



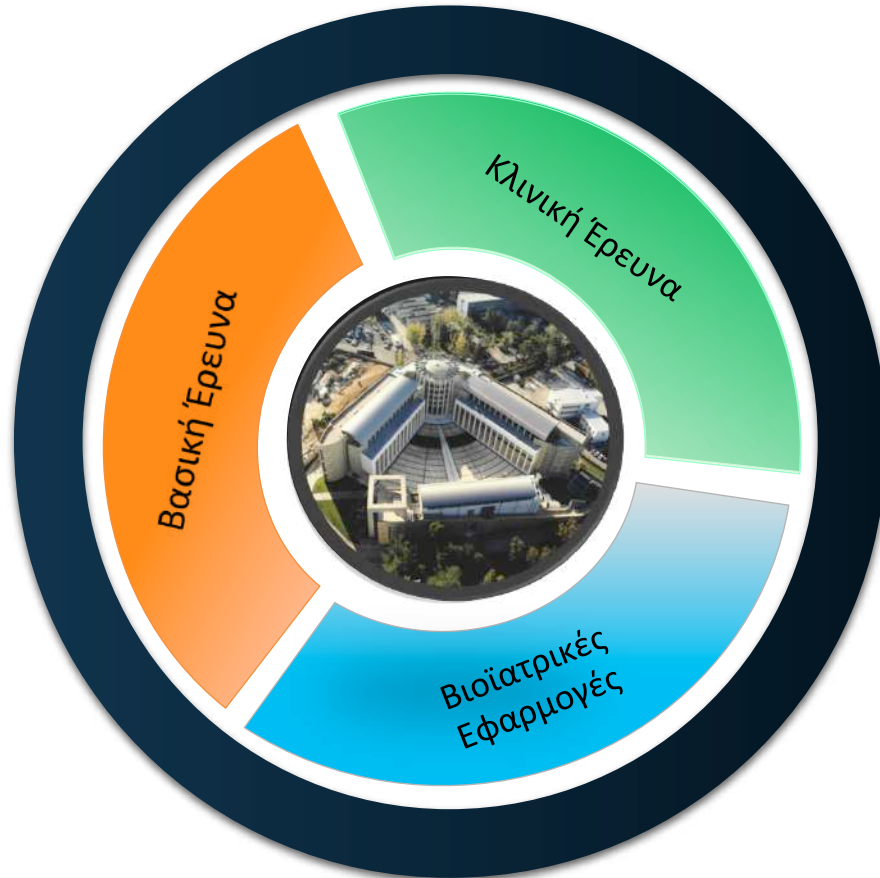
Παγκόσμια Πρωτοβουλία για τα Ερευνητικά Δεδομένα, RDA Ευρωπαϊκό Νέφος Ανοικτής Επιστήμης, EOSC



Δρ. Ζωή Κούρνια
zcournia@bioacademy.gr

COVID19 Workshop v.2

Ίδρυμα Ιατροβιολογικών Ερευνών Ακαδημίας Αθηνών





RDA COVID19 Working Group

<https://www.rd-alliance.org/groups/rda-covid19>

Presentation to

COVID-19 Workshop v.2

November 6, 2020

RDA COVID-19 Recommendations and Guidelines

DOI: <https://doi.org/10.15497/rda00052>

Zoe Cournia, Biomedical Research Foundation, Academy of Athens

Natalie Meyers, Navari Family Center for Digital Scholarship, University of Notre Dame



Research Data Alliance

THE RESEARCH DATA ALLIANCE

www.rd-alliance.org

building the social and technical bridges that enable open sharing and re-use of data

Vision

Researchers and innovators openly share and **re-use** data across technologies, disciplines, and countries to address the grand challenges of society.

Mission

RDA builds the **social and technical bridges** that enable open sharing and **re-use** of data.

50 FLAGSHIP OUTPUTS

including 8 ICT Technical Specifications

100+ ADOPTION CASES

across multiple disciplines, organisations & countries

94 GROUPS WORKING ON GLOBAL DATA INTEROPERABILITY CHALLENGES

37 Working Groups
57 Interest Groups

11,154 INDIVIDUAL MEMBERS FROM 146 COUNTRIES

69% Academia & Research
14% Public Administration
11% Enterprise & Industry

**52 ORGANISATIONAL MEMBERS
11 AFFILIATE MEMBERS**

<https://www.rd-alliance.org/about-rda>





What does RDA do?

Members come together through self-formed, volunteer and focused Working Groups and exploratory Interest Groups to exchange knowledge, share discoveries, discuss barriers and potential solutions, explore and define policies and test as well as harmonise standards to enhance and facilitate global data sharing & re-use.

RDA members collaborate together across the globe to tackle numerous infrastructure & data sharing challenges related to:

- Reproducibility
- Data preservation
- Best practices for domain repositories
- Legal interoperability
- Data citation
- Data type registries
- Metadata





Who Can Join RDA?

