

Large-scale Execution for Industry & Society





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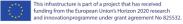
FEDERATED RESEARCH DATA **MANAGEMENT IN LEXIS**

EGI 2020 Conference Nov 2nd, 2020 Data Management Solutions-Part 1

JOHANNES MUNKE, MOHAMAD HAYEK (LRZ)

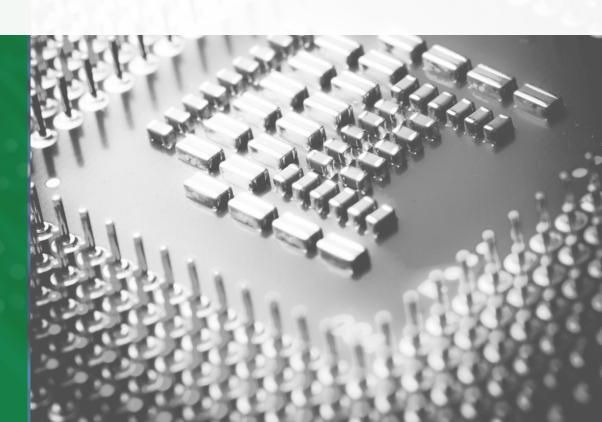
LEXIS DATA SYSTEM TEAM **CONSORTIUM**







CONTEXT:
QUICK OVERVIEW
OF LEXIS





Large-scale Execution for Industry & Society





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Topic:	HPC and Big Data enabled Large-scale Test-beds and Applications	
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Турє

LEXIS project, led by the IT4Innovations (CZ) Supercomputing Centre:

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(...) is building an advanced engineering platform at the confluence of HPC, Cloud and Big Data, which leverages large-scale geographically-distributed resources from existing HPC infrastructure, employs Big Data analytics solutions and augments them with Cloud services.

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Proje

Driven by the requirements of several pilot testcases, the LEXIS platform relies on best-in-class data management solutions (EUDAT) and advanced, distributed orchestration solutions (TOSCA), augmenting them with new, efficient hardware and platform capabilities (e.g. in the form of Data Nodes and federation, usage monitoring and accounting/billing support).

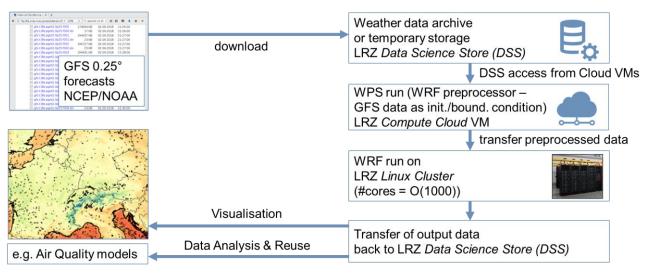
Thus realize, LEXIS realises an innovative solution (...)

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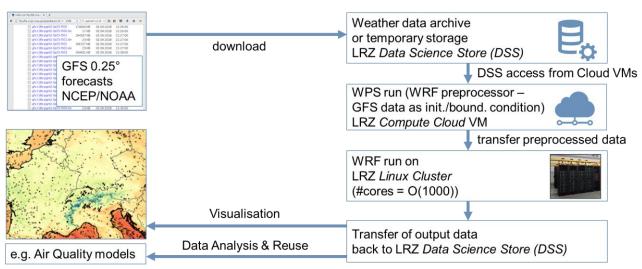
LEXIS: THE PROBLEM ADDRESSED

Typical High-Performance-Computing (HPC) / Big Data workflow: Weather prediction at LRZ



LEXIS: THE PROBLEM ADDRESSED

Typical High-Performance-Computing (HPC) / Big Data workflow: Weather prediction at LRZ



- Complicated!
 - multiple systems & data transfers to be set up
 - closed system, no flexible usage of European resources
- Not often leveraged by Industry, SMEs, unexperienced scientists





LEXIS H2020 PROJECT OBJECTIVES

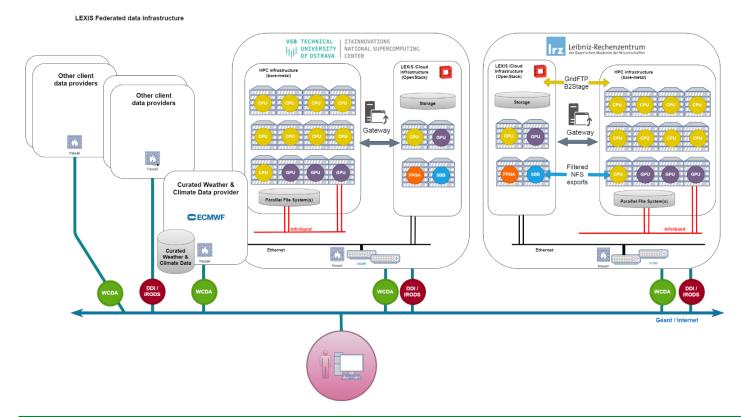
European Computing & Big Data Platform for Industry, Society, Science

