

Large-scale EXecution for Industry & Society

Deliverable D3.2

Mid-Term Infrastructure



Co-funded by the Horizon 2020 Framework Programme of the European Union Grant Agreement Number 825532 ICT-11-2018-2019 (IA - Innovation Action)

DELIVERABLE ID TITLE	D3.2 Mid-Term Infrastructure
RESPONSIBLE AUTHOR	Stephan Hachinger (LRZ)
WORKPACKAGE ID TITLE	WP3 LEXIS Data System
WORKPACKAGE LEADER	LRZ
DATE OF DELIVERY (CONTRACTUAL)	31/03/2020 (M15)
DATE OF DELIVERY (SUBMITTED)	01/04/2020 (M16)
VERSION STATUS	v 1.0 Final
TYPE OF DELIVERABLE	DEM (Demonstrator)
DISSEMINATION LEVEL	PU (Public)
AUTHORS (PARTNER)	LRZ; IT4I; Bull/Atos; LINKS; ECMWF; O24; Avio Aero; CEA; GFZ; CIMA; TESEO; BAY; CYC
INTERNAL REVIEW	Florin Apopei (TESEO), Olivier Terzo (LINKS)

Project Coordinator: Dr. Jan Martinovič – IT4Innovations, VSB – Technical University of Ostrava **E-mail:** jan.martinovic@vsb.cz, **Phone:** +420 597 329 598, **Web:** <u>https://lexis-project.eu</u>



DOCUMENT VERSION

VERSION	MODIFICATION(S)	DATE	AUTHOR(S)		
0.1	Table of Contents (first proposal) created	07/01/2020	Stephan Hachinger (LRZ)		
0.2	Fill-in draft created	20/01/2020	Stephan Hachinger (LRZ)		
0.3	Contribution from CYC on LEXIS Portal	27/01/2020	Sean Murphy (CYC)		
0.4	(i) Restructuring according to D3.3 changes, added content/summary(ii) Polishing	09/02/2020	(i) Stephan Hachinger (LRZ) (ii) Stephan Hachinger (LRZ)		
0.5	Figure 3, glossary, overview, and request for input	10/02/2020	Rubén Jesús García-Hernández (LRZ)		
0.6	Polishing	28/02/2020	Stephan Hachinger (LRZ)		
0.7	Ready for production editing	25/03/2020	Stephan Hachinger (LRZ)		
0.8	Final check	27/03/2020	Kateřina Slaninová (IT4I)		
1.0	Final check, update of Section 2.2.2	31/03/2020	Jan Matinovič (IT4I) Václav Svatoň (IT4I)		



GLOSSARY

ACRONYM	DESCRIPTION
AAI	Authentication and Authorization Infrastructure
ALIEN4CLOUD	Application LIfecycle ENablement for Cloud (cf. http://alien4cloud.org)
ΑΡΙ	Application Programming Interface
DDI	Distributed Data Infrastructure
НЕАРРЕ	High-End Application Execution Middleware
НРС	High-Performance Computing
HPDA	High-Performance Data Analytics
IRODS	Integrated Rule-Oriented Data System https://irods.org/
OAI-PMH	Open Archive Initiative Protocol for Metadata Harvesting
SCP	Secure Copy
SSH	Secure Shell
TOSCA	Topology and Orchestration Specification for Cloud Applications (by OASIS, cf. http://docs.oasis-open.org/tosca/TOSCA/v1.0/os/TOSCA-v1.0-os.html)
VM	Virtual Machine
YORC	Ystia Orchestrator (https://ystia.github.io/)



TABLE OF PARTNERS

ACRONYM	PARTNER
Avio Aero	GE AVIO SRL
AWI	ALFRED WEGENER INSTITUT HELMHOLTZ ZENTRUM FUR POLAR UND MEERESFORSCHUNG
BLABS	BAYNCORE LABS LIMITED
Bull/Atos	BULL SAS
CEA	COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES
СІМА	Centro Internazionale in Monitoraggio Ambientale - Fondazione CIMA
СҮС	CYCLOPS LABS GMBH
ECMWF	EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS
GFZ	HELMHOLTZ ZENTRUM POTSDAM DEUTSCHESGEOFORSCHUNGSZENTRUM GFZ
IT4I	VYSOKA SKOLA BANSKA - TECHNICKA UNIVERZITA OSTRAVA / IT4Innovations National Supercomputing Centre
ITHACA	ASSOCIAZIONE ITHACA
LINKS	FONDAZIONE LINKS / ISTITUTO SUPERIORE MARIO BOELLA ISMB
LRZ	BAYERISCHE AKADEMIE DER WISSENSCHAFTEN / Leibniz Rechenzentrum der BAdW
NUM	NUMTECH
024	OUTPOST 24 FRANCE
TESEO	TESEO SPA TECNOLOGIE E SISTEMI ELETTRONICI ED OTTICI



