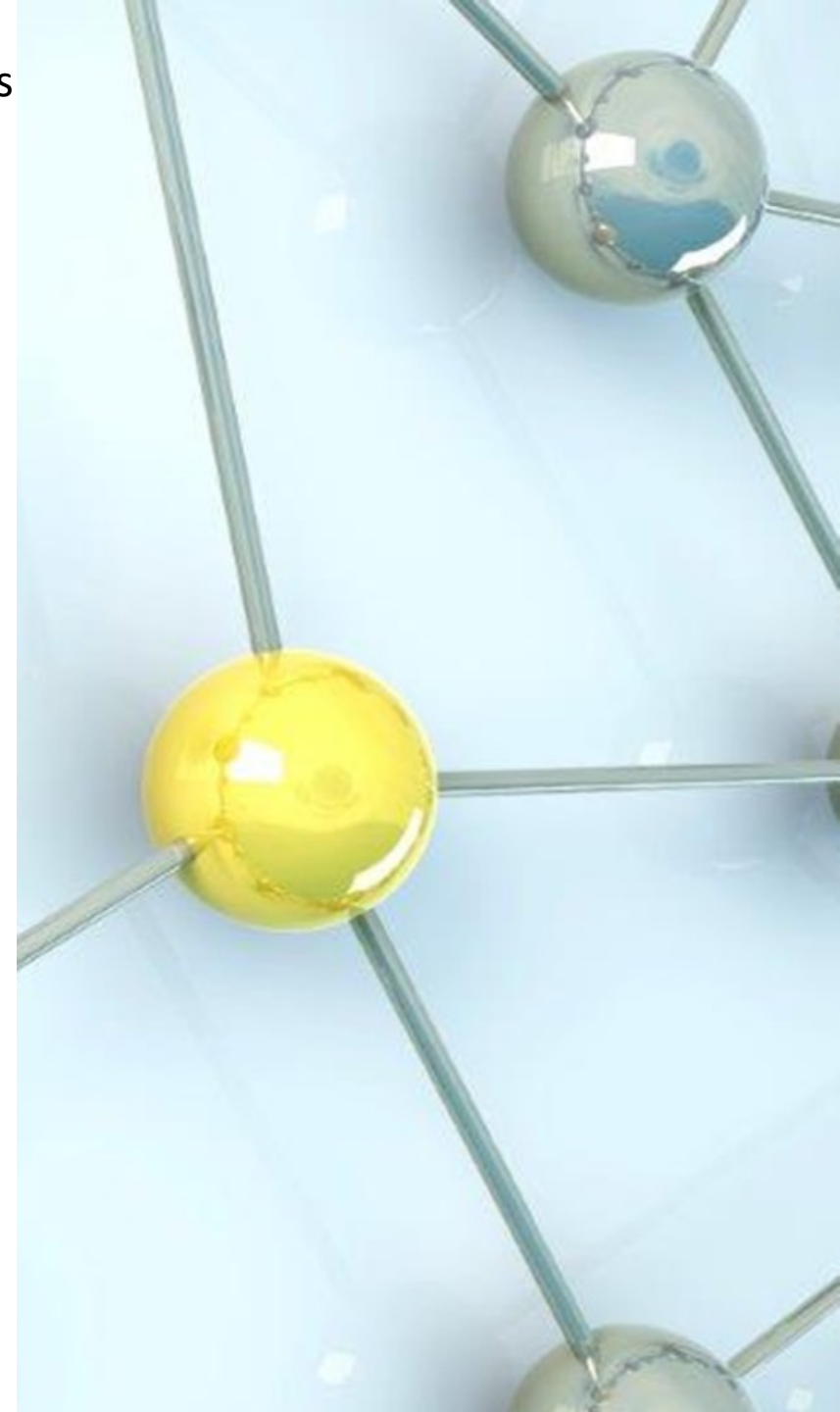





National Initiatives for Open Science in Europe

On-boarding thematic services

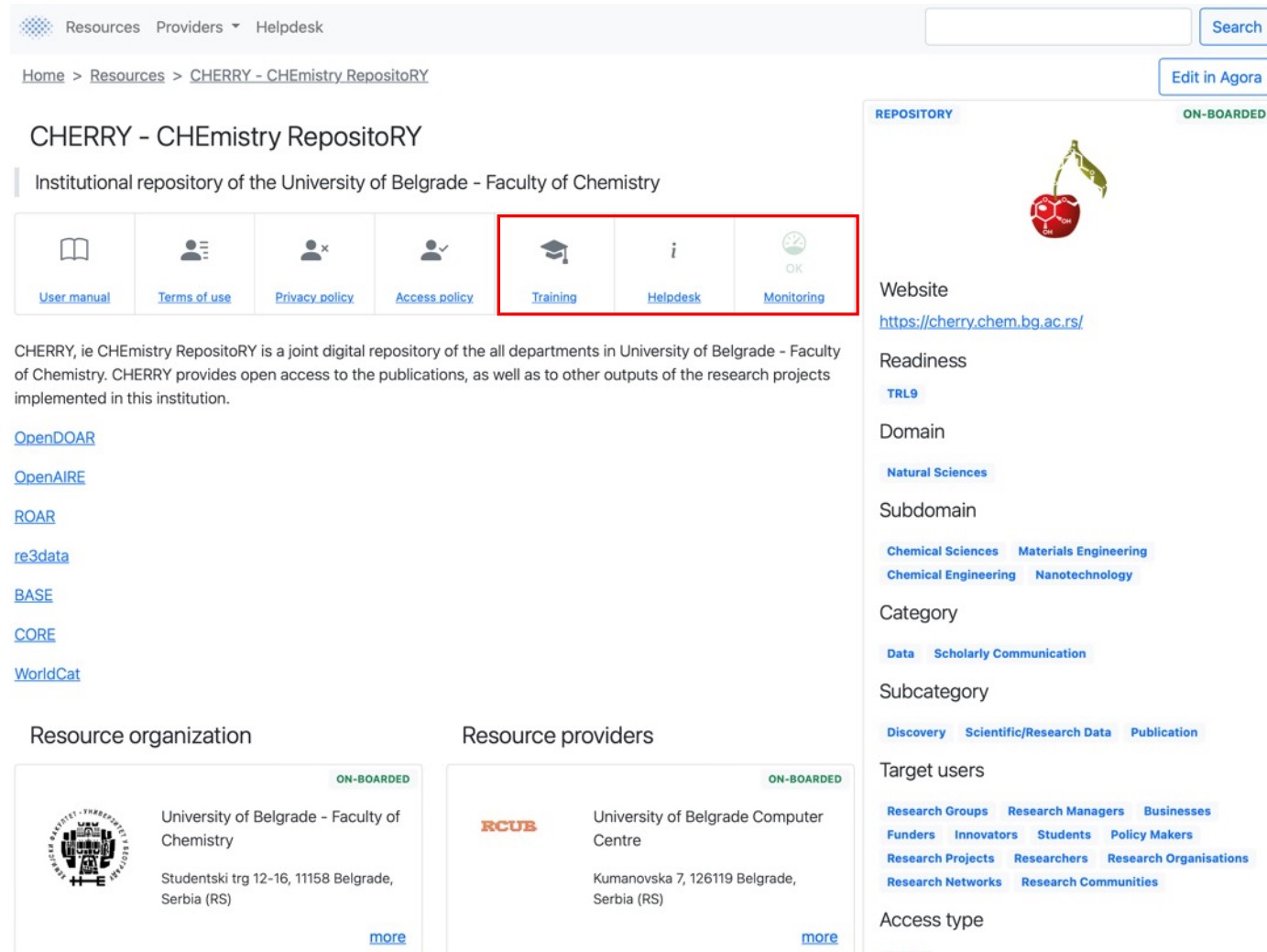
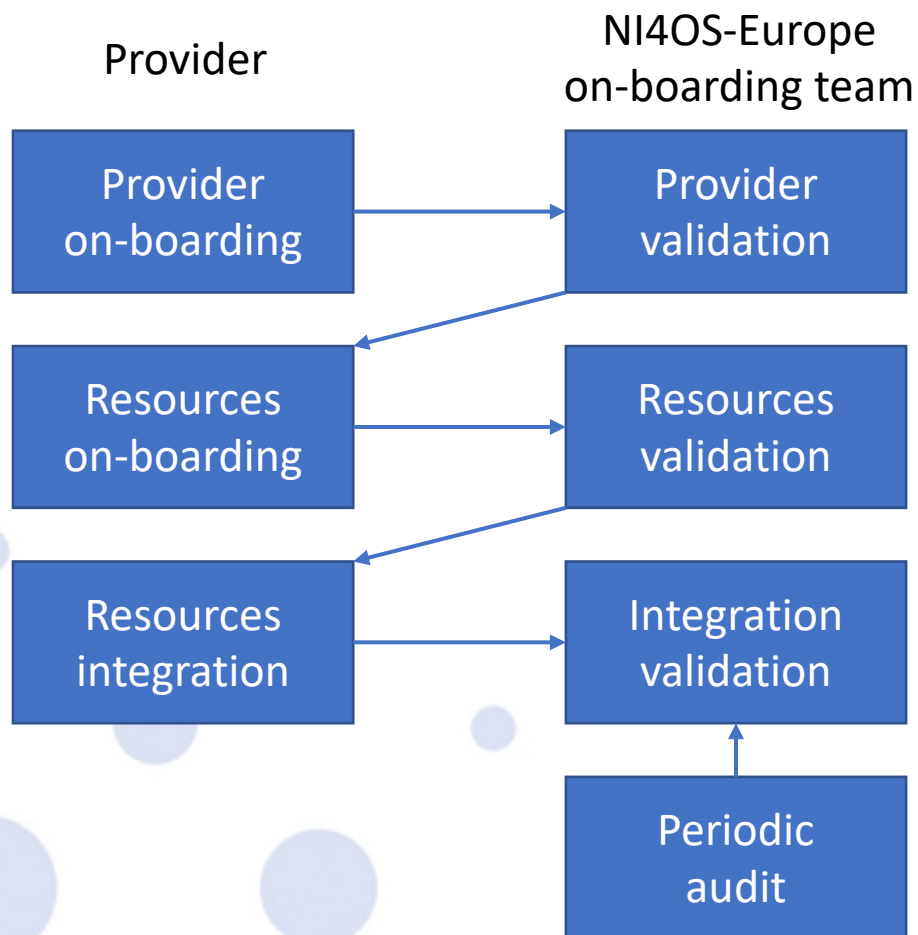
Bojana Koteska, University Ss. Cyril and Methodius in Skopje