Any individual or organisation, regardless of profession or discipline, with an interest in **reducing the barriers to the sharing and re-use of data** and who agrees to RDA's guiding principles of:

- 🌐 Openness
- 🌐 Consensus
- 🌐 Balance
- 🌐 Harmonization
- 🌐 Community-driven
- 🌐 Non-profit and technology-neutral

Individual Membership is free at <https://www.rd-alliance.org/user/register>





Why Join RDA as an Individual Member?

Individual Member Benefits

- **Contribute** to acceleration of data infrastructure development
- Work and **share experiences** with collaborators throughout the world
- **Access** to extraordinary network of colleagues with various levels of experience, perspectives and practices
- Gain greater **expertise** in data science regardless of whether one is a student, early or seasoned career professional
- **Enhance** the quality and effectiveness of personal work and activities
- **Improve** one's competitive advantage professionally and positioning oneself for leadership within the broader research community

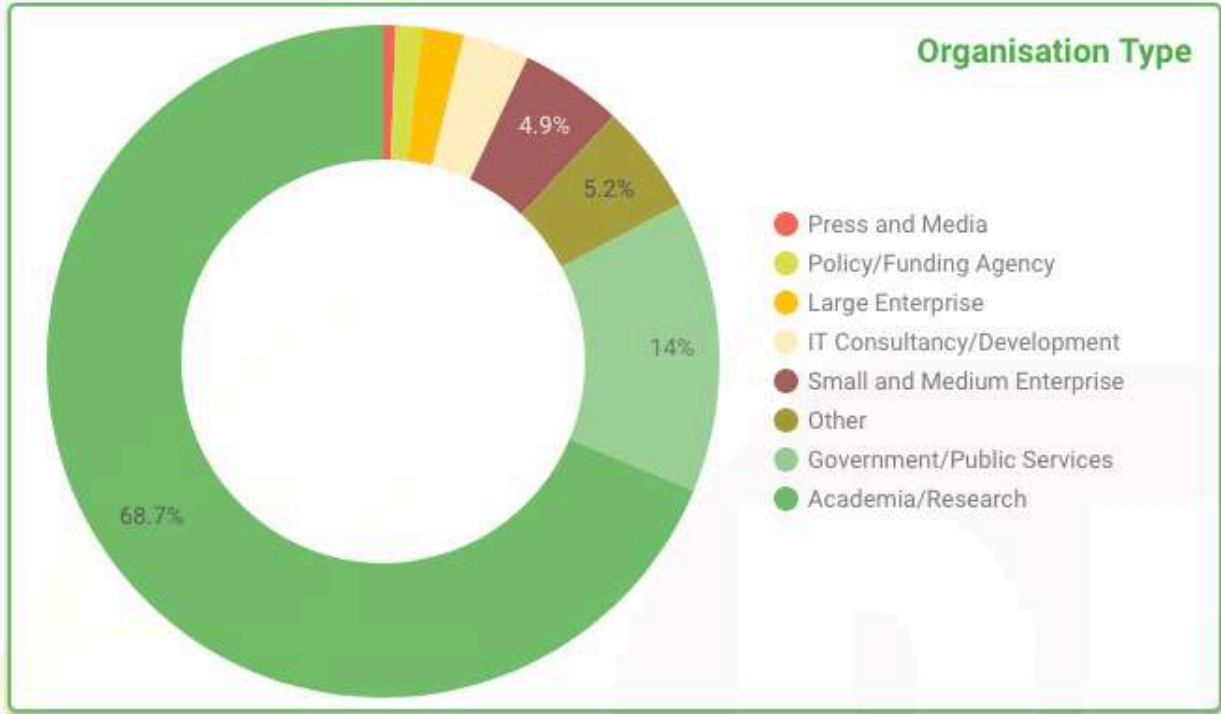
<https://www.rd-alliance.org/about-rda>

Individual RDA Members 11,154





Who is RDA – Organisation type



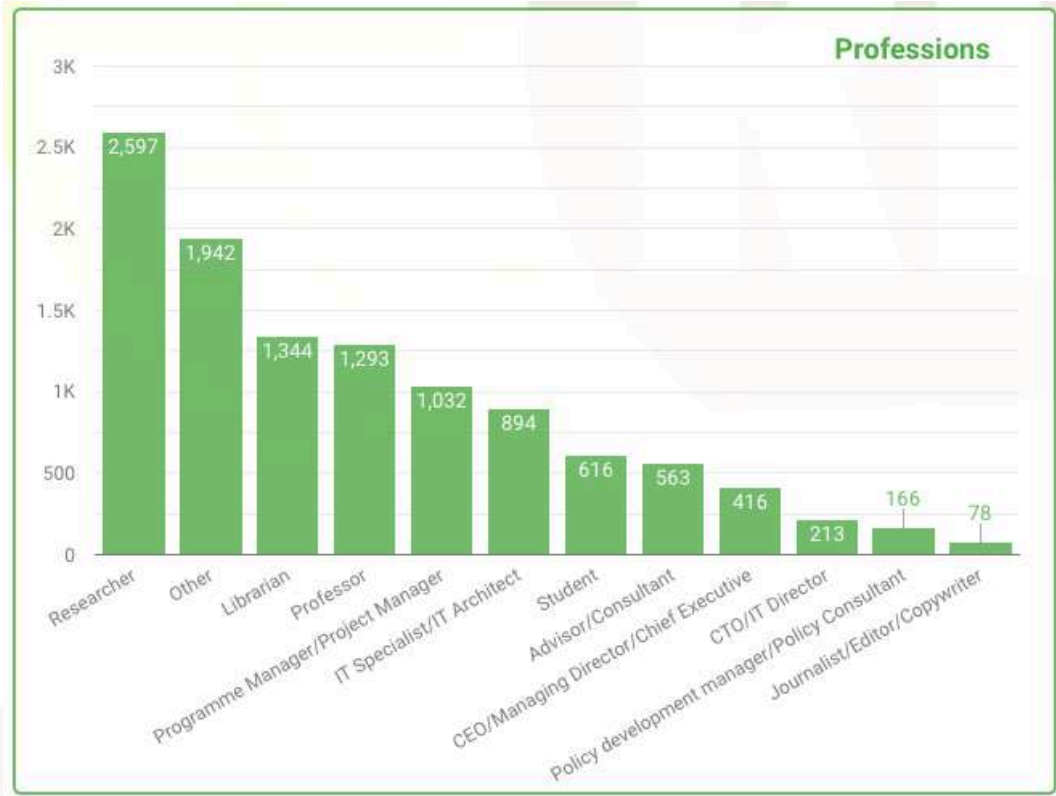
Organisation Type	%
1. Academia/Research	68.71%
2. Government/Public Services	14.05%
3. Other	5.24%
4. Small and Medium Enterprise	4.93%
5. IT Consultancy/Development	3.18%
6. Large Enterprise	2.02%
7. Policy/Funding Agency	1.26%
8. Press and Media	0.6%

1 - 8 / 8 < >



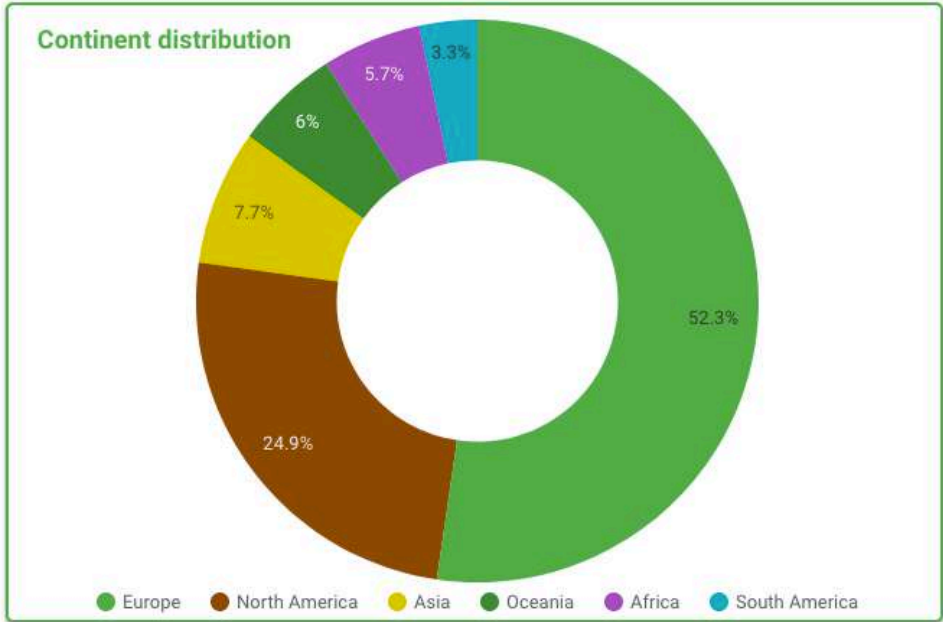
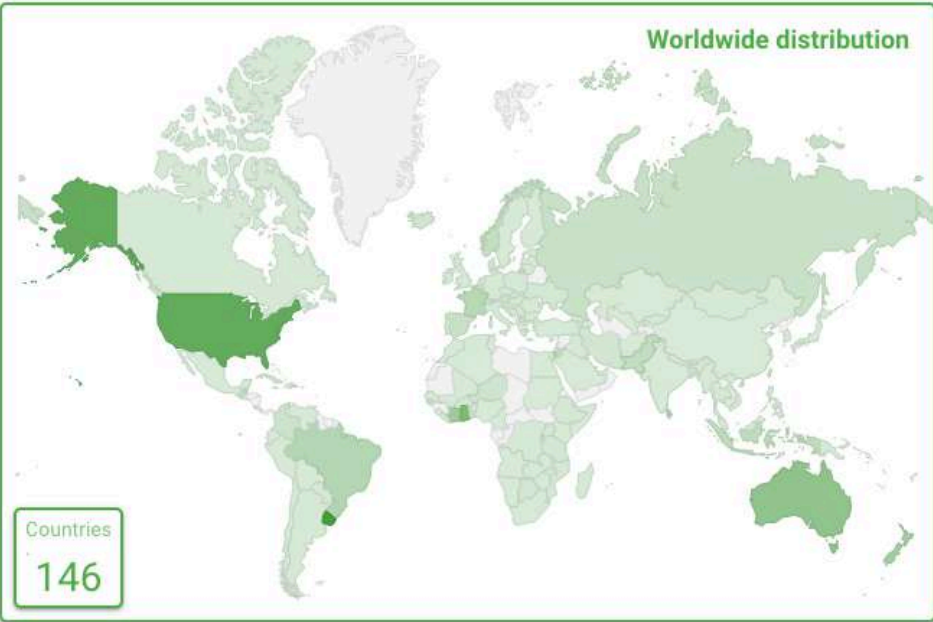