TABLE OF CONTENTS

EXECUTIVE SUMMARY	5
1 INTRODUCTION – LEXIS COMPONENTS	6
2 DEMONSTRATOR COMPONENTS	7
2.1 Novel computing systems at IT4I and LRZ	
2.2 LEXIS WORKFLOW-MANAGEMENT SOLUTIONS (YORC AND HEAPPE)	
2.2.1 Yorc	7
2.2.2 HEAppE middleware	9
2.2.1 TOTC	9
2.3.1 Low-level access	9
2.3.2 APIs	
2.4 Web Portal demonstrator components	11
2.4.1 Initial version of the Portal	11
2.4.2 Portal Revision R2 - Wireframes	11
3 SUMMARY	13
REFERENCES	14

LIST OF TABLES

TABLE 1 - LEXIS INFRASTRUCTURE COMPONENTS AS PRESENTED IN D3.3, AND DEMONSTRATORS. 6
--

LIST OF FIGURES

Figure 1: Alien4Cloud Application Builder	8
Figure 2: Alien4Cloud Workflow Builder	
FIGURE 3: HEAPPE REST API SWAGGER DESCRIPTION	9
FIGURE 4: SNAPSHOT FROM LEXIS VIDEO SHOWING THE DDI IN ACTION	10
FIGURE 5: SCREENSHOT SHOWING THE RESPONSE OF THE DATA-LISTING API (FIRST VERSION) WITH MOCK DATA.	11
FIGURE 6: MOCKUP (WIREFRAME) OF DDI INTERACTION FOR THE LEXIS PORTAL RELEASE R2 (UNDER CONSTRUCTION).	12
HOOKE O. MOCKOF (WINE KAME) OF DDINITERACTION FOR THE LEXIST ORTAL RELEASE RZ (ONDER CONSTRUCTION).	



EXECUTIVE SUMMARY

The LEXIS project, by month 15 of its activities, has deployed a wealth of hardware and software components. These components will help to turn the LEXIS vision of an ecosystem for optimised Cloud-HPC-HPDA workflows into reality. In D3.2, key components of LEXIS are made available in the form of a demonstrator. The installed hardware is shown and explained in the form of a video clip in order to make its capabilities clear. For the software and system components, test systems are deployed (e.g. Distributed Data Infrastructure test cluster and API preview systems), where access can be granted to interested parties. The portal of the LEXIS platform will be opened to the public (appropriate sections) when the LEXIS Open Call is issued. This deliverable does not discuss or demonstrate the LEXIS project web page¹, which is an important public component of LEXIS, but not considered a "LEXIS technical system".

Position of the deliverable in the whole project context

The deliverable describes the publicly available demonstration components (e.g. for dissemination purposes – WP9), and is thus complimentary to D3.3 [1], where technical details of the installed components are brought together. D3.2 and D3.3 thus represent the "Beta version of LEXIS technologies" (Milestone MS03, M15). The current system status reflects that the technologies/components presented in D2.2 [2] and the storage systems discussed in D3.1 [3] have been successfully integrated. MS3, D3.2 and D3.3 have a particular focus on the DDI, which must begin to interact with the orchestration system in order to allow for data transfers between itself and the HPC/Cloud systems.

Description of the deliverable

D3.2 begins with a short introduction and list of components, as they are described in D3.3. It then goes on describing the different demonstrator components:

- Novel computing systems at IT4I and LRZ (Section 2.1),
- Workflow-Management Solutions Integration of Yorc and HEAppE (Section 2.2),
- Video on LEXIS storage systems (Section 2.3),
- Preview of public parts of the LEXIS web portal (Section 2.4).

The deliverable closes with a short summary (Section 3). We remark that this report is only an addition to the actual demonstrator components to be delivered.