Agenda

-
- NI4OS-Europe on-boarding procedure (https://wiki.ni4os.eu/index.php/Service_onboarding_procedure)
 - Pre-production environment
 - Thematic services
 - On-boarding thematic services case study
- 

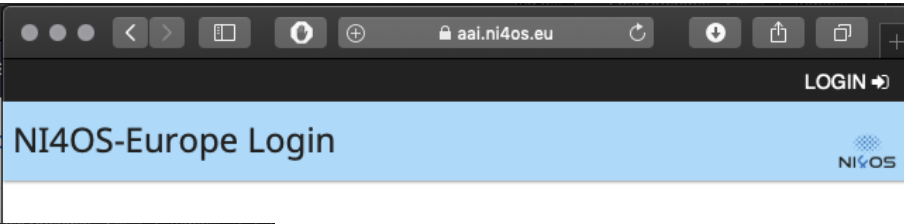
On-boarding workflow



The screenshot shows the website for the CHERRY - CHEmistry Repository. The page title is 'CHERRY - CHEmistry Repository' and the subtitle is 'Institutional repository of the University of Belgrade - Faculty of Chemistry'. The page features a navigation menu with 'Resources', 'Providers', and 'Helpdesk'. A search bar is located in the top right corner. The main content area includes a 'Training' link highlighted with a red box, along with 'Terms of use', 'Privacy policy', and 'Access policy'. The page also displays a 'REPOSITORY' status indicator and a 'Website' link: <https://cherry.chem.bg.ac.rs/>. The 'Readiness' section shows 'TRL9'. The 'Domain' is 'Natural Sciences'. The 'Subdomain' is 'Chemical Sciences', 'Materials Engineering', 'Chemical Engineering', and 'Nanotechnology'. The 'Category' is 'Data' and 'Scholarly Communication'. The 'Subcategory' is 'Discovery', 'Scientific/Research Data', and 'Publication'. The 'Target users' section lists 'Research Groups', 'Research Managers', 'Businesses', 'Funders', 'Innovators', 'Students', 'Policy Makers', 'Research Projects', 'Researchers', 'Research Organisations', 'Research Networks', and 'Research Communities'. The 'Access type' is 'Virtual'. The 'Resource organization' section lists 'University of Belgrade - Faculty of Chemistry' and 'Studentski trg 12-16, 11158 Belgrade, Serbia (RS)'. The 'Resource providers' section lists 'University of Belgrade Computer Centre' and 'Kumanovska 7, 126119 Belgrade, Serbia (RS)'. Both sections include 'ON-BOARDED' status indicators and 'more' links.

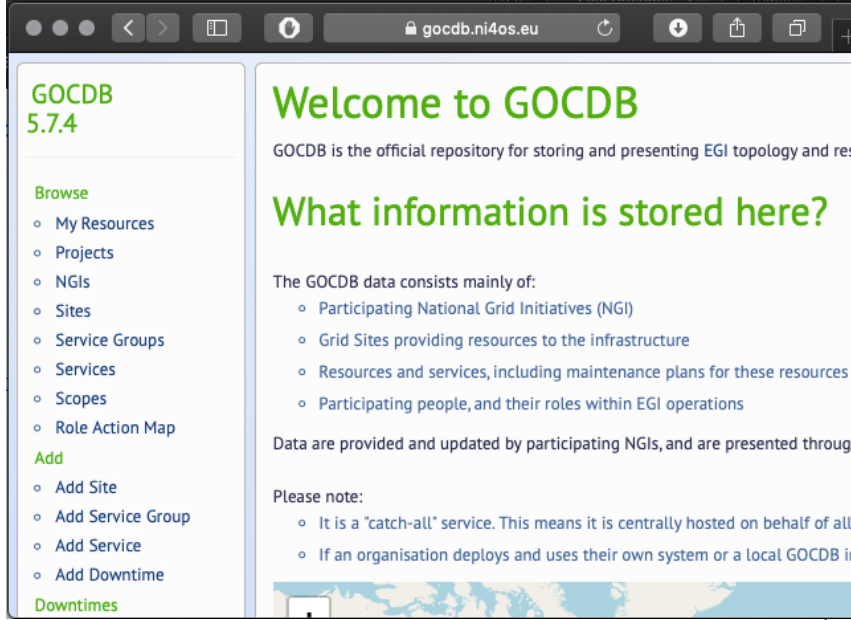
Technical architecture of the pre-production env.

- Service portfolio management system
 - Agora
- Helpdesk
 - Request tracker
- AAI
 - NI4OS Login
- Monitoring
 - Argo
- Inventory
 - GOCDDB
- Accounting
 - in-house
- Training
 - Moodle + BBB
- Wiki
 - MediaWiki
- Events
 - Indico



aa1.ni4os.eu LOGIN

NI4OS-Europe Login



gocdb.ni4os.eu

Welcome to GOCDDB

GOCDDB is the official repository for storing and presenting EGI topology and res

What information is stored here?

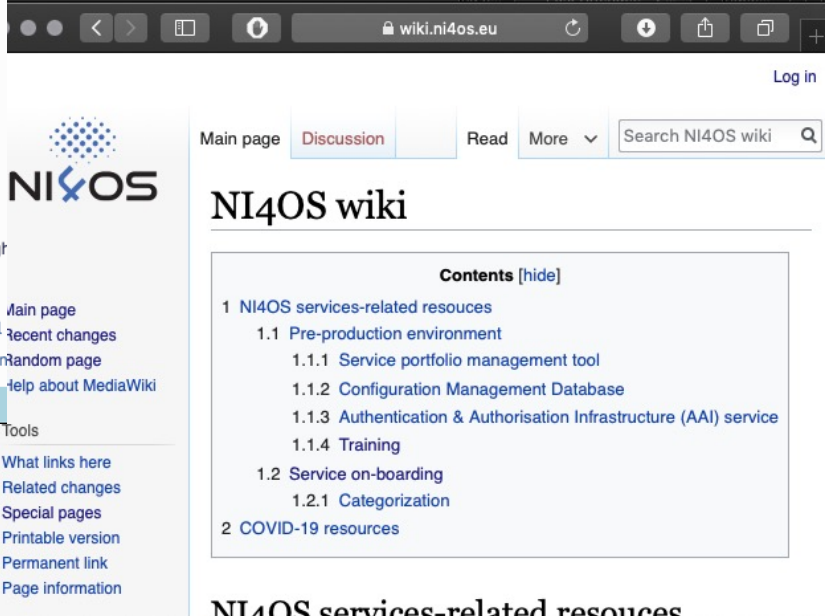
The GOCDDB data consists mainly of:

- Participating National Grid Initiatives (NGI)
- Grid Sites providing resources to the infrastructure
- Resources and services, including maintenance plans for these resources
- Participating people, and their roles within EGI operations

Data are provided and updated by participating NGIs, and are presented through

Please note:

- It is a "catch-all" service. This means it is centrally hosted on behalf of all
- If an organisation deploys and uses their own system or a local GOCDDB in



wiki.ni4os.eu

Welcome to NI4OS-Europe Login.

