Storage needs for long-term preservation will be covered mainly by GRNET and NIIF as these sites have offered plenty of tape resources.

It is expected that the initial iRODS federation will be deployed by M10 and the VAS is in production by M16 of the project.

5.4.4. VI-SEEM work storage space / local storage and data staging

Installation of GridFTP is mandatory at all sites with optional integration via iRODS. Initial sites to provide iRODS integration are: GRNET, IPB and NIIF.

For these sites GridFTP DSI component and GridFTP server installation is expected to be done approximately at the same time the iRODS federation is put in place (by M10 of the project). Partners offering work storage space are:

Partner	Country
GRNET	Greece
CYI	Cyprus
IICT-BAS	Bulgaria
IPB	Serbia
NIIF	Hungary
UVT	Romania
UKIM	FYR of Macedonia
RENAM	Moldova
IIAP-NAS-RA	Armenia
BA	Egypt
GRENA	Georgia
IUCC	Israel

Table 5 - Partners offering work storage space

5.4.5. VI-SEEM data discovery service

The data discovery service will implement data search and catalogue functionality.

The VI-SEEM data discovery service will be deployed in Bulgaria at IICT-BAS by M10 of the project. Integration with the other storage services in the region will begin immediately after that, aiming at having all existing data sources integrated by M12 of the project. VI-SEEM will also capitalize on the experience gained on the usage of such service from EUDAT and will utilize part of the code that has been developed around CKAN by EUDAT: source code is available at: <https://github.com/EUDAT-B2FIND>

5.4.6. VI-SEEM data analysis service

The Data analysis service based on Hadoop will be used. IPB will be the primary provider. IPB will offer a standalone Hadoop cluster, and initially, it will be deployed on 4 x 8-core machines (32-cores in total). This deployment will be in production by M10 of the project. Further to that GRNET's Orka service will be available to the users at a later stage if needed, and IUCC will provide facilities for data analytics as well.

5.4.7. VI-SEEM persistent identifier service

This service is already deployed at GRNET as discussed in section 5.2.1.

5.4.8. Further potential improvements

Apart from those mentioned above our further plans highly depend on community needs - although we already have some ideas how to move the generic services closer to the users, for example by letting them build into their data workflows by adopting e.g. the B2SHARE REST-API to bind it to community-specific portals, transparently converting data, enabling iRODS internal "mini-workflows", etc.

6. Conclusions

Using the results of the user survey conducted by WP5, WP4 has carried out a detailed analysis of data storage and management requirements of the scientific communities. Based on this analysis, it was identified that VI-SEEM needs to offer a comprehensive data management solution capable of storing and managing different types of data for different timeframes offered to different groups, and provide a stable set of data management functionalities to these communities.

In parallel, generic data services available in the region have been assessed in this deliverable, and suitable services were identified based on the user requirements.

Finally, the existing open-source solutions have been analysed, with the focus on the current trend in pan-European data management solutions.

The following generic types of services have been identified to be deployed:

- Simple data sharing
- Data repositories
- Data archiving
- Work storage space / local storage
- Data search and catalogue
- Data analysis

For these services a specific implementation has been identified based on the experience of the VI-SEEM partners as well as the pan-European trends in data related services (mainly based on the flagship EUDAT2020 project). From its inception VI-SEEM has committed to leveraging the existing solutions in related problem areas, and build on existing open source solutions.

Finally, an initial deployment plan has been set up for each of the envisaged data services. The sites in the table below will deploy services in this phase.

Partner	Service
GRNET	Repository, Archive, Scratch, Data Analysis
CYI	Repository, Archive, Scratch
IICT-BAS	Data Discovery, Archive, Scratch
IPB	Repository, Archive, Scratch, Data Analysis
NIIF	Repository, Archive, Scratch
UVT	Scratch
UKIM	Scratch
RENAM	Scratch
IIAP-NAS-RA	Scratch
BA	Scratch
GRENA	Scratch
IUCC	Scratch, Data Analysis

Table 6 - Services to be deployed by partners

A total of 330 TB of disk and 510 TB of tape capacity are offered by the partners to be utilized to support different services.

The proof of concept implementation for all services will be deployed by M08, and the services will go into production by M11.

The VRE portal will make use of VI-SEEM AAI developed by WP3 of the project. VI-SEEM generic data services with web interfaces will be accessible through the VRE portal.