Who is RDA – Professional Title





Who is RDA – Geographical Distribution



11,154 RDA members from 146 different countries





RDA in Greece

Taxonomy:



Posts



Wiki



Events



Repository



Outputs



Case
Statements



Plenaries



Members

create new content

Node Coordinators: Fotis Karagiannis, Elli Papadopoulou



This is a working area dedicated to the support and updates of RDA Greek Node. The Node is hosted at Athena Research and Innovation Information Technology, hence actively acting as a mediator and promoting RDA in Greece, south eastern Europe and beyond. Please register to RDA and join the RDA Greece group to follow all the updates!

<https://www.rd-alliance.org/groups/rda-greece>

Node starter kit

RDA Europe Node programme materials

- National node icons - Greece - for nodes websites, webpages and social media profiles
- National nodes Handbook - RDA Europe owncloud repository (restricted access)
- Flyers: National Nodes Flyer; RDA Europe Grants Flyer
- National Node ppt template - Greece
- Node folder - Greece - RDA Europe owncloud repository (restricted access)
- Membership country statistics - Greece - RDA Europe owncloud repository (restricted access)
- Events toolkit Google folder
- **NEW! European RDA Growth Dashboard**

RDA general materials

- RDA in a Nutshell slidedeck - updated statistics on the RDA Membership issued on a monthly basis.
- RDA Recommendations and Adoption cards - downloadable from RDA Communication kit

Documents available in country language

- About RDA (in Greek)

RDA local news, events and related reports/blogs





RDA Recommendations & Outputs



CATEGORIES OF RECOMMENDATIONS & OUTPUTS

1. Data Management
2. Data Collection
3. Data Description
4. Identity, Store & Preserve
5. Disseminate, Link & Find
6. Policy, Legal Compliance & Capacity

Search for Recommendations & Outputs

21 RDA Recommendations - of which 8 ICT Technical Specifications - & 23 Supporting Outputs currently in the RDA Catalogue:

<https://www.rd-alliance.org/recommendations-and-outputs/catalogue>





RDA active Interest Groups (IG) & Working Groups (WG): Discipline-focused and Partnerships

Total 94 groups:
37 Working Groups & 57 Interest Groups

Discipline focus

Working Groups

- [Agrisemantics WG](#)
- [Capacity Development for Agriculture Data WG](#)
- [Rice Data Interoperability WG](#)
- [Reproducible Health Data Services WG](#)
- [Preserving Scientific Annotation WG](#)
- [Blockchain Applications in Health WG](#)
- [Interoperable Descriptions of Observable Property Terminology WG \(I-ADOPT WG\)](#)
- [RDA-COVID19-Legal-Ethical](#)
- [RDA-COVID19-Software](#)
- [RDA-COVID19-Clinical WG](#)
- [RDA-COVID19-Community-participation WG](#)
- [RDA-COVID19-Epidemiology WG](#)
- [RDA-COVID19-Omics WG](#)
- [RDA-COVID19-Social-Sciences WG](#)
- [RDA-COVID19 WG](#)
- [Raising FAIRness in health data and health research performing organisations \(HRPOs\) WG](#)
- [Empirical Humanities Metadata Working Group](#)

Interest Groups

- [Agricultural Data IG \(IGAD\)](#)
- [Biodiversity Data Integration IG](#)
- [Chemistry Research Data IG](#)
- [Digital Practices in History and Ethnography IG](#)
- [ESIP/RDA Earth, Space, and Environmental Sciences IG](#)
- [Geospatial IG](#)
- [Global Water Information IG](#)
- [Health Data IG](#)
- [Linguistics Data IG](#)
- [RDA/CODATA Materials Data Infrastructure & Interoperability IG](#)
- [Research data needs of the Photon and Neutron Science community IG](#)
- [Small Unmanned Aircraft Systems' Data IG](#)
- [Social Sciences Research Data IG](#)
- [Research Data Management in Engineering IG](#)
- [RDA for the Sustainable Development Goals IG](#)

Partnerships

Working Groups

- [RDA/TDWG Metadata Standards for attribution of physical and digital collections stewardship WG](#)
- [RDA/World Data System \(WDS\) Scholarly Link Exchange WG](#)

Interest Groups

- [ELIXIR Bridging Force IG](#)
- [RDA/National Information Standards Organization \(NISO\) Privacy Implications of Research Data Sets IG](#)