LOGIN

Main page Discussion Read More Search NI4OS wiki

NI4OS wiki

Contents [hide]

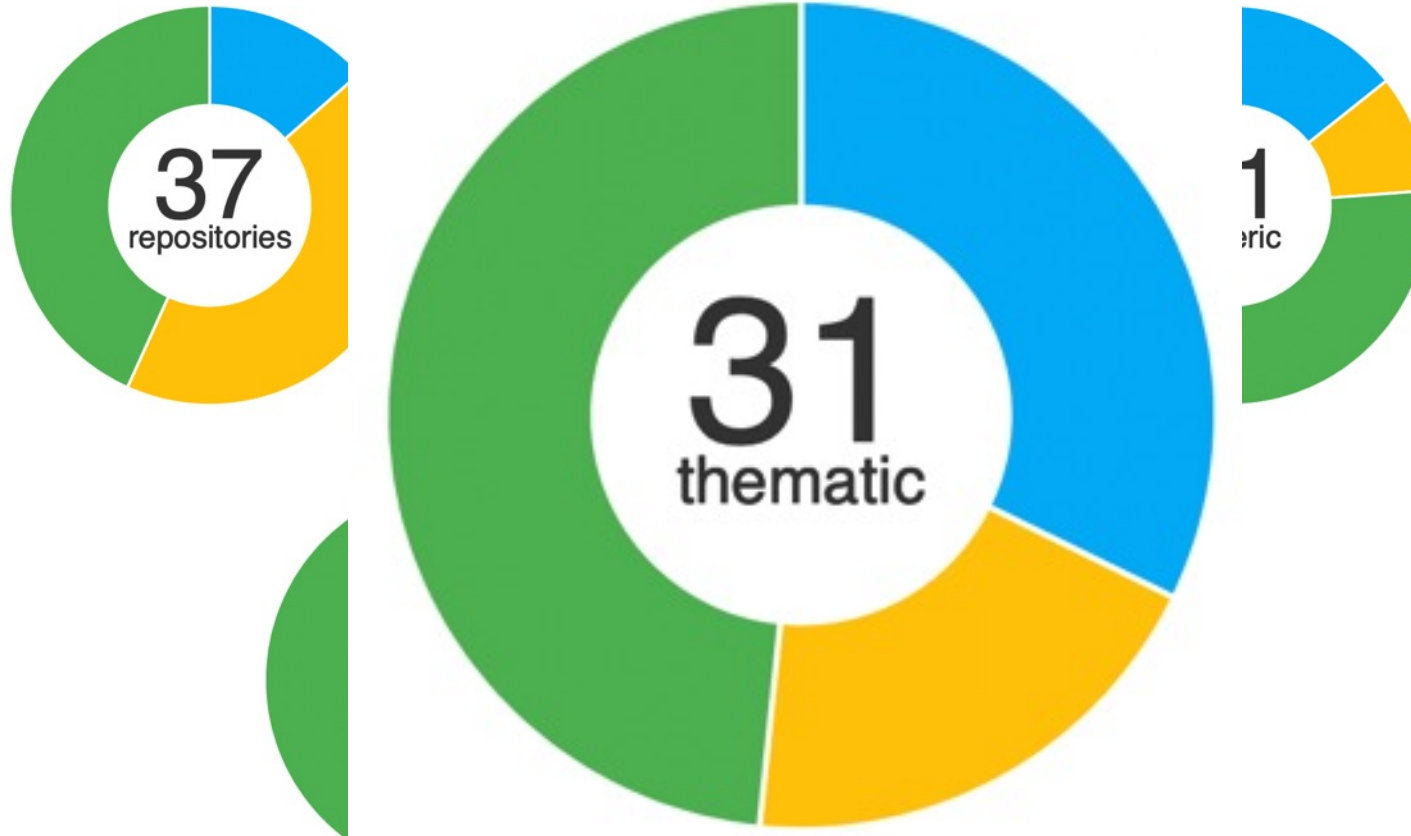
- 1 NI4OS services-related resources
 - 1.1 Pre-production environment
 - 1.1.1 Service portfolio management tool
 - 1.1.2 Configuration Management Database
 - 1.1.3 Authentication & Authorisation Infrastructure (AAI) service
 - 1.1.4 Training
 - 1.2 Service on-boarding
 - 1.2.1 Categorization
- 2 COVID-19 resources

NI4OS services-related resources

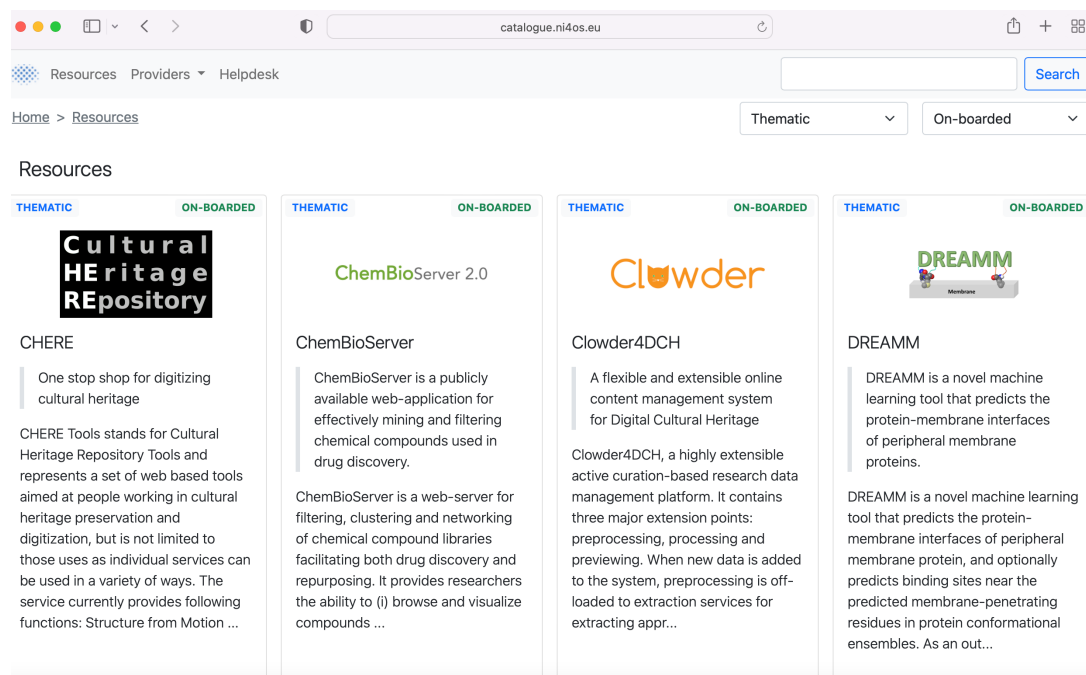
Pre-production environment

- Minimum set of federating services to support integration of the initial set of the regional service into the EOSC
- Environment equivalent to the EOSC Core
- Essential building blocks that will enable the integration of all the other service in the EOSC ecosystem
- Verify the services before EOSC on-boarding
- Regionally support the service providers through the process
 - Based on the previous experience of excellent regional cooperation

