

National Initiatives for Open Science in Europe

Εργαλειοθήκη NI4OS-Europe και
καλές πρακτικές στο EOSC

Μελέτη περίπτωσης από τον τομέα της
βιοϊατρικής

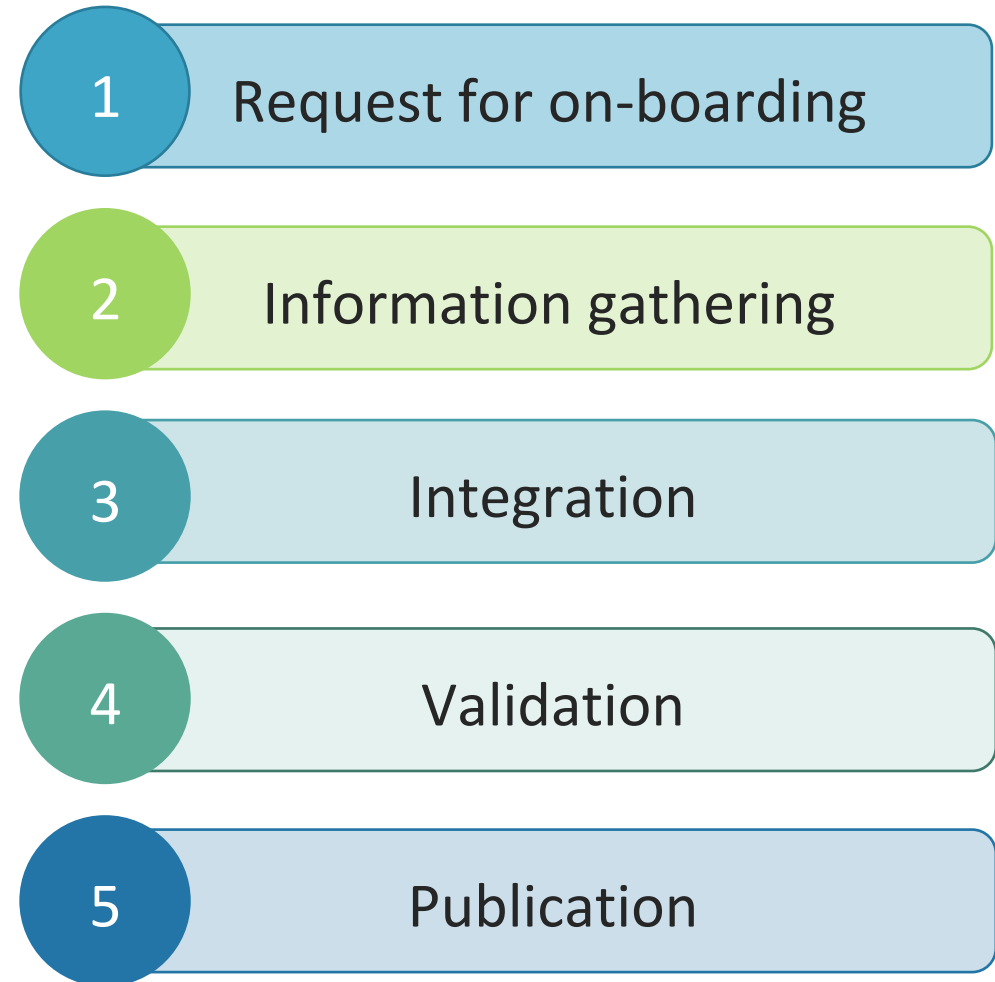
6 Δεκεμβρίου 2021

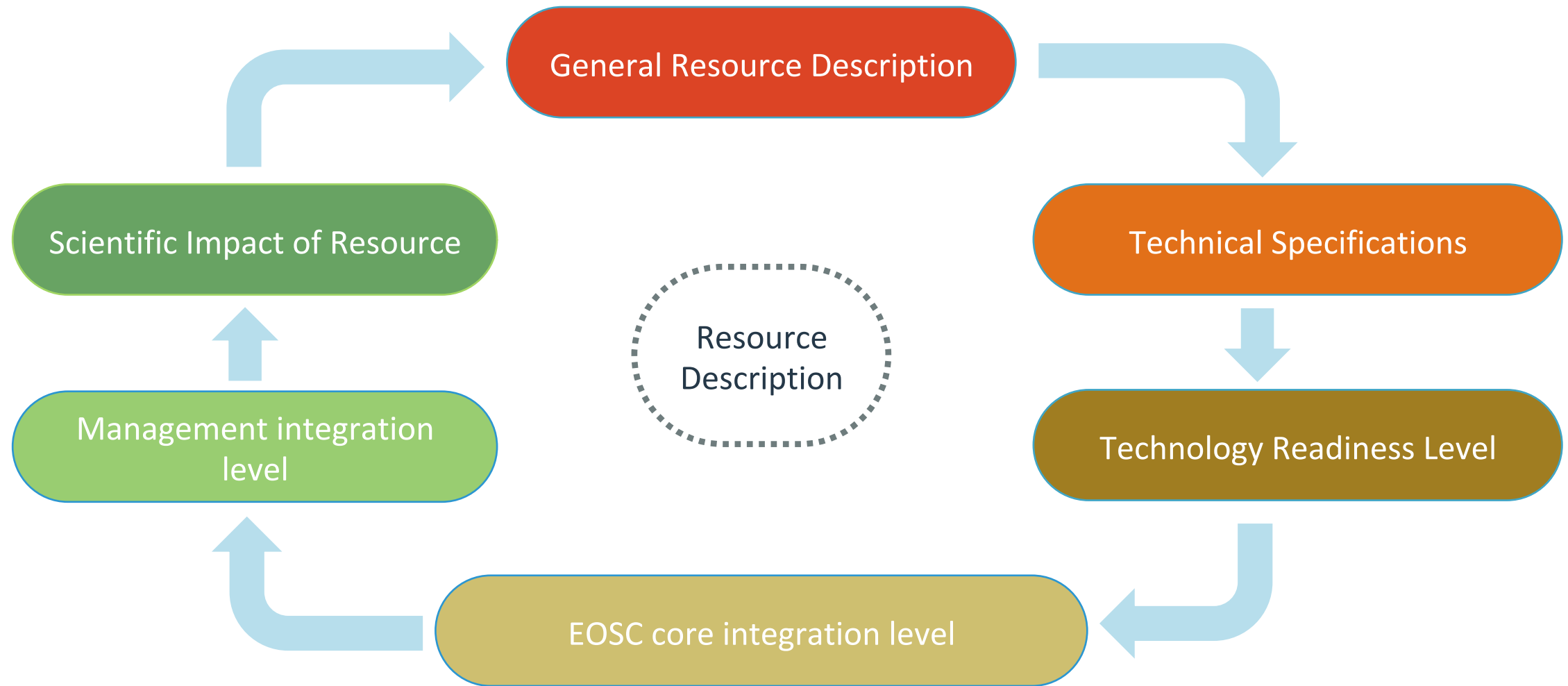
Ζωή Κούρνια, IIBEAA
Life Sciences Scientific Community Leader