- Access to the HPC/Cloud/Big Data resources for SMEs/Industry (incl. Billing model)
- **Web Portal** (easy entry point, unified AAI)
- **Orchestration** for easy, automatic and optimized workflows
 - Cloud and HPC resources at different European Computing Sites
 - convenient user interface to define workflows
 - boosted by acceleration techniques (Compute: GPU, FPGA: Data: Burst Buffers)
 - → Details in the talk of **Alberto Scionti** et al., 13:15 today, session **"Workflow Management Solutions"**
- Integration with European Infrastructure
- **Demand** for a strong Data Management backend LEXIS Work Package 3
 - unified data access from LEXIS Cloud and HPC resources across Europe
 - cross-site "Big Data" and metadata management
 - Data Discovery and FAIR ("Findable, Accessible, Interoperable, Reusable") Data
 - \rightarrow This is the scope of this talk





LEXIS PLATFORM



LEXIS PILOT PROJECTS

General information - https://lexis-project.eu/web/



Computation Fluid Dynamics (CFD), Rotating parts (gearboxes), 3D Visualization



Earthquakes & Tsunami prediction models, geographic and urban databases, emergency organization, urgent computing

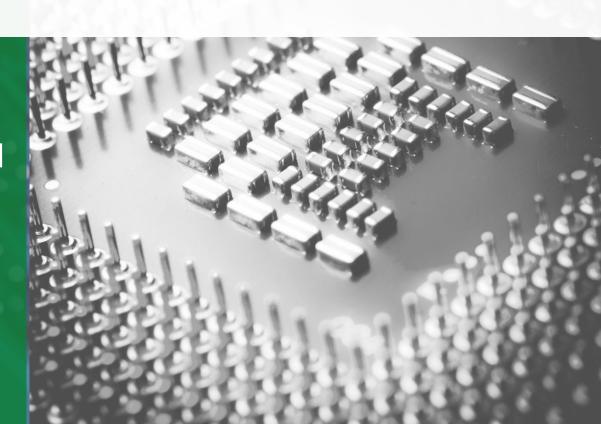


Weather & Climate models (WRF) and various post-processors for flood, wildfire & agriculture applications



LEXIS DATA SYSTEM

(WORK PACKAGE 3)



LEXIS DDI - DISTRIBUTED DATA INFRASTRUCTURE

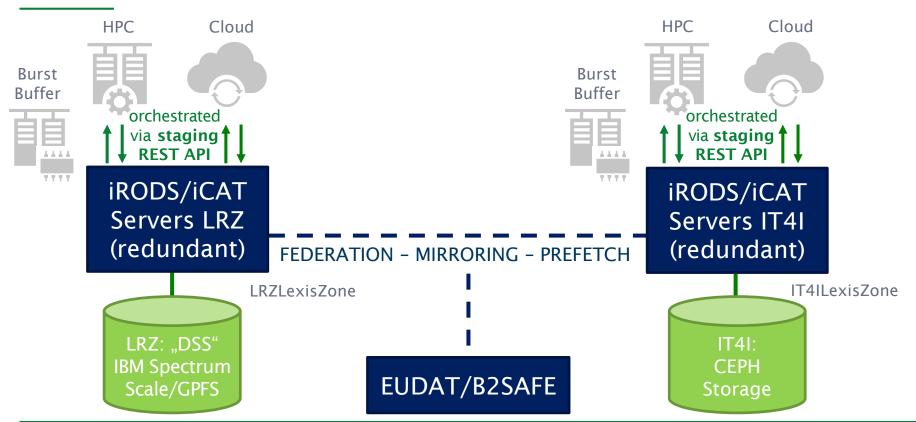
Key Points

- Idea: use an European system for LEXIS data
 → EUDAT/iRODS (Integrated Rule-Oriented Data System middleware)
- Unified view on data in LEXIS federated iRODS zones (IT4I, LRZ, ...)
 - "filesystem-like"; top-level directories e.g. /IT4ILexisZone
 - transparent access to all files via all iRODS servers
- Physical file storage policies implemented as iRODS rules, e.g.
 - cross-site mirroring
 - **low-level storage tiering** (in each computing/data centre)
- "Non-invasive" data-curation approach
 - DataCite-like metadata stored in iRODS, EUDAT-B2HANDLE PIDs
 - directory/access-rights structure fixed on project (top-)level
- Uses LEXIS cross-provider AAI



LEXIS DDI

Federation leveraging iRODS & EUDAT B2SAFE (and B2HANDLE, B2STAGE)







DATA PRESERVATION IN LEXIS: B2SAFE

B2SAFE is the data preservation module in EUDAT

- The B2SAFE service runs on top of LEXIS iRODS zone to:
 - provide data safety and resiliency in case of an issue at one of the federated centres, by implementing mirroring policies;
 - optimize the workflows execution by allowing the Orchestrator to get the data from the zone close to the computing resources; and to
 - trigger PID registration.