NI4OS-Europe resources



Overview of the thematic services



catalogue.ni4os.eu

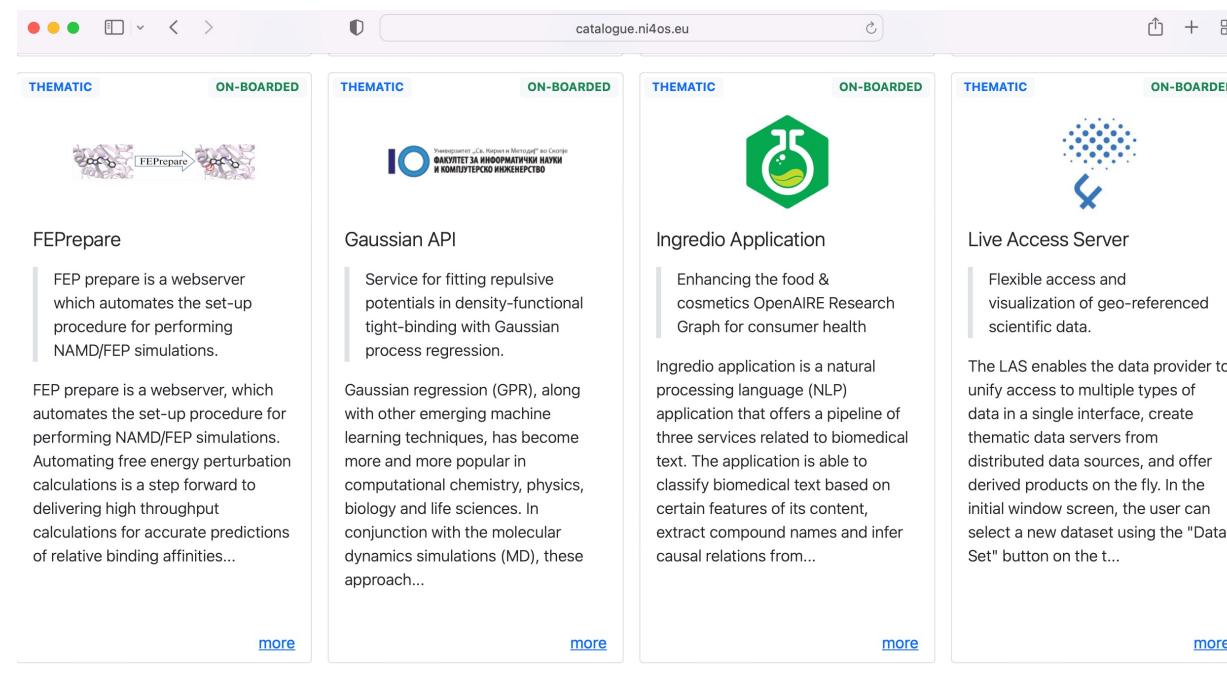
Resources Providers Helpdesk

Home > Resources

Thematic On-boarded

Resources

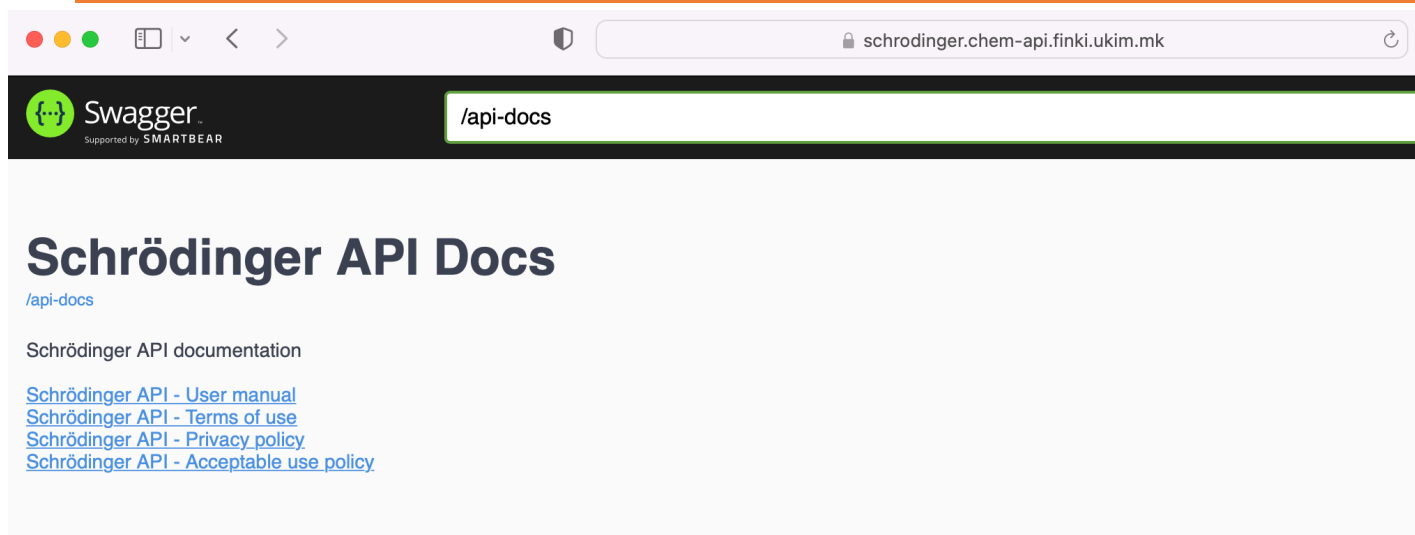
- Cultural Heritage REpository**
CHERE
One stop shop for digitizing cultural heritage
CHERE Tools stands for Cultural Heritage Repository Tools and represents a set of web based tools aimed at people working in cultural heritage preservation and digitization, but is not limited to those uses as individual services can be used in a variety of ways. The service currently provides following functions: Structure from Motion ...
- ChemBioServer 2.0**
ChemBioServer
ChemBioServer is a publicly available web-application for effectively mining and filtering chemical compounds used in drug discovery.
ChemBioServer is a web-server for filtering, clustering and networking of chemical compound libraries facilitating both drug discovery and repurposing. It provides researchers the ability to (i) browse and visualize compounds ...
- Clowder**
Clowder4DCH
A flexible and extensible online content management system for Digital Cultural Heritage
Clowder4DCH, a highly extensible active curation-based research data management platform. It contains three major extension points: preprocessing, processing and previewing. When new data is added to the system, preprocessing is off-loaded to extraction services for extracting appr...
- DREAMM**
DREAMM
DREAMM is a novel machine learning tool that predicts the protein-membrane interfaces of peripheral membrane proteins.
DREAMM is a novel machine learning tool that predicts the protein-membrane interfaces of peripheral membrane protein, and optionally predicts binding sites near the predicted membrane-penetrating residues in protein conformational ensembles. As an out...



catalogue.ni4os.eu

- FEPPrepare**
FEP prepare is a webserver which automates the set-up procedure for performing NAMD/FEP simulations.
FEP prepare is a webserver, which automates the set-up procedure for performing NAMD/FEP simulations. Automating free energy perturbation calculations is a step forward to delivering high throughput calculations for accurate predictions of relative binding affinities... [more](#)
- Gaussian API**
Service for fitting repulsive potentials in density-functional tight-binding with Gaussian process regression.
Gaussian regression (GPR), along with other emerging machine learning techniques, has become more and more popular in computational chemistry, physics, biology and life sciences. In conjunction with the molecular dynamics simulations (MD), these approach... [more](#)
- Ingredio Application**
Enhancing the food & cosmetics OpenAIRE Research Graph for consumer health
Ingredio application is a natural processing language (NLP) application that offers a pipeline of three services related to biomedical text. The application is able to classify biomedical text based on certain features of its content, extract compound names and infer causal relations from... [more](#)
- Live Access Server**
Flexible access and visualization of geo-referenced scientific data.
The 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, and offer derived products on the fly. In the initial window screen, the user can select a new dataset using the "Data Set" button on the t... [more](#)