RDA COVID19 Working group aims

- to clearly define detailed **guidelines on data sharing under the present COVID-19 circumstances** to help stakeholders follow best practices to maximize the efficiency of their work, and to act as a blueprint for future emergencies;
- to develop **recommendations for policymakers** to maximise timely, quality data sharing and appropriate responses in such health emergencies;
- to address the interests of **researchers, policy makers, funders, publishers,** and providers of **data sharing infrastructures.**





Community Participation for Data Sharing under COVID-19

Indigenous Data under COVID-19

Legal and Ethical Considerations under COVID-19

Research Software for Data Sharing under COVID-19



WG outputs

- Best practice guidelines per sub-group and overall
- Recommendations for researchers and policymakers to help maximise data sharing
- Catalogue of key resources to inform guidelines (e.g. key datasets, standards, tools, repositories etc)
- A decision tree tool to facilitate navigation to specific resources by different stakeholders





Omicns COVID-19 WG

<https://www.rd-alliance.org/groups/rda-covid19-omics>

Sub-groups/cross cutting themes	Challenges	Guidelines for researchers	Recommendations for funders/policymakers
Omicns	An increased need of rapid openness for omicns data to gain early insights into molecular biology of the processes at cellular level	Omicns research should be a collaborative effort to learn the genetic determinants of COVID-19 susceptibility, severity and outcomes	Promote use of domain-specific repositories to enable standardisation of terms and enforce metadata standards

Data Sharing in Omicns

- Focus and Description
- Scope
- Policy Recommendations
 - Researchers Producing Data
 - Policymakers & Funders
- Guidelines
 - Virus Genomics Data
 - Host Genomics Data
 - Structural Data
 - Metabolomics
 - Lipidomics





Omics COVID-19 WG

<https://www.rd-alliance.org/groups/rda-covid19-omics>

<https://covid.molssi.org>

Example: For Structural Data

- Repositories

- Protein Structures: wwPDB, EBI PDBe, EMDB for Europe, RCSB PDB for USA, PDBj for Japan
- GDHHI of China

- Locating Existing Data

- COVID-19 Molecular Structure and Therapeutics Hub by MOLSSI and BioExcel

- Data and Metadata Standards

- X-ray diffraction
- Electron Microscopy
- NMR
- Neutron Scattering
- Molecular Dynamics simulations
- Computer-aided Drug Design data

Targets:

3CLpro / Mpro Activity
 Inhibition of PLpro Protease Activity
 Host Immune Response
 Inhibition of Nsp13 Helicase Activity
 Blocking SARS-CoV-2 Spike Protein Binding to Human ACE2 Receptor
 Inhibiting Cleavage of the SARS-CoV-2 Spike Protein
 Inhibition of Formation of the Viral Fusion Core
 Inhibition of Viral Polymerases

Proteins:

3CLpro ACE2 BoAT1 E protein Fc receptor Furin Helicase IL6R M protein Macromodain N protein NSP1 NSP10 NSP11 NSP14 NSP15 NSP16 NSP2 NSP4 NSP6 NSP7 NSP8 NSP9 ORF10 ORF3a ORF6 ORF7a ORF7b ORF8 PD-1 PLpro RdRP TMPRSS2 fusion core p38 spike virion

Structures:

3CLpro ACE2 BoAT1 E protein Fc receptor Furin Helicase IL6R M protein Macromodain N protein NSP1 NSP10 NSP11 NSP14 NSP15 NSP16 NSP2 NSP4 NSP6 NSP7 NSP8 NSP9 ORF10 ORF3a ORF6 ORF7a ORF7b ORF8 PD-1 PLpro RdRP TMPRSS2 fusion core p38 spike virion

Models:

3CLpro ACE2 BoAT1 E protein Fc receptor Furin Helicase IL6R M protein Macromodain N protein NSP1 NSP10 NSP11 NSP14 NSP15 NSP16 NSP2 NSP4 NSP6 NSP7 NSP8 NSP9 ORF10 ORF3a ORF6 ORF7a ORF7b ORF8 PD-1 PLpro RdRP TMPRSS2 fusion core p38 spike virion

Therapeutics:

antibody antiviral immunotherapy peptide small molecule





Timeline

24 April	1st draft release
1 May	2nd draft release
8 May	3rd draft release
15 May	4th draft release
28 May	5th / Final draft release
8 June	Close of community comment and feedback (after 10 days)
15 June	Final document sent to RDA governance for endorsement
22 June	Deadline for RDA endorsement (Council, OAB, TAB)
29 June	Internal deadline for incorporation of RDA governance feedback, graphic design
30 June	Final endorsed document available





RDA-COVID19 Omics sub-group

RDA COVID19 UMBRELLA GROUP WEB PAGES	https://www.rd-alliance.org/groups/rda-covid19
RDA COVID19 CASE STATEMENT	https://www.rd-alliance.org/node/68704/case-statement
RDA COVID19 EVENTS (WEBINAR DETAILS)	https://www.rd-alliance.org/node/68704/events
RDA COVID19 WORKING & SUB-GROUP ORGANIZATION	https://www.rd-alliance.org/group/rda-covid19/wiki/working-sub-group-organization
RDA COVID19 OMICS SUBGROUP WEB PAGES	https://www.rd-alliance.org/groups/rda-covid19-omics
RDA COVID19 OMICS SUBGROUP GOOGLE FOLDER	https://drive.google.com/open?id=1bHzfxQLIMdsJtrbl_ZeoSeNZUnY0r2o1