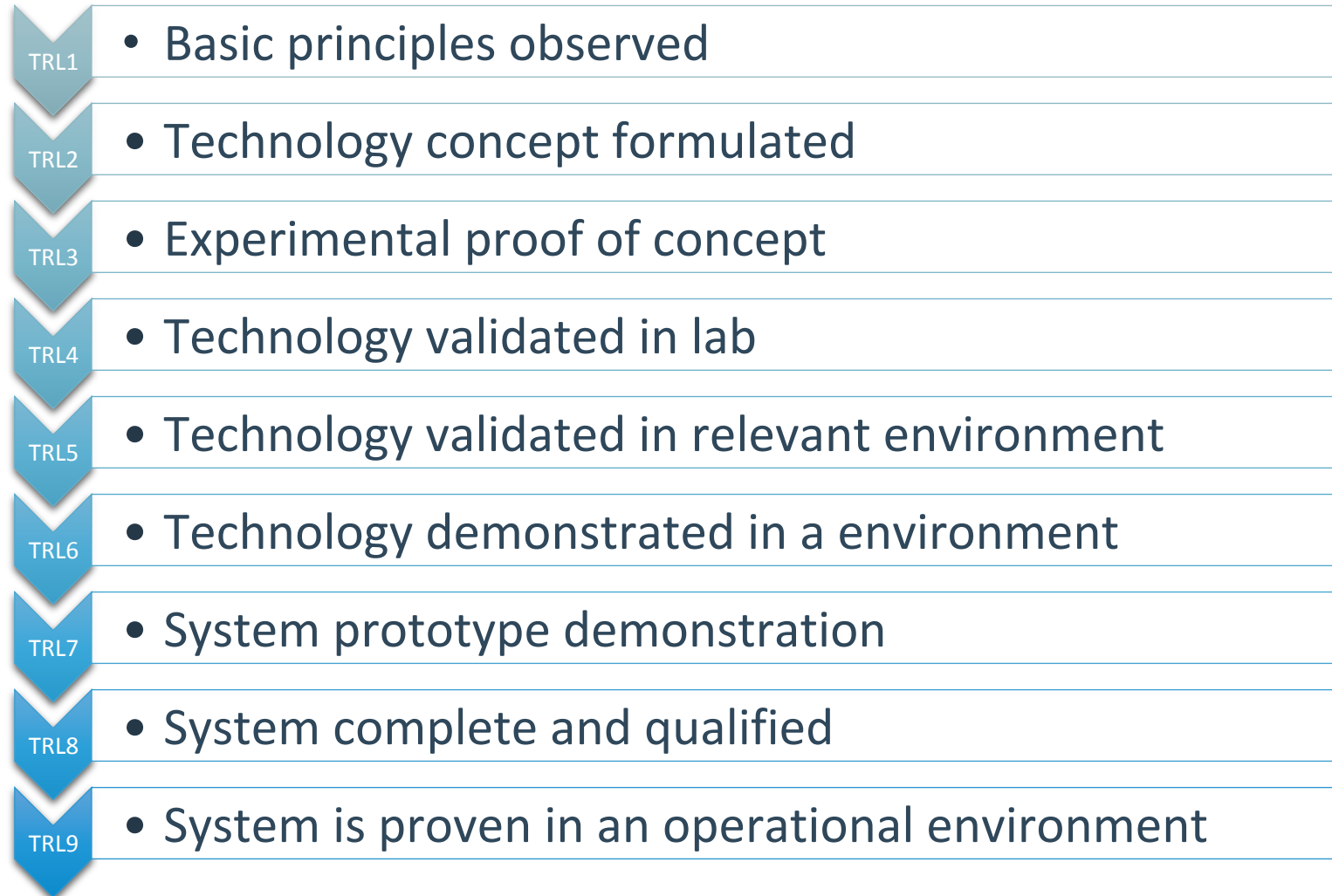


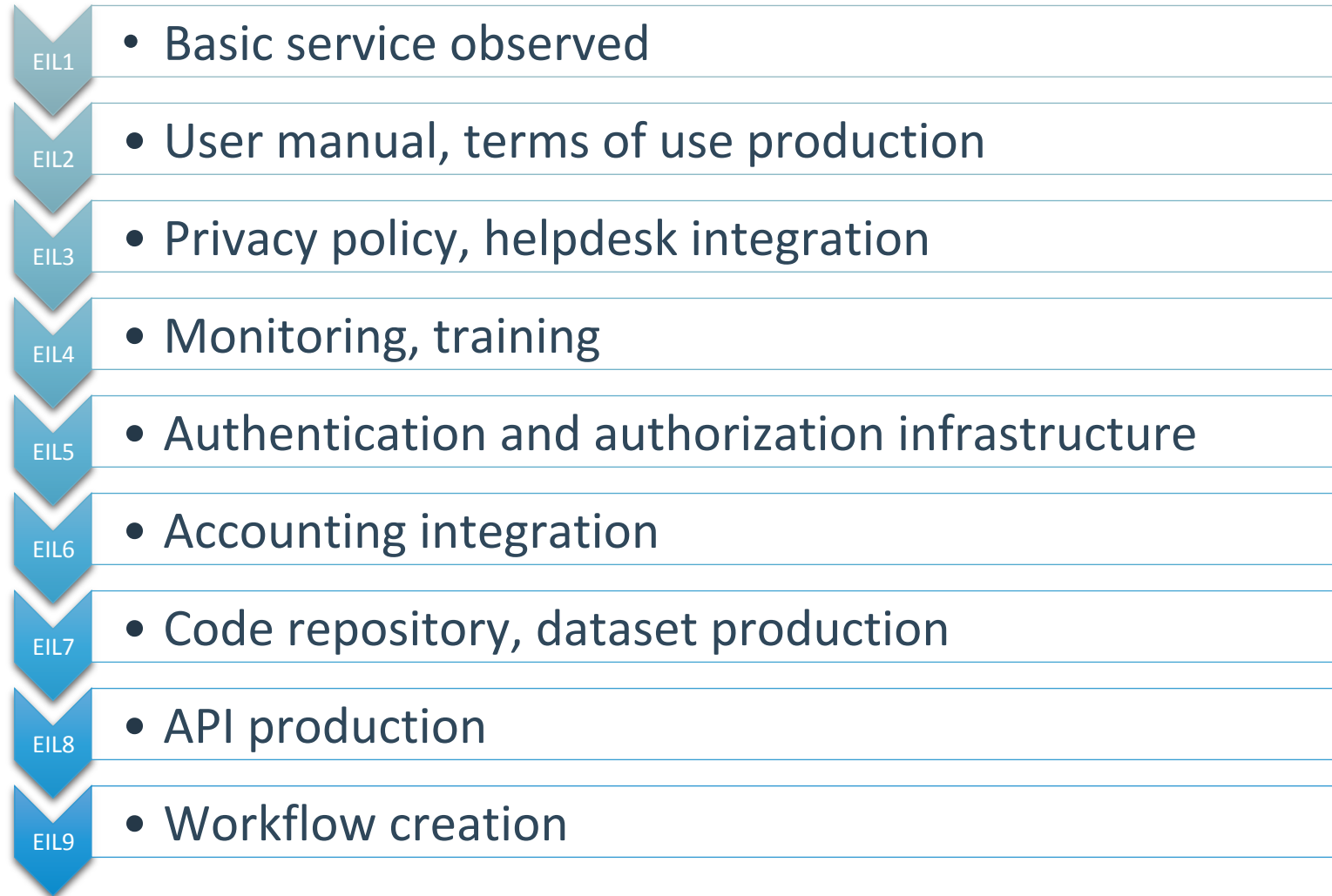
- ❑ Onboarding Procedure
- ❑ Examples of services that can be onboarded on NI4OS/EOSC
- ❑ Examples of BRFAA onboarded services
- ❑ From Software to Web-server
- ❑ Case study from NI4OS-Europe onboarding in Life Sciences

- ❑ **1. Request sent** by service provider [via e-mail](#) or submitted via a dedicated form that officially initiates the on-boarding process
- ❑ **2. Relevant information is gathered** by registering the service in [AGORA](#) using a service description template or a corresponding online form
- ❑ **3. a.** NI4OS-Europe proceeds with **pre-production environment integration**
- ❑ **3. b.** The resource is **integrated** with the existing EOSC tools and federated core, to be compatible with the rules of participation