On-boarding case study: Schrödinger API



Swagger
Supported by SMARTBEAR

/api-docs

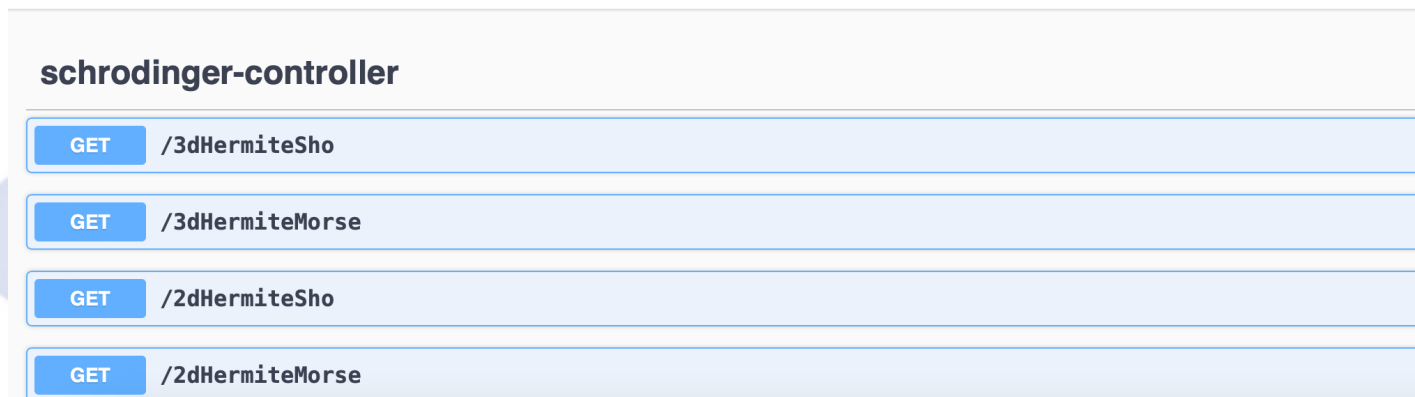
Schrödinger API Docs

/api-docs

Schrödinger API documentation

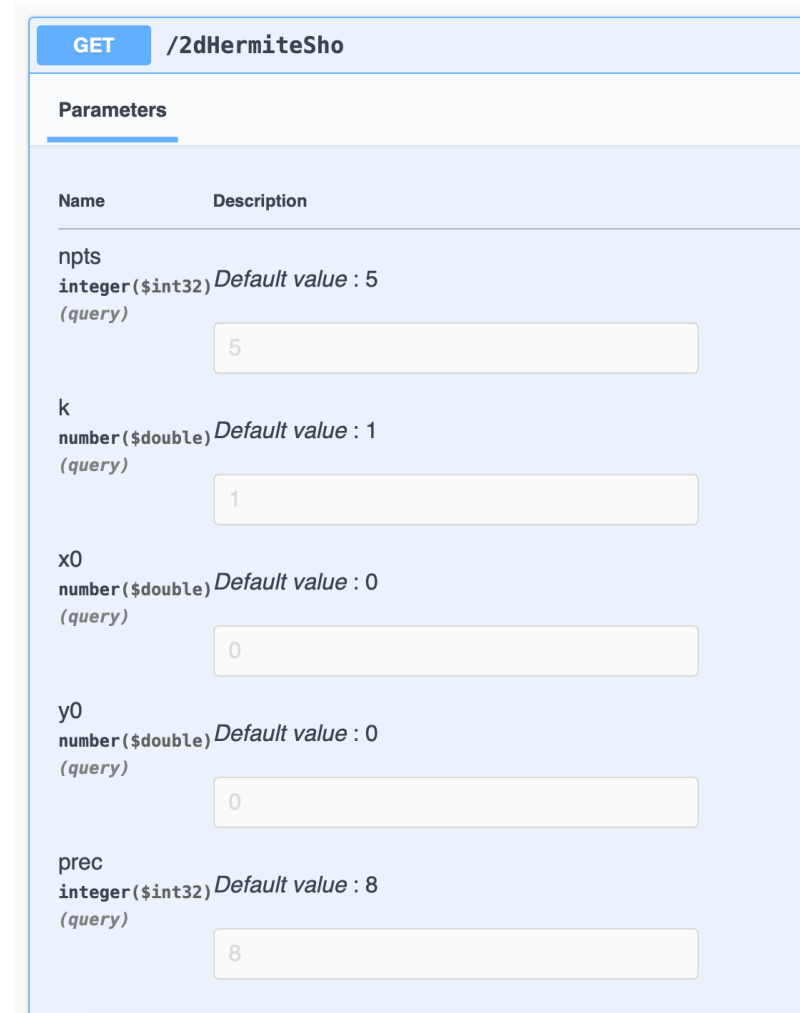
[Schrödinger API - User manual](#)
[Schrödinger API - Terms of use](#)
[Schrödinger API - Privacy policy](#)
[Schrödinger API - Acceptable use policy](#)

Servers
https://schrodinger.chem-api.finki.ukim.mk/



schrodinger-controller

- GET /3dHermiteSho
- GET /3dHermiteMorse
- GET /2dHermiteSho
- GET /2dHermiteMorse

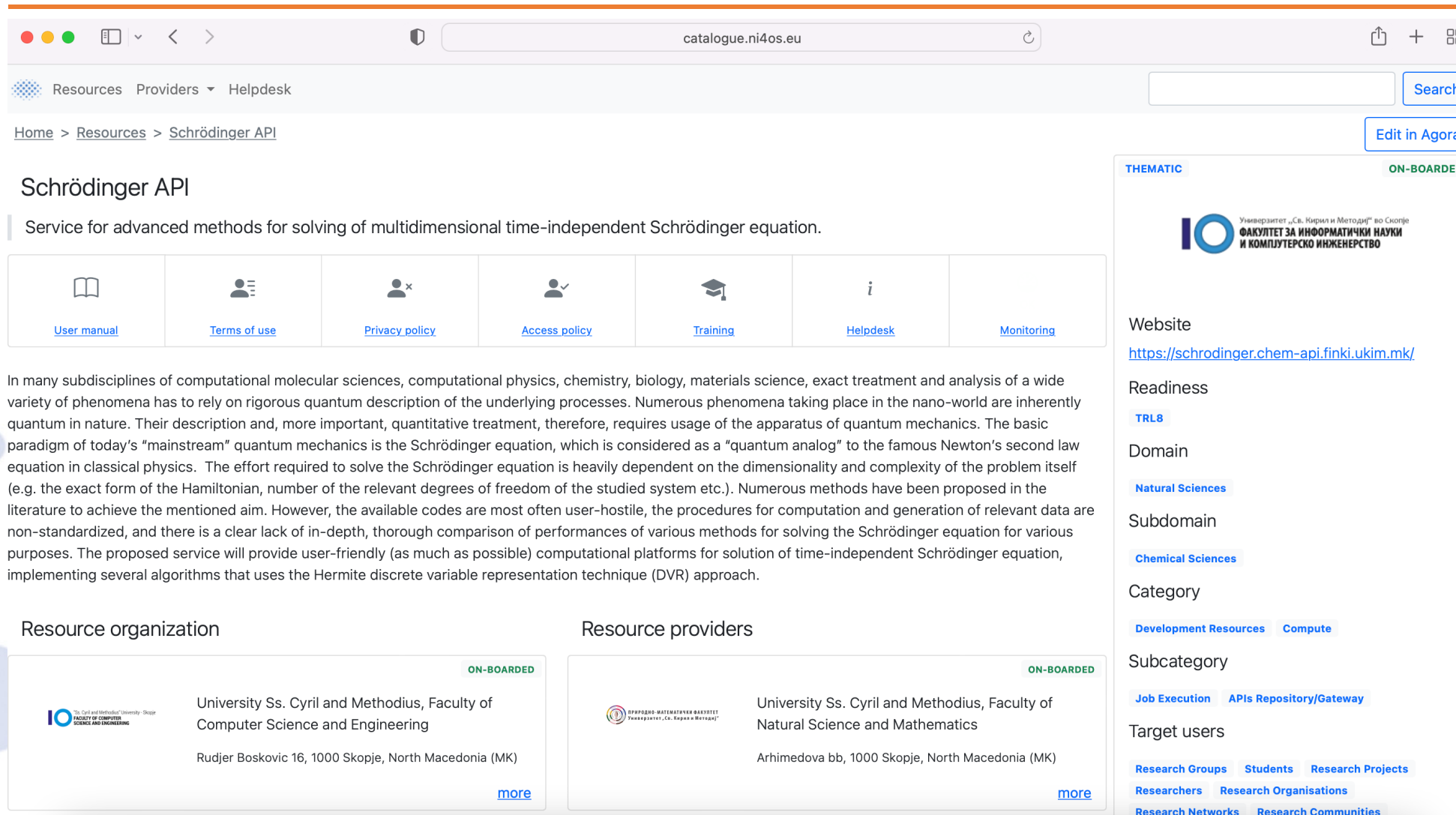


GET /2dHermiteSho

Parameters

Name	Description
npts	integer(\$int32) Default value : 5 (query)
k	number(\$double) Default value : 1 (query)
x0	number(\$double) Default value : 0 (query)
y0	number(\$double) Default value : 0 (query)
prec	integer(\$int32) Default value : 8 (query)

On-boarding case study: Schrödinger API



The screenshot shows a web browser window with the URL `catalogue.ni4os.eu`. The page title is "Schrödinger API". The breadcrumb navigation is "Home > Resources > Schrödinger API". The main content area describes the service as a tool for solving the multidimensional time-independent Schrödinger equation. Below the description is a row of seven icons with links: "User manual", "Terms of use", "Privacy policy", "Access policy", "Training", "Helpdesk", and "Monitoring". A detailed paragraph follows, explaining the importance of quantum mechanics in computational molecular sciences and the challenges of solving the Schrödinger equation. The page is organized into two columns: "Resource organization" and "Resource providers". The "Resource organization" section lists the University Ss. Cyril and Methodius, Faculty of Computer Science and Engineering, located at Rudjer Boskovic 16, 1000 Skopje, North Macedonia (MK). The "Resource providers" section lists the same university, Faculty of Natural Science and Mathematics, located at Arhimedova bb, 1000 Skopje, North Macedonia (MK). On the right side, there is a sidebar with a search bar, a "Search" button, and an "Edit in Agora" button. Below this, there is a "THEMATIC" section with an "ON-BOARDED" status. The sidebar also includes a "Website" link to `https://schrodinger.chem-api.finki.ukim.mk/`, a "Readiness" section with a "TRL8" tag, and a "Domain" section with a "Natural Sciences" tag. The "Subdomain" section has a "Chemical Sciences" tag. The "Category" section has "Development Resources" and "Compute" tags. The "Subcategory" section has "Job Execution" and "APIs Repository/Gateway" tags. The "Target users" section has "Research Groups", "Students", and "Research Projects" tags. At the bottom of the sidebar, there are links for "Researchers", "Research Organisations", "Research Networks", and "Research Communities".

Resources Providers Helpdesk

Home > Resources > Schrödinger API


Schrödinger API

Service for advanced methods for solving of multidimensional time-independent Schrödinger equation.


[User manual](#) [Terms of use](#) [Privacy policy](#) [Access policy](#) [Training](#) [Helpdesk](#) [Monitoring](#)

In many subdisciplines of computational molecular sciences, computational physics, chemistry, biology, materials science, exact treatment and analysis of a wide variety of phenomena has to rely on rigorous quantum description of the underlying processes. Numerous phenomena taking place in the nano-world are inherently quantum in nature. Their description and, more important, quantitative treatment, therefore, requires usage of the apparatus of quantum mechanics. The basic paradigm of today's "mainstream" quantum mechanics is the Schrödinger equation, which is considered as a "quantum analog" to the famous Newton's second law equation in classical physics. The effort required to solve the Schrödinger equation is heavily dependent on the dimensionality and complexity of the problem itself (e.g. the exact form of the Hamiltonian, number of the relevant degrees of freedom of the studied system etc.). Numerous methods have been proposed in the literature to achieve the mentioned aim. However, the available codes are most often user-hostile, the procedures for computation and generation of relevant data are non-standardized, and there is a clear lack of in-depth, thorough comparison of performances of various methods for solving the Schrödinger equation for various purposes. The proposed service will provide user-friendly (as much as possible) computational platforms for solution of time-independent Schrödinger equation, implementing several algorithms that uses the Hermite discrete variable representation technique (DVR) approach.