Omics Sub-group Moderators



**Omics Sub-group
Co-chair**

Juan Bicarregui
STFC



Omics

Rob Hooft, DTL &
Natalie Meyers, Uni of Notre Dame

Rob Hooft: rob.hooft@dtls.nl | @rwwh
Natalie Meyers: natalie.meyers@nd.edu | @nkmeyers





RDA-COVID19 Omics sub-group

Members

Alecia Naidu
Andrea Zaliani
Bartha Maria Knoppers
Calvin Chan
Christopher Harrison
Dara Hallinan
Eric Piver
Galia Weidl
Hilary Hanahoe
Isabelle PERSEIL
Juliane Fluck
Korbinian Bösl
Lynn Schriml
Marta Teperek
Paolo Manghi
Pieter Heyvaert
Ram Gouripeddi
Rodrigo Sara
Stéphanie Rennes
Thomas Duflet
Vivien Bonazzi

Alejandra Gonzalez-Beltran
Andrew Harrison
Brian Corrie
Caterina Tomulescu
Claire Austin
David Molik
Fanny Sébire
George Papastefanatos
Hugh Shanahan
Jeremy Geelen
Justine Vandendorpe
Laurence DELHAES
Mark Leggott
Mary O'Brien Uhlmansiek
Patrick Dunn
Piotr Dabrowski
Richard Milne
Rosanna Babagiannou
Steve Tsang
Tim Smith
Wolmar Nyberg Åkerström

Alessandra Renieri
Anupama Gururaj
Brian Corrie
Catherine Chronaki
Clara Amid
Deepti Mittal
Felix Bach
Heidi Laine
Hussein Sherief
Jonathan Tedds
Kara Woo
Lawrence Nderu
Mark Taylor
Miguel Rocha
Paula Martinez Lavanchy
Priyanka Pillai
Rob Hooft
Simon Hodson
Susanna-Assunta Sansone
Venkata Satagopam
Yasemin Turkyilmaz-van der
Velden

Alexander Bernier
Artur Rocha
Bridget Walker
Christian Busse
Daniel Mietchen
Emmanuelle Rial-Sebbag
Fotis Psomopoulos
helene blasco
Idris Sulaiman
Juan Bicarregui
Konrad Förstner
Leyla Garcia
Marta Marin
Natalie Meyers
Philippe Rocca-Serra
Rajini Nagrani
Robert Quick
Sophie Limou
Susheel Varma
Victor Greiff
Zoe Cournia