- ❑ **4.** The resource is **validated** using tools from the federated core
- ❑ **5.** The resource is **published** in the EOSC catalogue
[More info here](#)











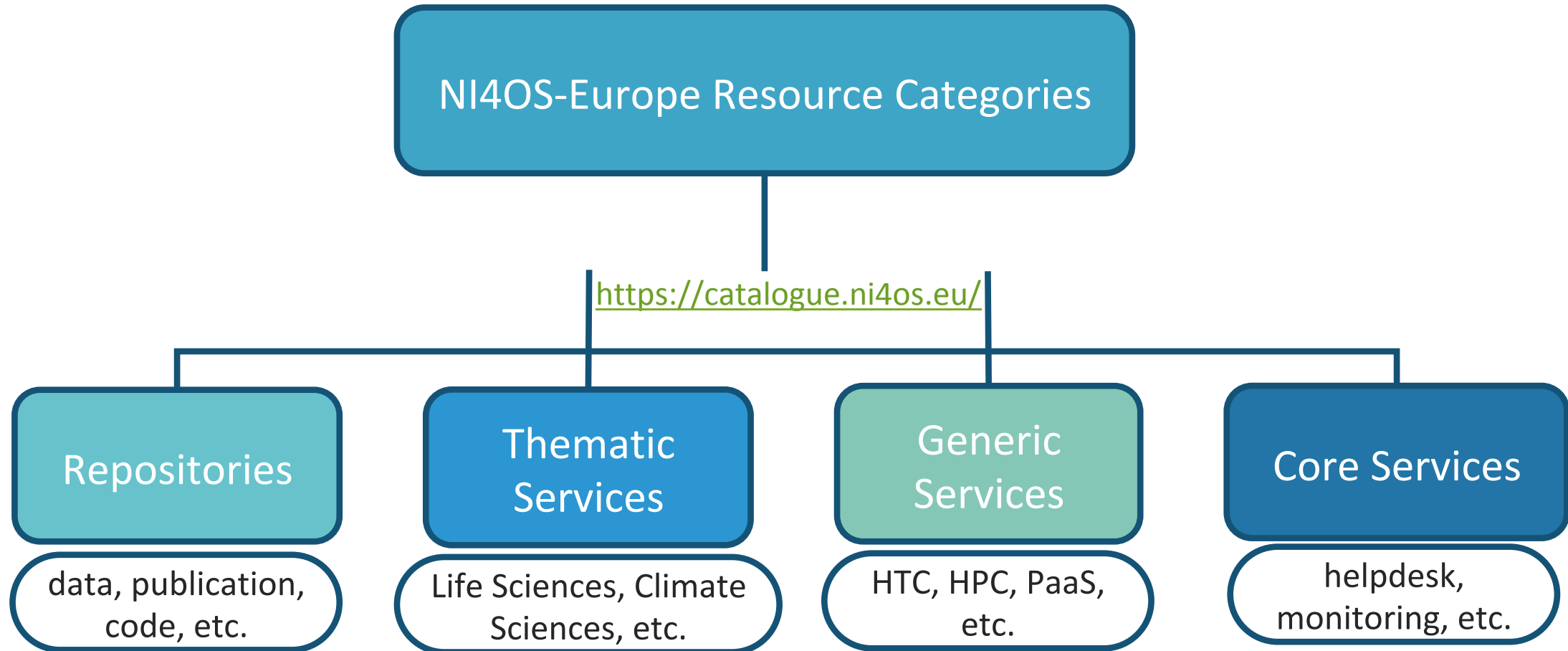
- Creation of provider's AGORA account, via AGORA catalogue
- Authorization of provider's AGORA account
- Provider registration using AGORA
- Publish provider information
- Creation of resource provider's AGORA account
- Authorization of resource provider's AGORA account
- Basic description of resource
- User manual
- Terms of use: template available [here](#)
- Access policy
- Privacy policy: guidelines and a template document available [here](#)
- Acceptable use policy
- Helpdesk integration process
- Integration with the monitoring system
- Publication of the resource within the catalogue