Resource organization

 University Ss. Cyril and Methodius, Faculty of Computer Science and Engineering
Rudjer Boskovic 16, 1000 Skopje, North Macedonia (MK)
[more](#)

Resource providers

 University Ss. Cyril and Methodius, Faculty of Natural Science and Mathematics
Arhimedova bb, 1000 Skopje, North Macedonia (MK)
[more](#)

THEMATIC ON-BOARDED

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

Website
<https://schrodinger.chem-api.finki.ukim.mk/>

Readiness
TRL8

Domain
Natural Sciences

Subdomain
Chemical Sciences

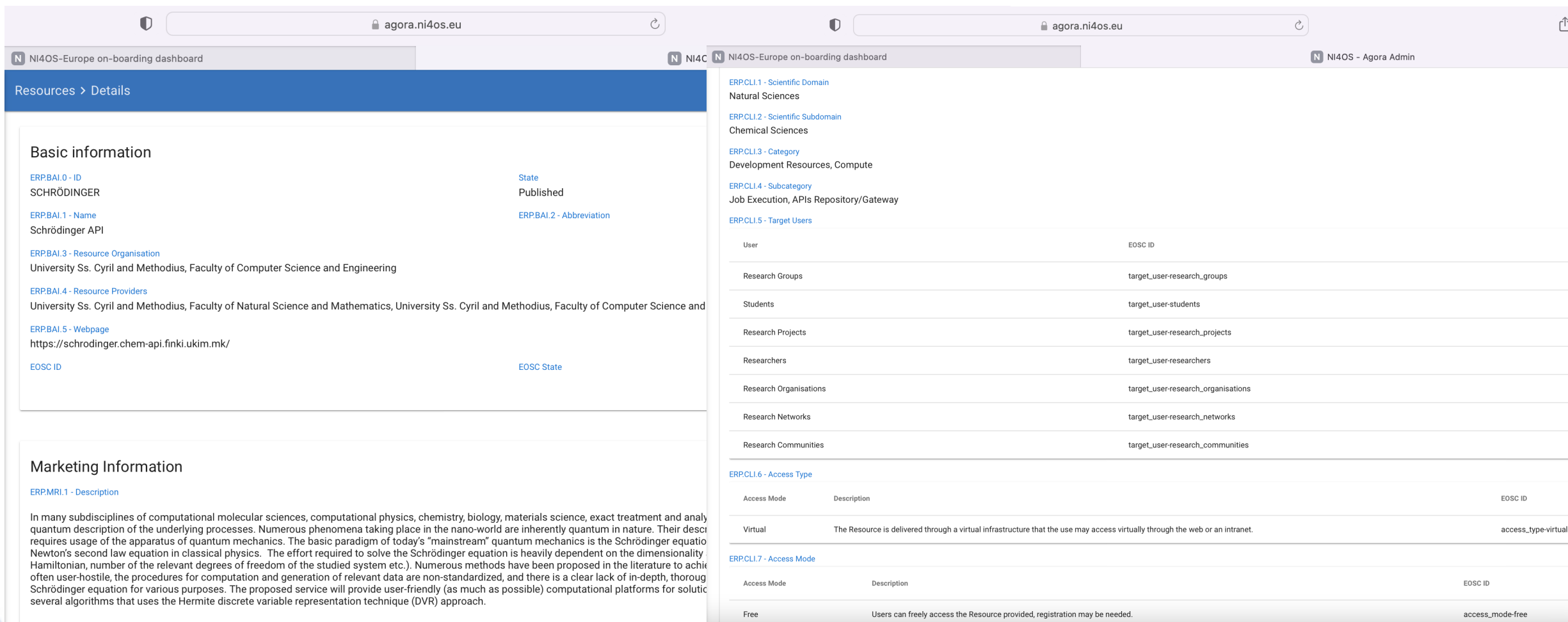
Category
Development Resources Compute

Subcategory
Job Execution APIs Repository/Gateway

Target users
Research Groups Students Research Projects
Researchers Research Organisations
Research Networks Research Communities

Registering a service in AGORA

- <https://grnet.github.io/agora-sp/>



The screenshot displays the AGORA registration interface. The left sidebar shows the navigation menu with 'Resources > Details' selected. The main content area is divided into two sections: 'Basic information' and 'Marketing Information'.

Basic information

ERPBAI.0 - ID SCHRÖDINGER	State Published
ERPBAI.1 - Name Schrödinger API	ERPBAI.2 - Abbreviation
ERPBAI.3 - Resource Organisation University Ss. Cyril and Methodius, Faculty of Computer Science and Engineering	
ERPBAI.4 - Resource Providers University Ss. Cyril and Methodius, Faculty of Natural Science and Mathematics, University Ss. Cyril and Methodius, Faculty of Computer Science and	
ERPBAI.5 - Webpage https://schrodinger.chem-api.finki.ukim.mk/	
EOSC ID	EOSC State

Marketing Information

[ERP.MRI.1 - Description](#)

In many subdisciplines of computational molecular sciences, computational physics, chemistry, biology, materials science, exact treatment and analytical quantum description of the underlying processes. Numerous phenomena taking place in the nano-world are inherently quantum in nature. Their description requires usage of the apparatus of quantum mechanics. The basic paradigm of today's "mainstream" quantum mechanics is the Schrödinger equation Newton's second law equation in classical physics. The effort required to solve the Schrödinger equation is heavily dependent on the dimensionality Hamiltonian, number of the relevant degrees of freedom of the studied system etc.). Numerous methods have been proposed in the literature to achieve often user-hostile, the procedures for computation and generation of relevant data are non-standardized, and there is a clear lack of in-depth, thorough Schrödinger equation for various purposes. The proposed service will provide user-friendly (as much as possible) computational platforms for solution of several algorithms that uses the Hermite discrete variable representation technique (DVR) approach.

ERPCLI.1 - Scientific Domain

Natural Sciences

ERPCLI.2 - Scientific Subdomain

Chemical Sciences

ERPCLI.3 - Category

Development Resources, Compute

ERPCLI.4 - Subcategory

Job Execution, APIs Repository/Gateway

ERPCLI.5 - Target Users

User	EOSC ID
Research Groups	target_user-research_groups
Students	target_user-students
Research Projects	target_user-research_projects
Researchers	target_user-researchers
Research Organisations	target_user-research_organisations
Research Networks	target_user-research_networks
Research Communities	target_user-research_communities

ERPCLI.6 - Access Type

Access Mode	Description	EOSC ID
Virtual	The Resource is delivered through a virtual infrastructure that the user may access virtually through the web or an intranet.	access_type-virtual

ERPCLI.7 - Access Mode

Access Mode	Description	EOSC ID
Free	Users can freely access the Resource provided, registration may be needed.	access_mode-free

Helpdesk registration

- https://wiki.ni4os.eu/index.php/NI4OS_wiki#Helpdesk

Resources Providers ▾ Helpdesk

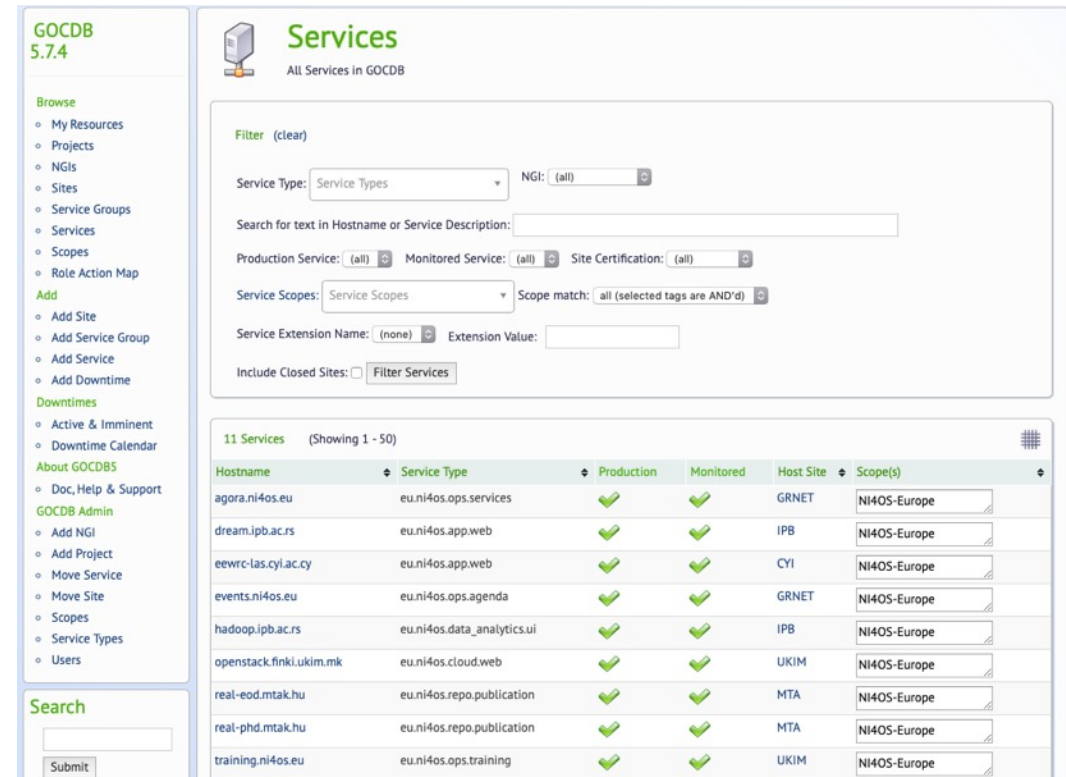
[Home](#) > [Helpdesk](#)