National Initiatives for Open Science in Europe

NI4OS-EU vs COVID-19

International COVID19 HPC Knowledge
Exchange Group

4 June 2020

Zoe Cournia, BRFAA
Life Sciences Scientific Community Leader



Current model of European data infrastructures

- Data
- Computing
- Storage
- Applications
- Software



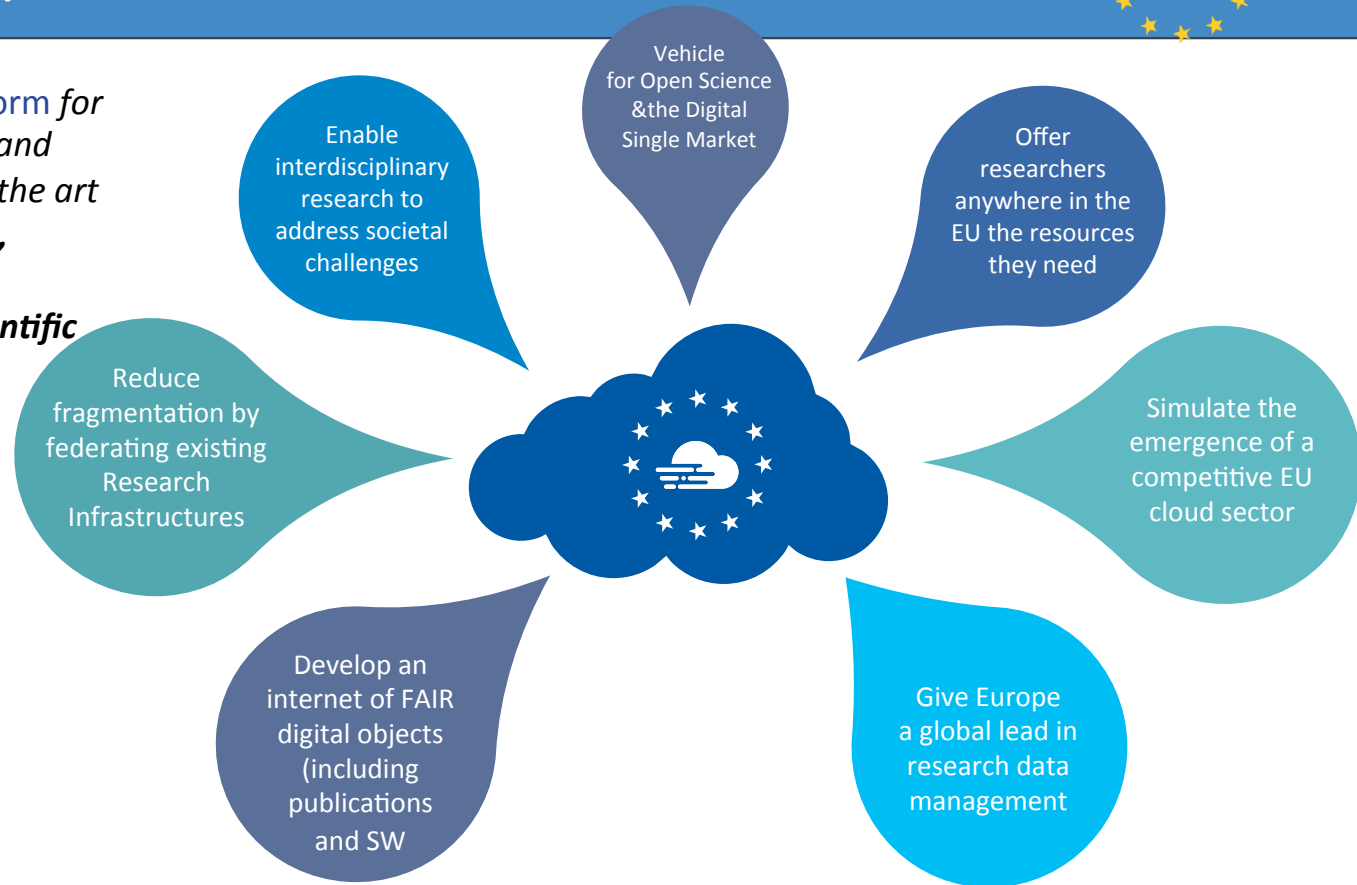
Source: EOSC Strategic Implementation Roadmap 2018-2020, May 2018, European Commission

From fragmentation and uneven access to information to a federated model, where access to data would be universal, building on a strong legacy