TRL > 8,9

EIL > 4

MIL >3

[More info here](#)



Repositories



NI4OS-Europe repository service

NI4OS-Europe general-purpose data repository.

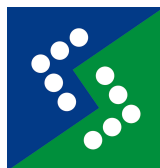
Thematic Services



Nanocrystal

NanoCrystal is a novel web-based crystallographic tool that creates nanoparticle coordinates from any material crystal structure.

Generic Services



Data analysis service

Data exchange service for the scientific communities.

Core Services



Agora Resource Portfolio Management Tool

Resource portfolio management tool.

1) Have you created/Do you own any of the following?

- A. Repository/Database
- B. Software (Thematic Service)
- C. Generic Service (Computing resources)
- D. Core Service (Archival services, heldesk, monitoring etc)
- E. Both A and B or Both C and D
- F. All


2) Have you onboarded your service?

A. YES

B. NO

- ❑ Best practices for on-boarding and related policies (D3.1)
- ❑ Provider landscape analysis and provider categorization (D5.1)
- ❑ NI4OS-Europe Best practices for on-boarding and related policies 2nd version (D3.4)
- ❑ All NI4OS resources can be found [here](#).

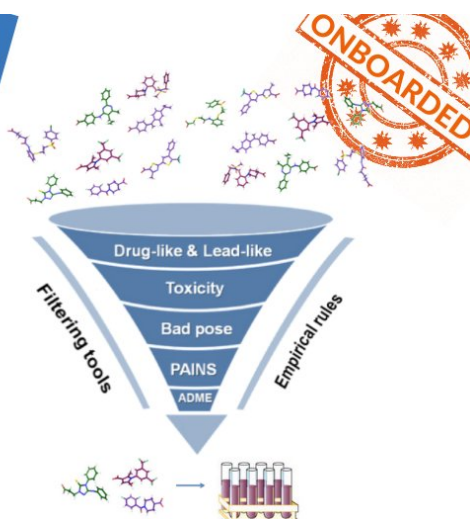
Examples of BRFAA onboarded services


 **EXPLORE**
NI4OS-Europe Catalogue

Thematic services

ChemBioServer is a publicly available web application for effectively **filtering and clustering chemical compounds** used in drug discovery.

<http://chembioserver.vi-seem.eu/>

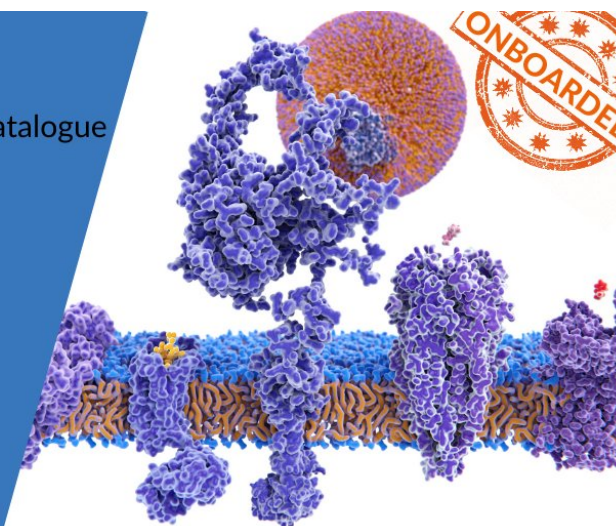


 **EXPLORE**
NI4OS-Europe Catalogue

Thematic services

DREAMM is a novel web-based tool that **predicts the protein-membrane interfaces of peripheral membrane proteins** using ensemble machine learning.

<http://dreamm-ni4os.eu/>

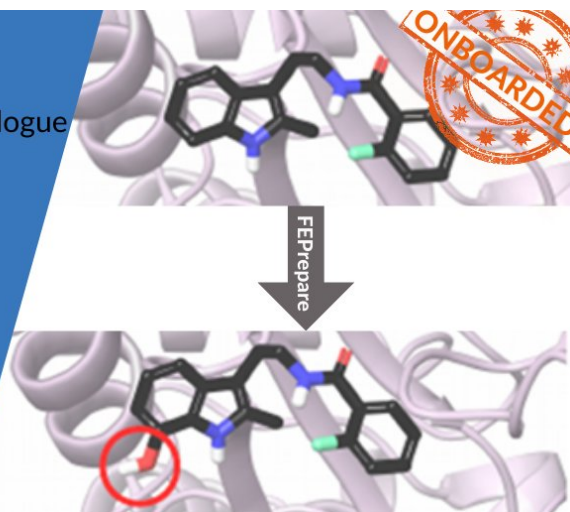


 **EXPLORE**
NI4OS-Europe Catalogue

Thematic services

FEPprepare is a webserver, which automates the set-up procedure for performing **NAMD/FEP simulations**.