Helpdesk

Your name	Your e-mail address
<input type="text"/>	<input type="text"/>
Resource type	Resource
Thematic resources ▾	Schrödinger API ▾
Subject	
<input type="text"/>	
Message	
<input type="text"/>	
<input type="button" value="Send"/>	

Defining service type in GOCDDB

Name	Description
argo.ams	ARGO AMS service.
argo.mon	ARGO MON service.
argo.webui	ARGO UI service.
eu.eudat.itsm.spm	Agora UI.
eu.ni4os.aai.oidc.login	Enables federated access to an OpenID Connect Relying Party using login credentials managed by Identity Provider(s) provided via configuration.
eu.ni4os.aai.saml.login	Enables federated access to a SAML Service Provider using login credentials managed by Identity Provider(s) provided via configuration.
eu.ni4os.app.api	API based thematic service.
eu.ni4os.app.web	Web based thematic services.
eu.ni4os.cloud.api	Cloud service API interface.
eu.ni4os.cloud.web	Cloud service web interface.
eu.ni4os.data_analytics.ui	UI to the analytics generic service.
eu.ni4os.hpc.ui	HPC User Interface (login, gateway node) machine.
eu.ni4os.ops.aai	The AAI service type.
eu.ni4os.ops.accounting	Accounting service.
eu.ni4os.ops.agenda	Agenda system.
eu.ni4os.ops.code	Source code repository.
eu.ni4os.ops.gocdb	GOC DB Service.
eu.ni4os.ops.mon.ARGO	ARGO monitoring instance.
eu.ni4os.ops.mon.ARGO.api	ARGO API.
eu.ni4os.ops.mon.ARGO.webui	ARGO Web UI.
eu.ni4os.ops.services	Service Catalogue service.
eu.ni4os.ops.support	Support/helpdesk service.
eu.ni4os.ops.training	Training platform.
eu.ni4os.ops.web	Project web site.
eu.ni4os.ops.wiki	Project wiki pages.
eu.ni4os.repo.data	Data repository.
eu.ni4os.repo.publication	Publication repository.
eu.ni4os.xml	XML service type.
gr.noa.astro.hesperia	Prediction tool.



GOCDDB 5.7.4

Services
All Services in GOCDDB

Filter (clear)

Service Type: Service Types NGI: (all)

Search for text in Hostname or Service Description:

Production Service: (all) Monitored Service: (all) Site Certification: (all)

Service Scopes: Service Scopes Scope match: all (selected tags are AND'd)

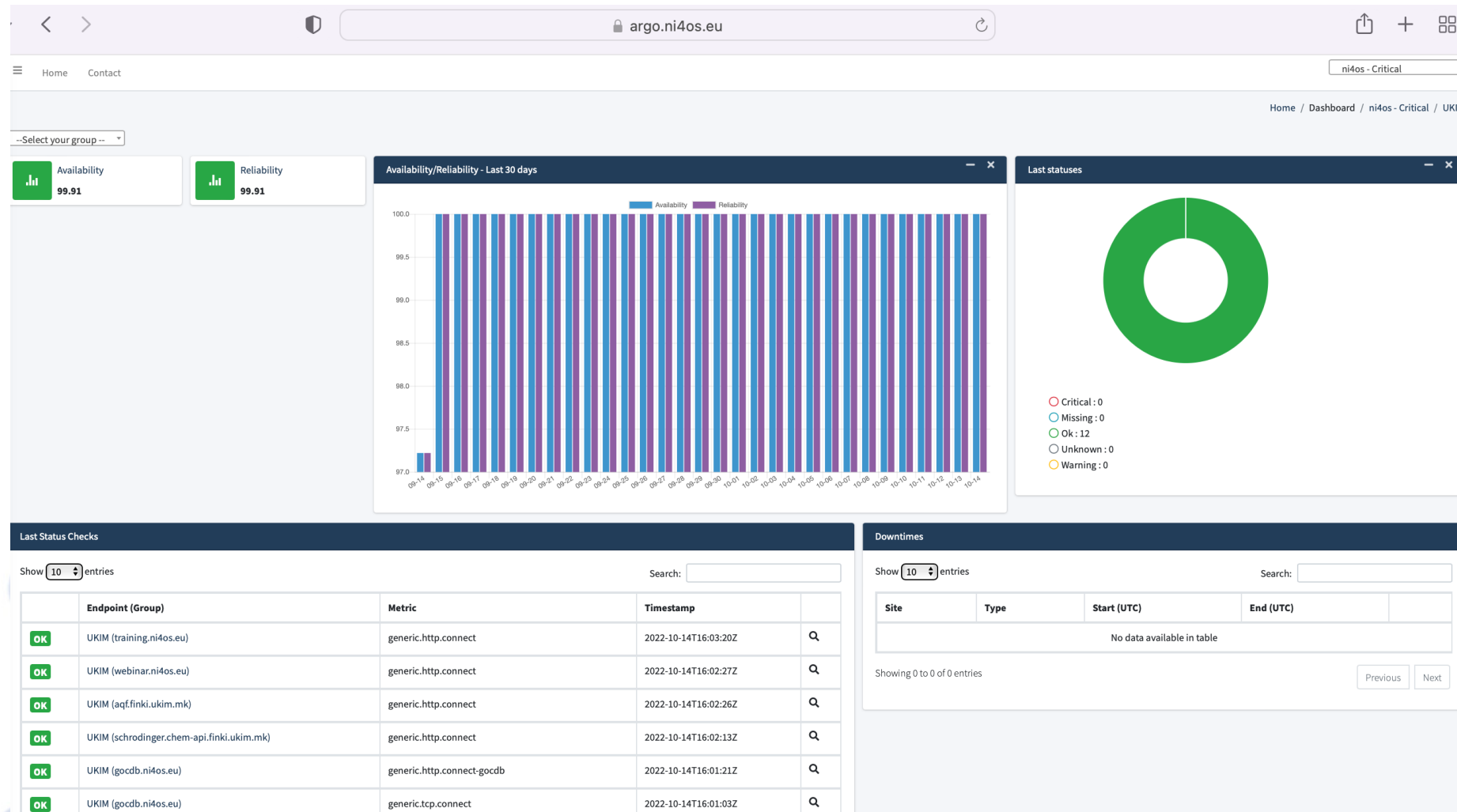
Service Extension Name: (none) Extension Value:

Include Closed Sites: Filter Services

11 Services (Showing 1 - 50)

Hostname	Service Type	Production	Monitored	Host Site	Scope(s)
agora.ni4os.eu	eu.ni4os.ops.services	✓	✓	GRNET	NI4OS-Europe
dream.ipb.ac.rs	eu.ni4os.app.web	✓	✓	IPB	NI4OS-Europe
eewrc-las.cyl.ac.cy	eu.ni4os.app.web	✓	✓	CYI	NI4OS-Europe
events.ni4os.eu	eu.ni4os.ops.agenda	✓	✓	GRNET	NI4OS-Europe
hadop.ipb.ac.rs	eu.ni4os.data_analytics.ui	✓	✓	IPB	NI4OS-Europe
openstack.finki.ukim.mk	eu.ni4os.cloud.web	✓	✓	UKIM	NI4OS-Europe
real-eod.mtak.hu	eu.ni4os.repo.publication	✓	✓	MTA	NI4OS-Europe
real-phd.mtak.hu	eu.ni4os.repo.publication	✓	✓	MTA	NI4OS-Europe
training.ni4os.eu	eu.ni4os.ops.training	✓	✓	UKIM	NI4OS-Europe

Monitoring



Accounting

<https://accounting.ni4os.eu/dashboard>

NI4OS Accounting Data

Compute Data Cloud Data Storage Data Repository Data WebScience

Data type: Number of workflows
Period: from 07-2022 to 10-2022
Table: rows Application columns Date
show