EUDAT Collaborative Data Infrastructure, "B2SAFE - EUDAT," EUDAT Ltd, 2020. [Online]. Available: https://www.eudat.eu/services/b2safe.

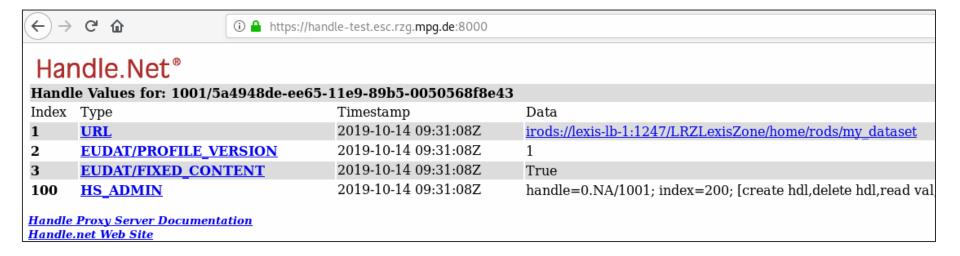




PERSISTENT IDENTIFIERS IN LEXIS (PIDs): B2HANDLE

B2HANDLE is the PID module in EUDAT

- The LEXIS DDI makes use of B2HANDLE PIDs to guarantee data access via long-lasting unique identifiers, in order to to
 - facilitate publication of data; and
 - facilitate data retrieval in the long term.





THE LEXIS DDI PROMOTES FAIR DATA MANAGEMENT

Findable, Accessible, Interoperable, Reusable Research Data

- Two of the most basic FAIR requirements:
 - 。 metadata
 - a (world-)unique identifier for the data
- Metadata in LEXIS:
 - stored in iRODS Attribute-Value(-Unit)
 store for each data set
 - schema oriented at the basics from DataCite (schema.datacite.org)

```
@lexis-lb-1:~$ ils
/LRZLexisZone/home/rods/my dataset:
       @lexis-lb-1:~$ iput opensearch.txt
      @lexis-lb-1:~$ ils
/LRZLexisZone/home/rods/my dataset:
  opensearch.txt
       @lexis-lb-1:~$ irule -F eudatPidsColl.r
newPID = 1001/5a4948de-ee65-11e9-89b5-0050568f8e43
       @lexis-lb-1:~$ imeta ls -C /LRZLexisZone/home/rods/my dataset
AVUs defined for collection /LRZLexisZone/home/rods/my dataset:
attribute: EUDAT/FIXED CONTENT
value: True
units:
attribute: PID
value: 1001/5a4948de-ee65-11e9-89b5-0050568f8e43
units:
```



THE DDI IN THE LEXIS ECOSYSTEM

Communication via APIs

Portal Data / Workflows / Visualisation



Monitoring System



Data Discovery API



Data Transfer API



Monitoring/ Billing API



DDI

(Distributed Data Infrastructure with Metadata Handling / FAIR)



Local Storage Systems











AAI (Authentication & Authorization

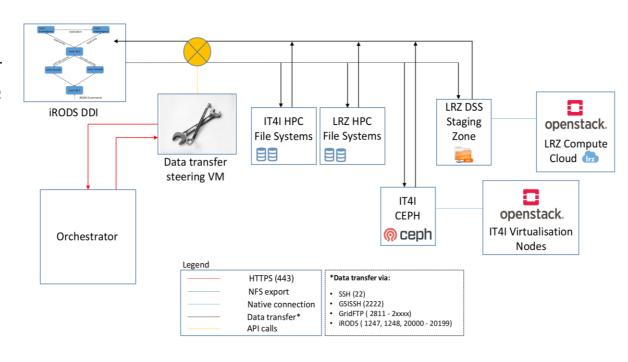
Infrastructure)