¹ LEXIS project web page: <u>https://lexis-project.eu/web/</u>



1 INTRODUCTION – LEXIS COMPONENTS

In this deliverable, outstanding LEXIS system components are picked for demonstration, and it is described in the way they can be demonstrated to the public. In parts, the actual demonstrators are publicly accessible 24/7 - as it is the case with YouTube videos, for example. Other components, such as the DDI test system can only be accessed on request, with possible time and audience limitations (e.g. to colleagues in the field) for security reasons.

Table 1 lists all LEXIS systems as discussed in D3.3, indicates the availability (or unavailability) of a respective demonstrator component, and refers to the later sections of the present deliverable where the demonstrator components are described.

COMPONENT	DEMO ?	SHORT DESCRIPTION OF DEMO	CF. D3.3 SECTION	SEE SECTION BELOW
Burst Buffers	Y	Novel computing systems at IT4I and LRZ	2.1	2.1
AAI Machines	Ν	-	2.2	-
Storage Systems, Management VMs/Systems	Y	Novel computing systems at IT4I and LRZ	2.3	2.1
Cloud and Accelerator Nodes, HPC Systems used	Y	Novel computing systems at IT4I and LRZ	2.4	2.1
Network	N	-	2.5	-
LEXIS AAI System (Keycloak)	Ν	-	3.1	-
DDI – Core	Y	Small DDI test system on LRZ Compute Cloud (time-limited access to researchers in the field on request).	3.2.1- 3.2.5	2.3.1
DDI – APIs	Y	Access via web browser for listing datasets on a test cluster, prospectively also served as a standard OAI-PMH catalogue.	3.2.6- 3.2.7	2.3.2
LEXIS Workflow & Code- Execution MGMT	Y	Publicly-accessible GitHub repositories and web pages with documentation for functionality preview.	3.3	2.2
LEXIS Portal and Monitoring Software Components	Y	Public sections of LEXIS portal.	3.4	2.4
Remote Visualisation	Ν	-	3.5	-
LEXIS Pilot Software Components	Ν	-	3.6	-

Table 1 - LEXIS infrastructure components as presented in D3.3, and demonstrators.



2 DEMONSTRATOR COMPONENTS

2.1 NOVEL COMPUTING SYSTEMS AT IT4I AND LRZ

Offering high-profile hardware, as installed for LEXIS, as a direct demonstrator to the public is not straightforward.

IT4I and LRZ have thus decided to create an attractive video, introducing the supercomputing centres and server rooms and showing LEXIS hardware and installation work there. Systems shown include Burst Buffers, Storage, Cloud and HPC systems. The video is made publicly available on the LEXIS YouTube Channel²

Complementary to this visual material, a press release³ has been issued containing some technical details and presenting the LEXIS strategy.

2.2 LEXIS WORKFLOW-MANAGEMENT SOLUTIONS (YORC AND HEAPPE)

LEXIS Workflow-Management solutions centre around Yorc (Ystia Orchestrator, including Alien4Cloud and other components) and HEAppE (High-End Application Execution Middleware). These pieces of software are discussed in Deliverable D3.3 and thoroughly described in Deliverable D4.2 [4] on the Design and Implementation of the HPC-Federated Orchestration System.

2.2.1 Yorc

Yorc, Ystia orchestrator⁴, provides a platform allowing to deploy applications modelled in TOSCA (Topology and Orchestration Specification for Cloud Applications) on Hybrid HPC/Cloud infrastructures. TOSCA is a standard language from the OASIS consortium to describe an application made of components, with their relationships, requirements, capabilities, and operations. Workflows - sequences of operations involving application components - can be executed and monitored by the Orchestration system.

Its front-end, Alien4Cloud⁵, provides a studio allowing to create applications from an extensible catalogue of TOSCA components, deploy these applications, run and monitor workflows.

Both the Ystia and Alien4Cloud GitHub pages provide extensive information on the software and easy instructions to install the software.

Before the LEXIS Portal can be used to run workflows, an internal test system is installed at LRZ. It allows to create hybrid Cloud/HPC applications. Such applications are made of Jobs that Yorc submits on the LRZ/IT4 HPC infrastructures through HEAppE and of software components that Yorc installs and starts on Virtual Machines that it creates on the IT4I/LRZ OpenStack infrastructures.