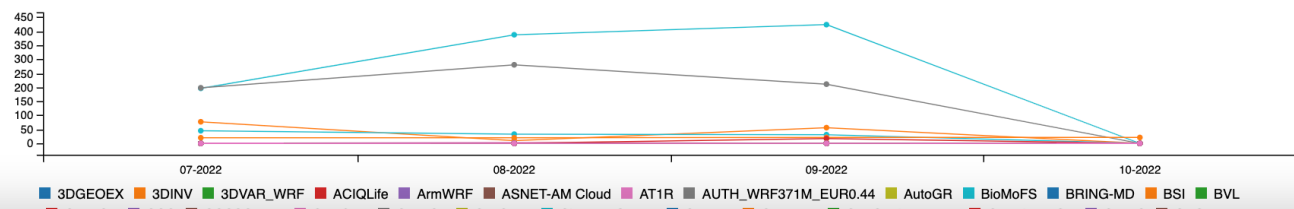
Filter records: sch

application	07-2022	08-2022	09-2022	10-2022
Schrödinger API	0	0	17	0

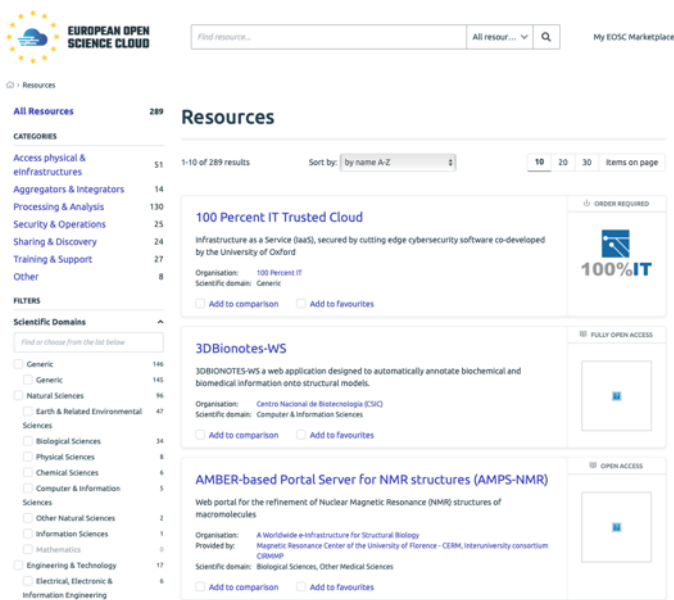
Showing 1 to 1 of 1 entries (filtered from 97 total entries)

CSV Excel

webscience usage by Application and Date



Integration with the EOSC marketplace



Find resource... All resour... My EOSC Marketplace

Resources

1-10 of 289 results

Sort by: by name A-Z

10 20 30 Items on page

100 Percent IT Trusted Cloud

Infrastructure as a Service (IaaS), secured by cutting edge cybersecurity software co-developed by the University of Oxford

Organization: 100 Percent IT

Scientific domain: Generic

3DBionotes-WS

3DBIONOTES-WS a web application designed to automatically annotate biochemical and biological information onto structural models.

Organization: Centro Nacional de Biotecnología (CNB)

Scientific domain: Computer & Information Sciences

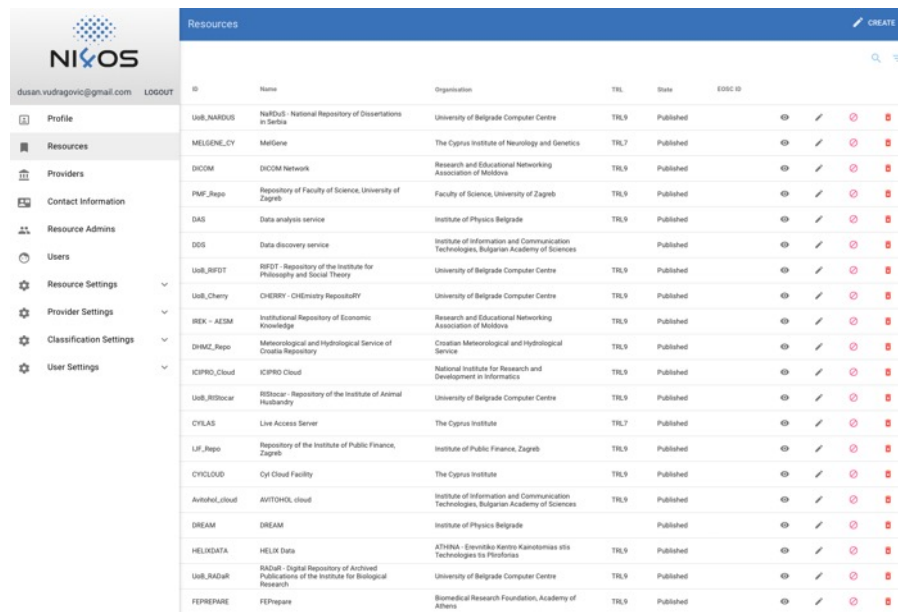
AMBER-based Portal Server for NMR structures (AMPS-NMR)

Web portal for the refinement of Nuclear Magnetic Resonance (NMR) structures of macromolecules

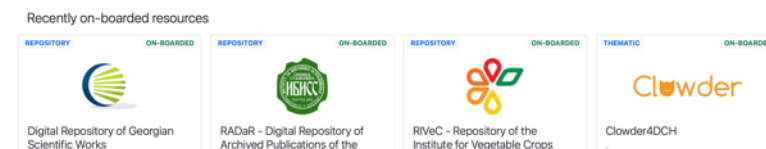
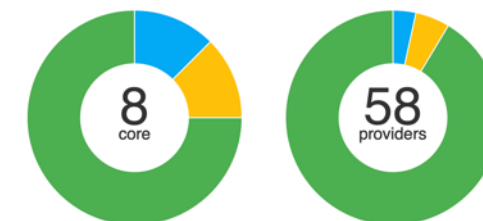
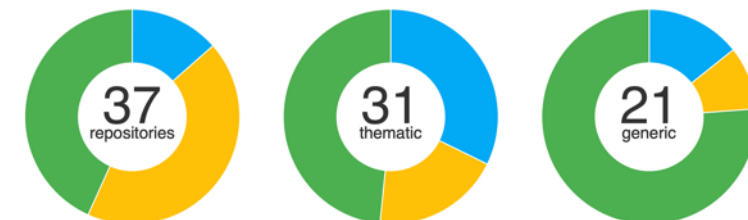
Organization: A Worldwide e-Infrastructure for Structural Biology

Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CERN

Scientific domain: Biological Sciences, Other Medical Sciences



ID	Name	Organization	TRL	Status	EOSC ID
UuB_NARDUS	NARDUS: National Repository of Dissertations in Serbia	University of Belgrade Computer Centre	TRL9	Published	
MELGENE_CV	MelGene	The Cyprus Institute of Neurology and Genetics	TRL7	Published	
DICOM	DICOM Network	Research and Educational Networking Association of Moldova	TRL9	Published	
PMP_Repo	Repository of Faculty of Science, University of Zagreb	Faculty of Science, University of Zagreb	TRL9	Published	
DAS	Data analysis service	Institute of Physics Belgrade	TRL9	Published	
DOS	Data discovery service	Institute of Information and Communication Technologies, Bulgarian Academy of Sciences		Published	
UuB_RFDIT	RFDIT - Repository of the Institute for Philosophy and Social Theory	University of Belgrade Computer Centre	TRL9	Published	
UuB_Cherry	ChERRY - ChEMistry Repository	University of Belgrade Computer Centre	TRL9	Published	
IREK - AEMM	Institutional Repository of Economic Knowledge	Research and Educational Networking Association of Moldova	TRL9	Published	
DHMZ_Repo	Meteorological and Hydrological Service of Croatia Repository	Croatian Meteorological and Hydrological Service	TRL9	Published	
ICPRO_Cloud	ICPRO Cloud	National Institute for Research and Development in Informatics	TRL9	Published	
UuB_RISocar	RISocar - Repository of the Institute of Animal Husbandry	University of Belgrade Computer Centre	TRL9	Published	
CYCLAS	Live Access Server	The Cyprus Institute	TRL7	Published	
LIF_Repo	Repository of the Institute of Public Finance, Zagreb	Institute of Public Finance, Zagreb	TRL9	Published	
CYCLCLOUD	Cy Cloud Facility	The Cyprus Institute	TRL9	Published	
Avitohol_Cloud	AVITOHOL_Cloud	Institute of Information and Communication Technologies, Bulgarian Academy of Sciences	TRL9	Published	
DREAM	DREAM	Institute of Physics Belgrade		Published	
HELIXDATA	HELIX Data	ATHINA - Eleni Kiriaki-Kiriakidou site Technologies to Piroforas	TRL9	Published	
UuB_RADAR	RADAR: Digital Repository of Archived Publications of the Institute for Biological Research	University of Belgrade Computer Centre	TRL9	Published	
FEPREPARE	FEPrepares	Biomedical Research Foundation, Academy of Athens	TRL9	Published	



Recently on-boarded resources

REPOSITORY ON-BOARDED

REPOSITORY ON-BOARDED

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