LEXIS DATA SYSTEM APIs: TRANSFER/STAGING API

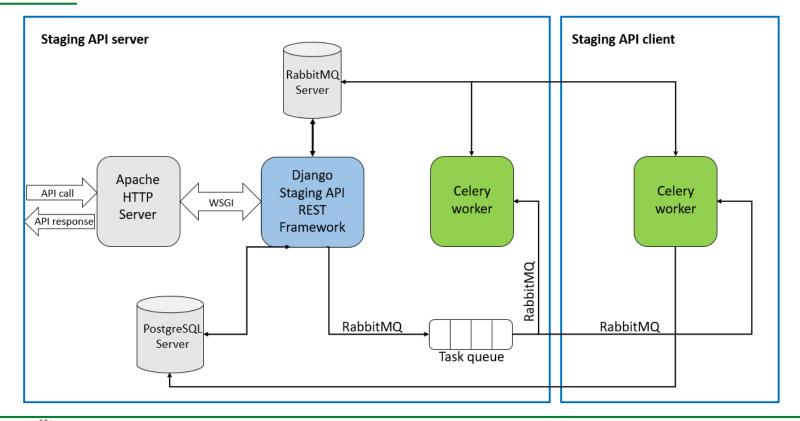
- Django-based RESTful API
- Purpose: LEXIS orchestrator can move data between the DDI and distributed computing resources by a simple HTTP request.
- Uses LEXIS AAI and the HEAppE middleware to authenticate the requests and authorize access.
- Uses Celery and RabbitMQ to handle requests asynchronously.





LEXIS DATA TRANSFER/STAGING API (continued)

Architecture



DATA MANAGEMENT VIA LEXIS PORTAL

Work Package 8, Task 8.1 - "Work in Progress"

- Login using LEXIS AAI (Keycloak-based)
- User accesses DDI data with rights encoded in token:

LEXIS DDI validates token using strongly customized iRODS-OpenID Plugin.

Next months:

from working demonstrator to convenient everyday data management!

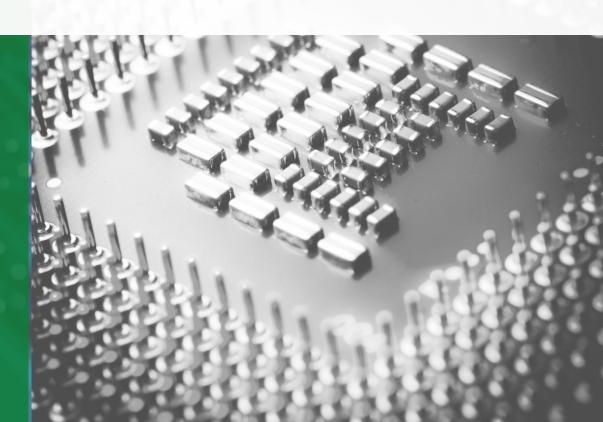








LEXIS OPEN CALL,
EUROPEAN
COLLABORATION &
OUTLOOK



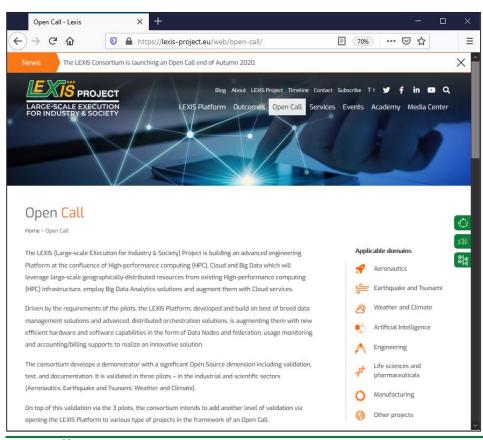
LEXIS - OPEN CALL: OBJECTIVES

- Idea: additional validation of platform via various "external" use cases
- Selected Open Call projects have the opportunity to
 - access HPC/Cloud workflow orchestration & data platform with large resources, and
 - get technical support and training (individual "project manager" from LEXIS team).
- These projects also include other EU projects (e.g. CompBioMed2) \rightarrow collaboration
- **Current stage**: Further applicants are submitting their projects and the Open Call Board will select the best ones
 - larger focus on Industry / Private sector (but not exclusive)
 - collaboration & integration with European & third party infrastructures (Computing/Data)





LEXIS - OPEN CALL ON PROJECT WEBSITE



For further information and registration visit:

lexis-project.eu/web/open-call/

CONCLUSIONS AND OUTLOOK

- LEXIS European Cloud-HPC Workflow Platform (H2020) works with a Distributed Data Infrastructure based on iRODS/EUDAT-B2SAFE
- Philosophy: **Easy usability** via Portal, **clean architecture** (REST APIs...)
- Data Federation of IT4I (CZ) and LRZ (DE) to be extended to further participants
- Platform to be further immersed with EUDAT and beyond (ideas: BDVA, EGI federated cloud, EOSC, ...)
- We are aiming at (and open for) collaborations!
 - with centres joining the LEXIS platform
 - with EU projects and initiatives
 - ... in the frame of the **LEXIS Open Call and in general.**
- Focus in 2021: benchmarking, optimisation & sustainability of the platform (operation & funding model, etc.)



CONTACT

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Thanks for your attention!

GFZ



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