<http://fepprepare.vi-seem.eu>

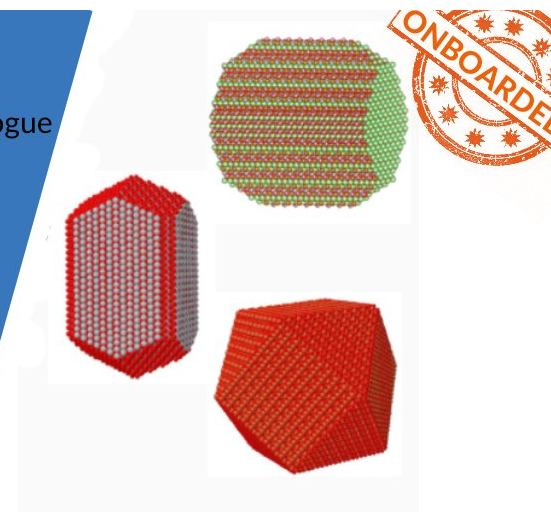


 **EXPLORE**
NI4OS-Europe Catalogue

Thematic services

NanoCrystal is a novel web-based **crystallographic tool** for the construction of nanoparticles from any material crystal structure.

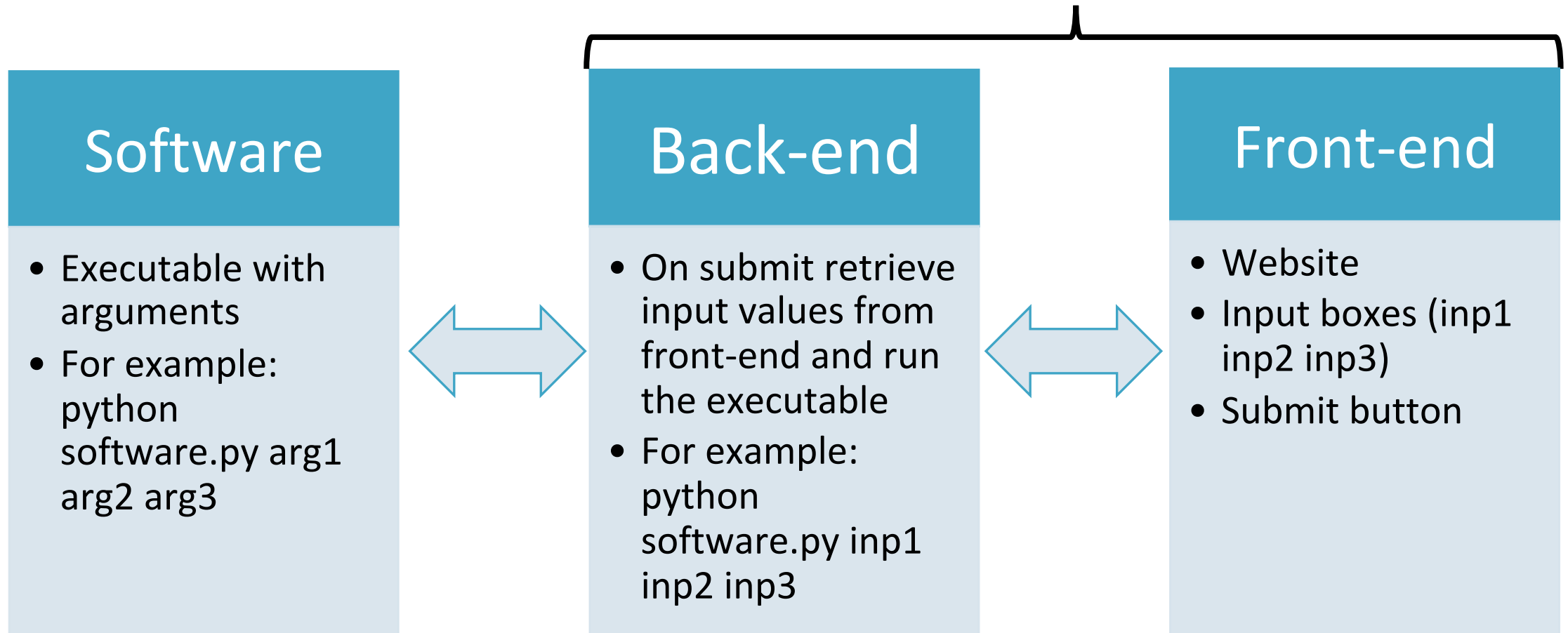
<http://nanocrystal-seem.eu>



From software to web-server example

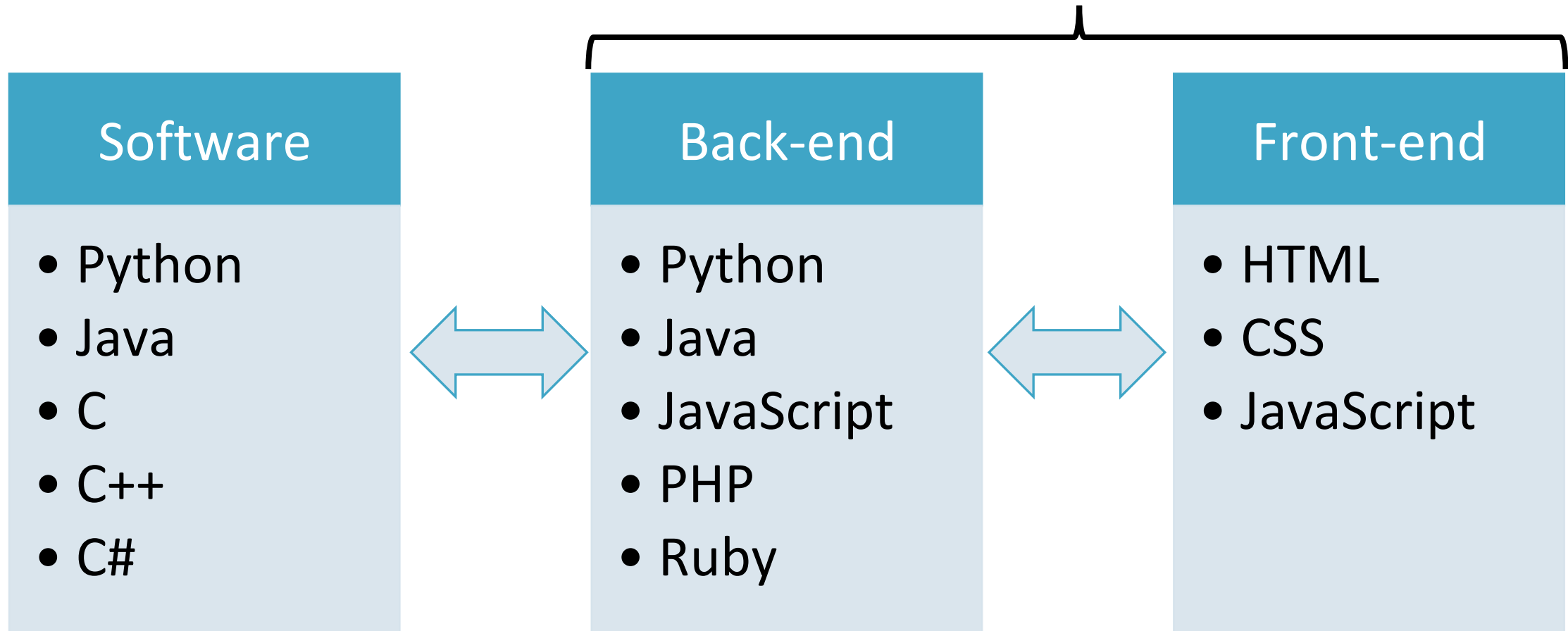
□ Make a software easily accessible

Web-service

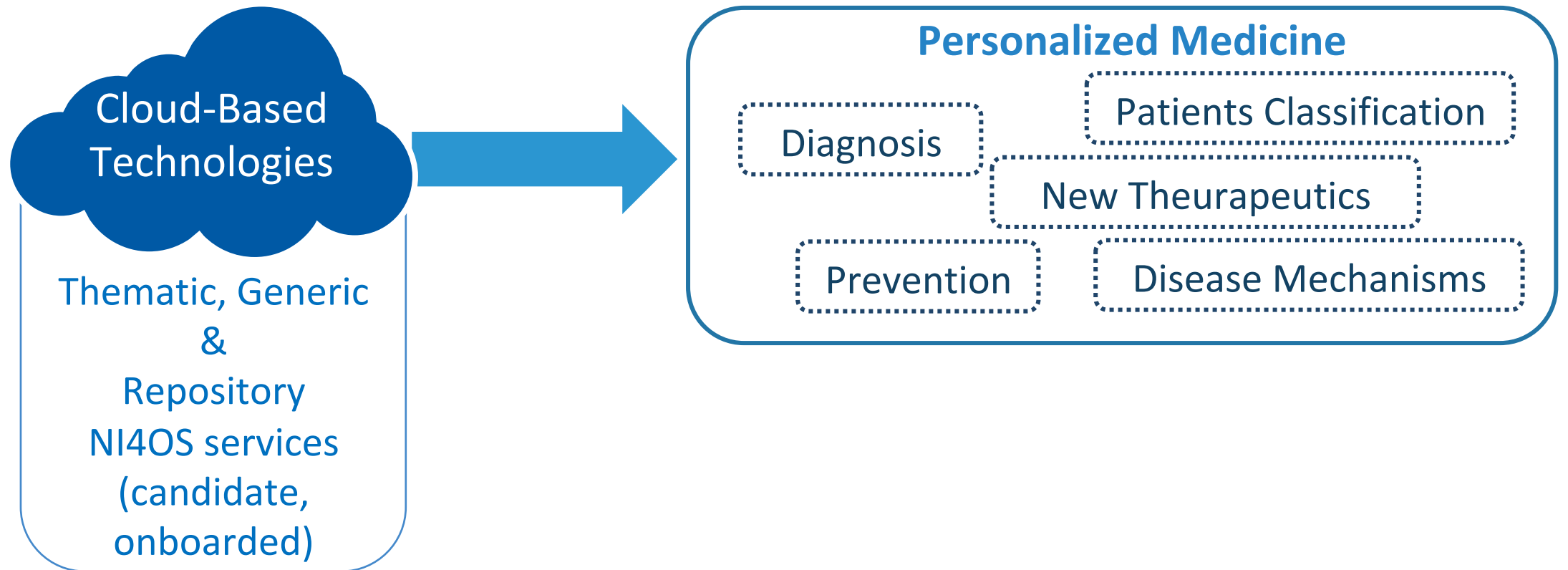


□ Make a software easily accessible

Web-service



- ❑ A computer acting as a server: Provided by NI4OS-Europe
- ❑ Server IP address and domain name: Provided by NI4OS-Europe
- ❑ An architecture similar to LAMP stack:
 - ❑ Linux: The operating system
 - ❑ Apache: The HTTP web-server software delivering content to the browser
 - ❑ MySQL: The database engine for database driven websites
 - ❑ PHP: The back-end software
- ❑ SSL certificate for secure websites: Provided by NI4OS-Europe



Use Case: “Extracting correlations for patient stratification using machine learning”