Using this internal test system, LEXIS partners can design their application like shown below in the Alien4Cloud Application Builder, selecting components (node templates in TOSCA terminology) from a catalogue of components in the right pane, and dragging/dropping these components in the main pane, then drawing relationships between components to describe how a requirement of a component is fulfilled by the capability of another component, as shown in the following screenshot of the Application Builder (Figure 1):

² LEXIS YouTube Channel: <u>https://m.youtube.com/channel/UCiU3w-dw9-eaOCD4Zlf8qVw/videos</u> (publicly available from Q2 2020)

³ LEXIS press release: <u>https://lexis-project.eu/web/press-releases</u>

⁴ Ystia orchestrator: <u>https://ystia.github.io/</u>

⁵ Alien4Cloud: <u>https://alien4cloud.github.io/</u>



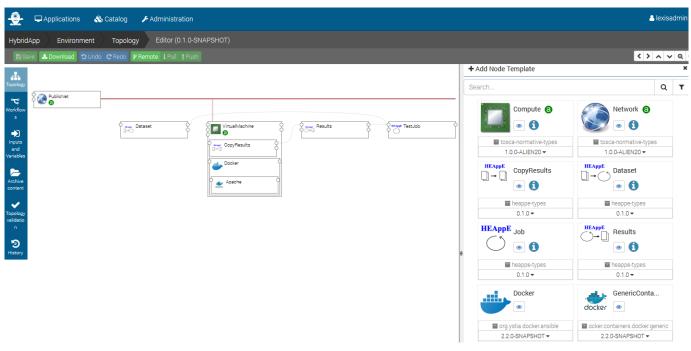


Figure 1: Alien4Cloud Application Builder.

A Workflow Builder then allows to build sequences of operations to execute on these components, as shown in the following screenshot (Figure 2):

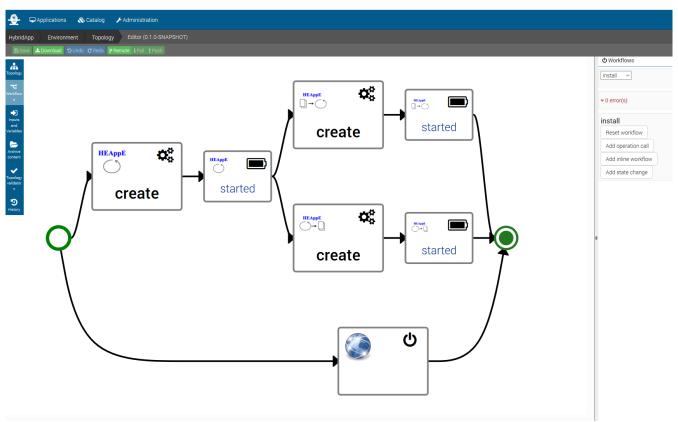


Figure 2: Alien4Cloud Workflow Builder.

Once done, this application can be deployed, its workflows are executed and monitored from this front-end. All these orchestration functions are also available through an API that will be used by the LEXIS portal.



For additional details, the reader is referred to deliverable D4.2 (Design and Implementation of the HPC-Federated Orchestration System - Intermediate).

2.2.2 HEAppE middleware

Home page of the HEAppE Middleware project is located at <u>http://heappe.eu</u>. Besides the code and documentation, the swagger's REST-API description & demonstrator is automatically available for each deployed middleware instance: IT4I's⁶ and LRZ's⁷ (see a screenshot in Figure 3).

⊖ swagger	Select a spec	Web API V1	~
HEAppE Web API [Base URL: heappe.lexis.lrz.de/lexis] /swagger/v1/swagger/son			
Schemes V V			
ClusterInformation		~	/
GET /heappe/ClusterInformation/ListAvailableClusters			
POST /heappe/ClusterInformation/CurrentClusterNodeUsage			
FileTransfer		~	/
POST /heappe/FileTransfer/GetFileTransferMethod			
POST /heappe/FileTransfer/EndFileTransfer			
POST /heappe/FileTransfer/DownloadPartsOfJobFilesFromCluster			
POST /heappe/FileTransfer/ListChangedFilesForJob			
POST /heappe/FileTransfer/DownloadFileFromCluster			
JobManagement		~	/
POST /heappe/JobManagement/CreateJob			

Figure 3: HEAppE REST API swagger description

2.3 DISTRIBUTED DATA INFRASTRUCTURE DEMO SYSTEM

2.3.1 Low-level access

On the LRZ Compute Cloud, a demonstration system has been installed, consisting of two iRODS zones (simulating LRZ/IT4I) with one iRODS-provider-server and one client machine for each. Access can be given on request for two weeks maximally, by creating a local user on the client systems and a corresponding iRODS user. The Client system is then reachable via SSH private-/public-key access via the internet, so that the requesting person can try out whatever he likes on the system. Original system images are retained such that all four machines can be reset afterwards.