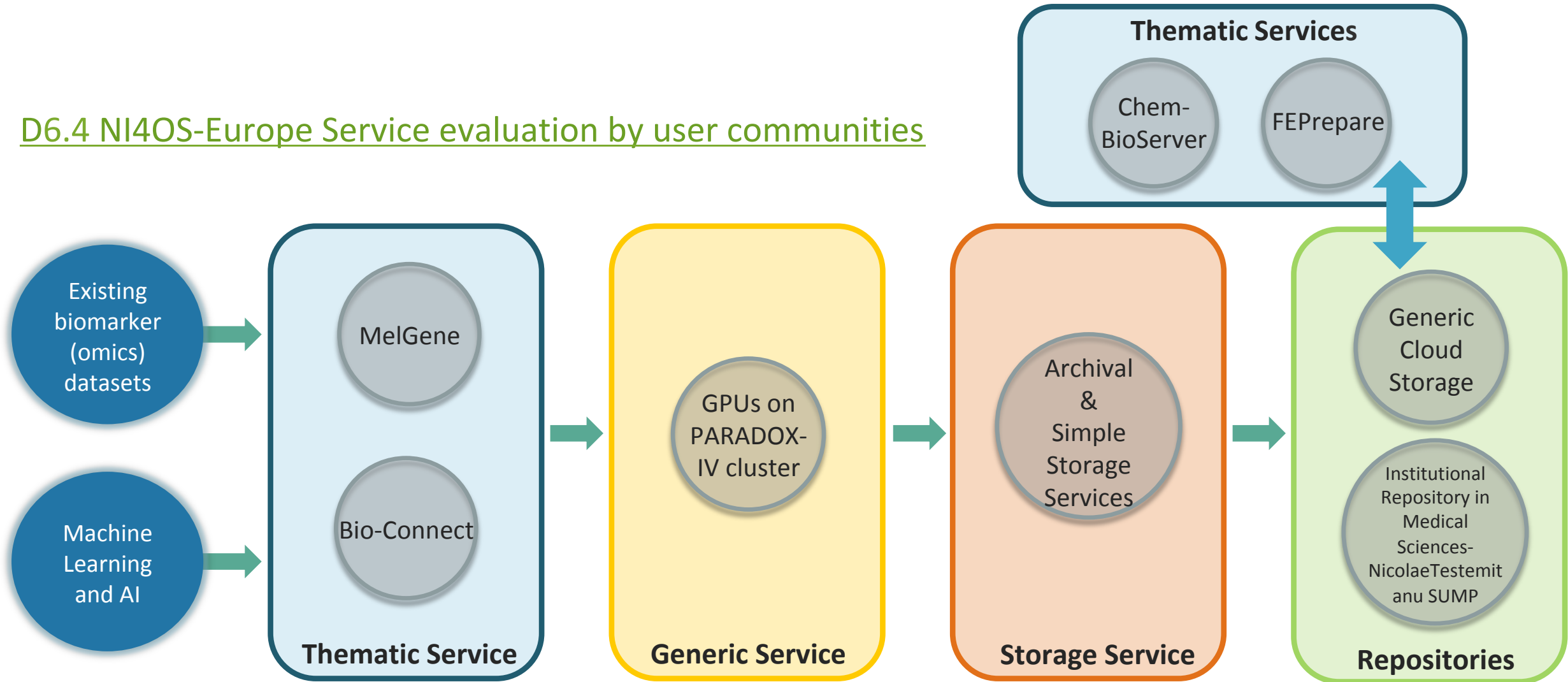
Extracting correlations for patient stratification using machine learning

- ❑ Classifying subgroups of patients according to their disease mechanism
- ❑ → provide them with the right drug at the right time and the right dose.
- ❑ Efficacy and response rates should improve.
- ❑ AI platforms can be trained to analyze remarkable breadths of biological information.
- ❑ A virtual infrastructure can enable the capacity & throughput to collect, process, screen, and target alongside the input resources.



Pipeline of Life-Sciences Use-Case

D6.4 NI4OS-Europe Service evaluation by user communities



Services expected to be evaluated

| Name of Service | Providing Country |
|--|-------------------|
| Bio-Connect* | Cyprus |
| MelGene | Cyprus |
| PARADOX-IV cluster | Serbia |
| ChemBioServer | Greece |
| FEPrepare | Greece |
| Archival Service* | Serbia |
| Simple Storage Service* | Greece |
| Institutional Repository in Medical Sciences-Nicolae Testemitanu SUMP* | Moldova |

- ❑ **Four services (*)** which were **not on-boarded on NI4OS-Europe** at the time of the testing.
 - ❑ **Bio-Connect** was accessible via a VPN connection to the Cyprus Institute's network.

| Service | Link to Service | NI4OS Status | | | Type of Service |
|---------------------------------------|---|------------------|-----------|----------------|-----------------|
| | | Fully on-boarded | Candidate | Not on-boarded | |
| Melgene | http://bioinformatics.cing.ac.cy/MelGene/ | | ✓ | | Thematic |
| Bio-Connect | (N/A) | | | ✓ | Thematic |
| PARADOX-IV cluster | https://www.scl.rs/PARADOX_User_Guide/p4-user-guide.html | ✓ | | | Generic |
| ChemBioServer | https://chembioserver.vi-seem.eu/ | ✓ | | | Thematic |
| FEPprepare | https://fepprepare.vi-seem.eu/ | ✓ | | | Thematic |
| FINKI Cloud | https://openstack.finki.ukim.mk/ | ✓ | | | Generic |
| NI4OS-Europe Repository Service | https://helpdesk.ni4os.eu/otrs/index.pl | ✓ | | | Repository |
| Data Analysis Service- PARADOX Hadoop | https://www.scl.rs/PARADOX_User_Guide/hadoop-user-guide.html | ✓ | | | Generic |



The NI4OS-Europe helpdesk is the main tool of the project's support system. It is used by:

- resource users
- resource owners
- project management.