The user transfers his own data via SCP to the machines, where he can ingest them into iRODS.

⁶ IT4I HEAppE Middleware REST API: <u>https://heappe.it4i.cz/lexis/index.html</u>

⁷ LRZ HEAppE Middleware REST API: <u>https://heappe.lexis.lrz.de/lexis/index.html</u>



A video showing the system in action, more of interest to researchers than a general public, has been put on Zenodo⁸, and a screenshot is displayed below (Figure 4). The video shows DDI in action - the left-hand and right-hand virtual machines both access the data in projtest001/GFS on the "IT4I Zone" and "LRZ zone" of the test-DDI (irods-lexis-demo-new-3 reads, irods-lexis-demo-new-4 writes). The video will be refined in the next few months and then also be put on the LEXIS YouTube Channel mentioned in Sec. 2.1.

←								
Datal Baarbaitan Asal	Virtual Machine "IT4!" side cht Terminal Reiter Hilfe	• • • ×	Datei Bearbeiten Ansicht Term	Virtual Machine "L	RZ" side			+ ×
		wp3/proitect001/CE	ubuntu@irods-lexis-demo-					_
S /IT4ItestLexisZone C- /IT4ItestLexi	s-demo-new-3:-\$ ils /IT4ItestLexisZone/main/ e/main/wp3/projtest001/GFS: isZone/main/wp3/projtest001/GFS/GFS-20180824 isZone/main/wp3/projtest001/GFS/GFS-20180825 s-demo-new-3:-5	18	ubuntu@irods-lex1s-demo- Filesystem udev tmpfs /dev/vda1 tmpfs tmpfs p tmpfs 0 141.40.254.10:/weatherda ubuntu@irods-lexis-demo- t001/GFS./01-download ubuntu@irods-lexis-demo- GFS-2018082418 GFS-2018082518 GFS-2018082518 GFS-2018082618	1K-blocks 4594304 920716 101584140 4603576 5120 4603576 920716 tta 106552684288 1 new-4:-5 cd ./01	8884 14802604 29308 0 0 0 0073700352 -w /IT4Ites - download/	4594304 911832 86765152 4574268 5120 4603576 920716 867706112 stLexisZon	1% /dev/s 0% /run/l 0% /sys/f 0% /run/u 97% /mnt e/main/wp3/	shm lock fs/cgrou user/100 /projtes
00:00:52								00:00:51

Figure 4: Snapshot from LEXIS video showing the DDI in action

2.3.2 APIs

A machine where API-based access to the LEXIS DDI can be demonstrated has been set up at: <u>https://lexis-ddi.srv.lrz.de</u>.

This machine runs the data-listing API and shows the user a list of datasets, where a selection can be made via the API. In this way, interested parties can gain a glimpse on the prospective style of LEXIS Data System APIs. A screenshot of this, based on mock data sets, is shown in Figure 5.

⁸ LEXIS video at ZENODO: <u>https://doi.org/10.5281/zenodo.3733761</u>



JSON Rohdaten Kopf	zeilen
Speichern Kopieren Alle ein	klappen Alle ausklappen 🖓 JSON durchsuchen
▼ 0:	
access_permission:	"public"
▼ contributor:	
0:	"1"
▼ creator:	
0:	"1"
group:	"wp5"
identifier:	"doi://lexis-datasets/wp5/datasetpublicx1"
name:	"datax5"
▼ owner:	
0:	"1"
project:	"proj51"
publicationYear:	"1900"
<pre>vublisher:</pre>	
0:	"1"
relatedIdentifier:	"doi://lexis-datasets/wp5/datasetpublicx1"
title:	"wp5/dataset"

Figure 5: Screenshot showing the response of the data-listing API (first version) with mock data.