It supports ticket management, including:

- ticket creation
- assignment/reassignment to the appropriate unit
- escalation, closing, searching, etc.

Organizers of use-cases

Dr. Z. Cournia, Dr. V. Constantinou, Dr. A. Athenodorou

4 Evaluators with scientific background in Life Sciences

Multidisciplinary Backgrounds

- 1 medical doctor
- 2 bioinformaticians
- 1 pharmacist

Research Experience

- 1 Postdoc Researcher
- 1 MSc student
- 1 PhD Candidate
- 1 Research Assistant

Team Meetings



4 Use Cases

1st Step

Acquire access to the services

2nd Step

Evaluate the services

- Accessibility:** How easy is it to access the service?
- Functionality of the service:**
 - User interface experience and documentation.
 - Service credibility, data sources and methods.
- Technical problems encountered**
- Overall experience**
- It was also agreed that recommendations regarding changes and improvements of the services should also be reported.

3rd Step

Provide reports

Each evaluator will provide **8 reports**, one for each tested service.

Accessibility

- Access through AAI
- NI4OS-Europe Helpdesk

Functionalities

- User manuals
- Tutorials
- The significance of an existing tutorial was indicated in cases where the evaluators had no prior experience with a similar service.

Technical Problems

- All technical problems discovered throughout the testing phase of each service were directed to the providers via the NI4OS-Europe Helpdesk
- Direct report to the provider

Recommendations

- Overall experience of using each service
- Recommendations for improvements
- Specific changes were proposed based on each researcher's expertise

MelGene

- Useful tool providing:
 - Useful synopsis and meta-analysis of peer-reviewed genetic association studies performed on Cutaneous Melanoma.
- Enrichment of its database.**
- User manual & tutorial.**
- Better representation of the results in order to be interpretable.**
- Integration of additional features.**

Bio-Connect

- Useful tool for sharing and visualizing genomic data, without sharing raw data.
- None of the services currently available offers a similar service.
- User manual & tutorial.**
- Modifications in the UI.**
- Integration of additional features.**

ChemBioServer

- ❑ Useful and practical tool for filtering, clustering and analyzing compounds resulting from virtual screening.
- ❑ Well documented (example test sets and tutorials available).
- ❑ Accelerates a time-consuming procedure, facilitating drug discovery.

FEPrepare

- ❑ Useful and practical tool.
- ❑ Automates a time-consuming procedure.
- ❑ Functional and well-documented.
- ❑ User manual, Tutorial & video demonstration.

PARADOX-IV cluster

- Functional, useful and well-organized service.
- Sufficient documentation.
- Easily accessible using the NI4OS-Europe helpdesk.

NI4OS-Europe Repository Service

- Well-organized and potentially useful tool for sharing and accessing experimental data, code, etc.
- It can be combined with other on-boarded NI4OS services and grow a strong research community.
- Well constructed and maintained.
- FAIR Data principles.
- Authentication problems** with some academic logins.

PARADOX Hadoop

- Functional, useful and well documented service.
- Detailed tutorial.
- No functionality problems addressed.

FINKI Cloud

- Well-organized and documented service.
- Detailed service manual.
- No functionality problems addressed.
- Useful tool for the scientific community.
- Enrichment of the tutorial.**

Through the Use-Case of Life Sciences :

- ❑ Insights regarding the fully on-boarded services.
 - ❑ Major and minor faults or weaknesses of on-boarded services were indicated.
 - ❑ Recommendations on fine-tuning of the on-boarded services were made.
- ❑ Development needs for candidate services before these are fully on-boarded in NI4OS-Europe.
- ❑ Identifications of major faults of not on-boarded services.

- ❑ The fully on-boarded services do not suffer any major weaknesses.
 - They are providing added value to NI4OS-Europe service catalogue due to unique functionalities.

- ❑ Candidate services require minor fixing or development of flawed operations to become fully on-boarded on NI4OS-Europe.

Thanks!



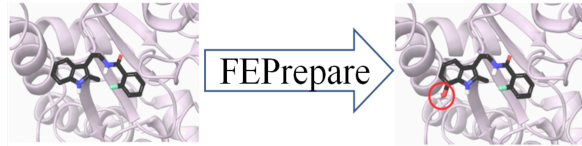
<https://ni4os.eu/ni4os-europe-vs-covid19/>



https://twitter.com/NI4OS_eu



<https://www.facebook.com/NI4OS/>

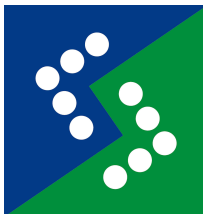


FEPPrepare: webservice, which automates the setup procedure for performing NAMD/FEP simulations.

ChemBioServer 2.0

ChemBioServer: web-server for filtering, clustering and networking of chemical compound libraries facilitating both drug discovery and repurposing.

MelGene: database providing a comprehensive and regularly updated field synopsis and meta-analysis of published genetic association studies performed in Cutaneous Melanoma (CM).



PARADOX-IV cluster:

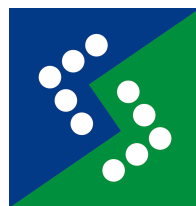
Cluster at the Scientific Computing Laboratory of Institute of Physics Belgrade, consisting of 106 compute nodes (1696 CPU cores and 106 GPUs) interconnected by the QDR InfiniBand network.



Универзитет „Св. Кирил и Методиј“ во Скопје
ФАКУЛТЕТ ЗА ИНФОРМАТИЧКИ НАУКИ
И КОМПЈУТЕРСКО ИНЖЕНЕРСТВО

FINKI Cloud:

Cloud service provided by the University Ss. Cyril and Methodius, Faculty of Computer Science & Engineering in Skopje. The infrastructure is based on OpenStack cloud computing platform and is hosted on 15 Huawei servers.



PARADOX Hadoop cluster: Designed to overlap computation and data storage operations, i.e., to enable performing of computation on the same machine(s) that store the corresponding data.