2.4 WEB PORTAL DEMONSTRATOR COMPONENTS

The LEXIS WP8 Portal provides access to LEXIS Infrastructure and Data Sets, such that interaction with datasets is facilitated, and controlling and monitoring job deployment are possible. Internal demonstrators for this portal have been made in the form of wireframes, as shown below.

As the LEXIS Portal will be used in the Open Calls, the LEXIS Portal will in the coming months be made open and publicly accessible. The functionality provided by the portal will clearly be limited for users which have no access to HPC resources, but e.g. public datasets can be listed and the user-friendly approach to HPC/Cloud/Big Data will be conveyed.

2.4.1 Initial version of the Portal

An initial internal version of the LEXIS portal was provided in M10 of the project; this had minimal support for Keycloak based login, adding information to user profiles, creating an organization that a user is affiliated with, etc.

The initial variant of the LEXIS Portal provided support for the listing Data Sets and associated meta data within the LEXIS DDI. More specifically, it provided support for interacting with an initial iRODS deployment which contained sample data, and which could be shown within the portal interface.

2.4.2 Portal Revision R2 - Wireframes

The WP8 team is working on R2 of the portal to be delivered in M15. This release will contain enhanced capabilities for interacting with the LEXIS DDI. More specifically, it will differentiate between:

- public data,
- project specific data,
- private data available to a single user,

and provide support for listing and viewing data of the above types. An example of a wireframe of this work can be seen in Figure 6.



< ⇒ × ☆ ⊡	ttp://lexis.portal.eu	LEXIS Portal - Manage Resources			
				<u>User: David Hruby</u>	Logout
Dashboard Projects Orgazation Jobs	GridFTF Dataset description: Me	P Transfer Request			\leq
Workflows Data sets	DataCite minimal metadata attributes	Identifier - (normally a DOI, can be left empty and will be filled when DOI is requested)	Id		
About LEXIS		Creator - (main researchers involved in producing the data)	Rubén García-Hernández		
		Title - (of the data set)	Earthquake region B run 1		
	8	Publisher - (entity which holds/archives/publishes/produces data)	LRZ		
	1.7	PublicationYear - (year when data became/become/will become public, if this is not available, use the date preferred from a citation perspective)	2020		
		ResourceType - (e.g. data set of weather simulation data)	Dataset / GIS		
	data-service-swagger metadata	Description			
		Owner	Rubén García-Hernández		
		Contributor	Rubén García-Hernández		
		Related Identifier(s)	2342	Earthquake region B run 2	
	8		5442	Earthquake region B run 3	
		Further metadata as needed			
	Data Set Access Mode	Public			
		Click here to request a globus data transfer			

Figure 6: Mockup (Wireframe) of DDI interaction for the LEXIS Portal Release R2 (under construction).



3 SUMMARY

This deliverable has centred on our efforts to give internal and external interested parties a grasp on LEXIS technology, i.e. installed hard- and software systems up to M15. To this end, videos, systems, and documentation hubs have been put together. This report just contains links and pointers to the actual demonstrator components.

Novel computing systems have been installed at IT4Innovations and LRZ. In order to present them in an easy way to the wider public audience, we have decided to produce a public video and press release about these computing systems. The Orchestration component of the platform (centred around HEAppE and Yorc) is presented in repositories, with user-friendly documentation, and instructions for everyone interested to do local demo installations. HEAppE also features REST-API definition/demo pages, as the DDI does. The lower-level DDI demonstration focuses on a test system, which is accessible on request and presented in a public, commented screen video. For the "face of LEXIS", the LEXIS portal, finally, wireframes are available for demonstration purposes and a public section is being prepared.

We are confident that with the components presented, we have found an adequate and attractive way to spark the interest in the LEXIS platform. Clearly, as LEXIS matures, also the demonstrator components will reflect the advanced status and thus become a tool to show the project's progress to the public.



- [1] LEXIS Deliverable, D3.3 Mid-Term Infrastructure (Deployed System Hard/Software).
- [2] LEXIS Deliverable, D2.2 Key parts LEXIS Technology Deployed on Existing Infrastructure and Key Technologies Specification.
- [3] LEXIS Deliverable, D3.1 Local Storage Solutions Report.
- [4] LEXIS Deliverable, D4.2 Design and Implementation of the HPC-Federated Orchestration System -Intermediate.

More specific, thematic references are to be given in Deliverable D3.3.