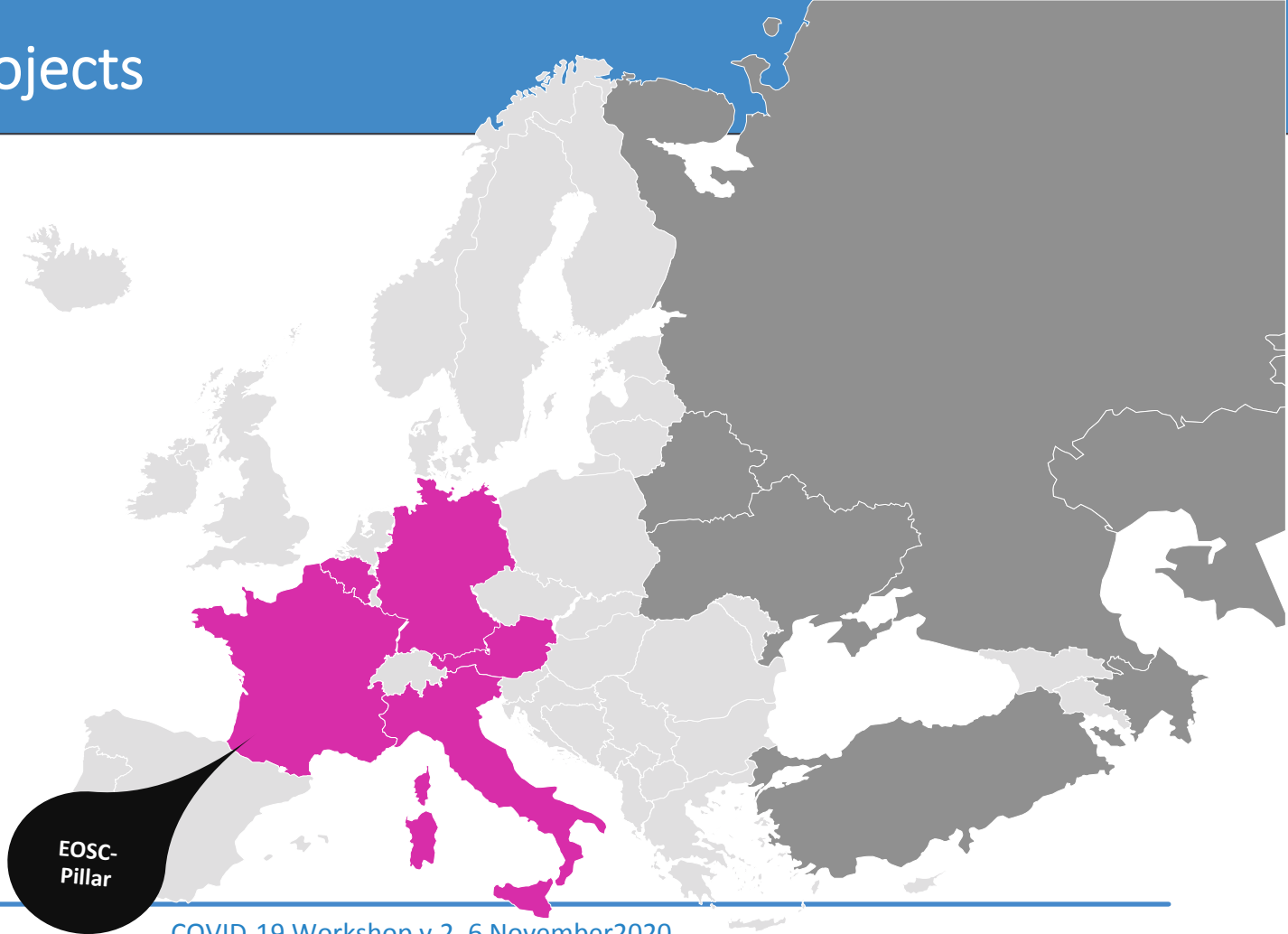


Future EOSC model: federation of data infrastructures

One federated platform for producing, curating and distributing state of the art **Findable, Accessible, Interoperable and Reusable (FAIR) scientific data.**

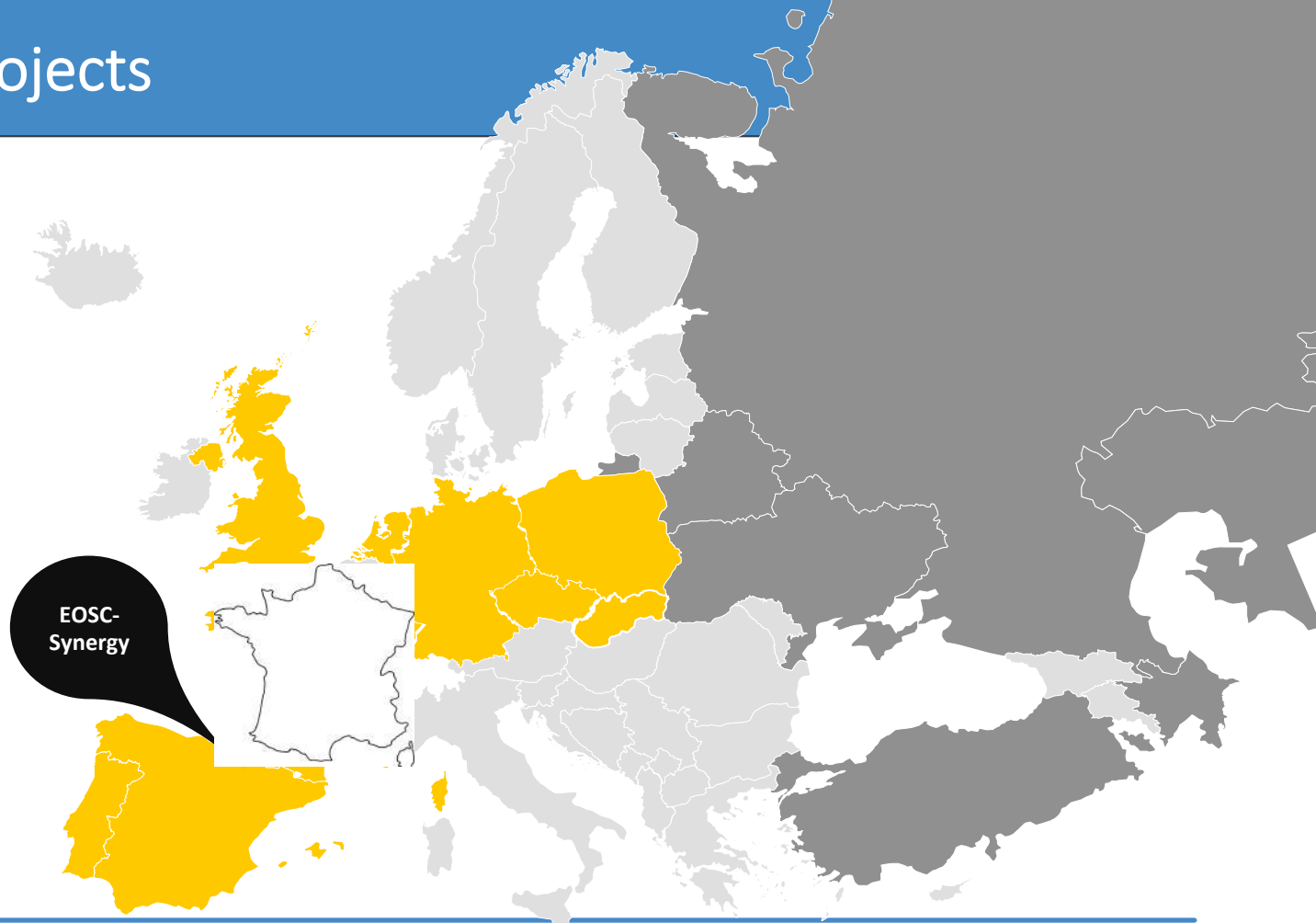


Regional projects



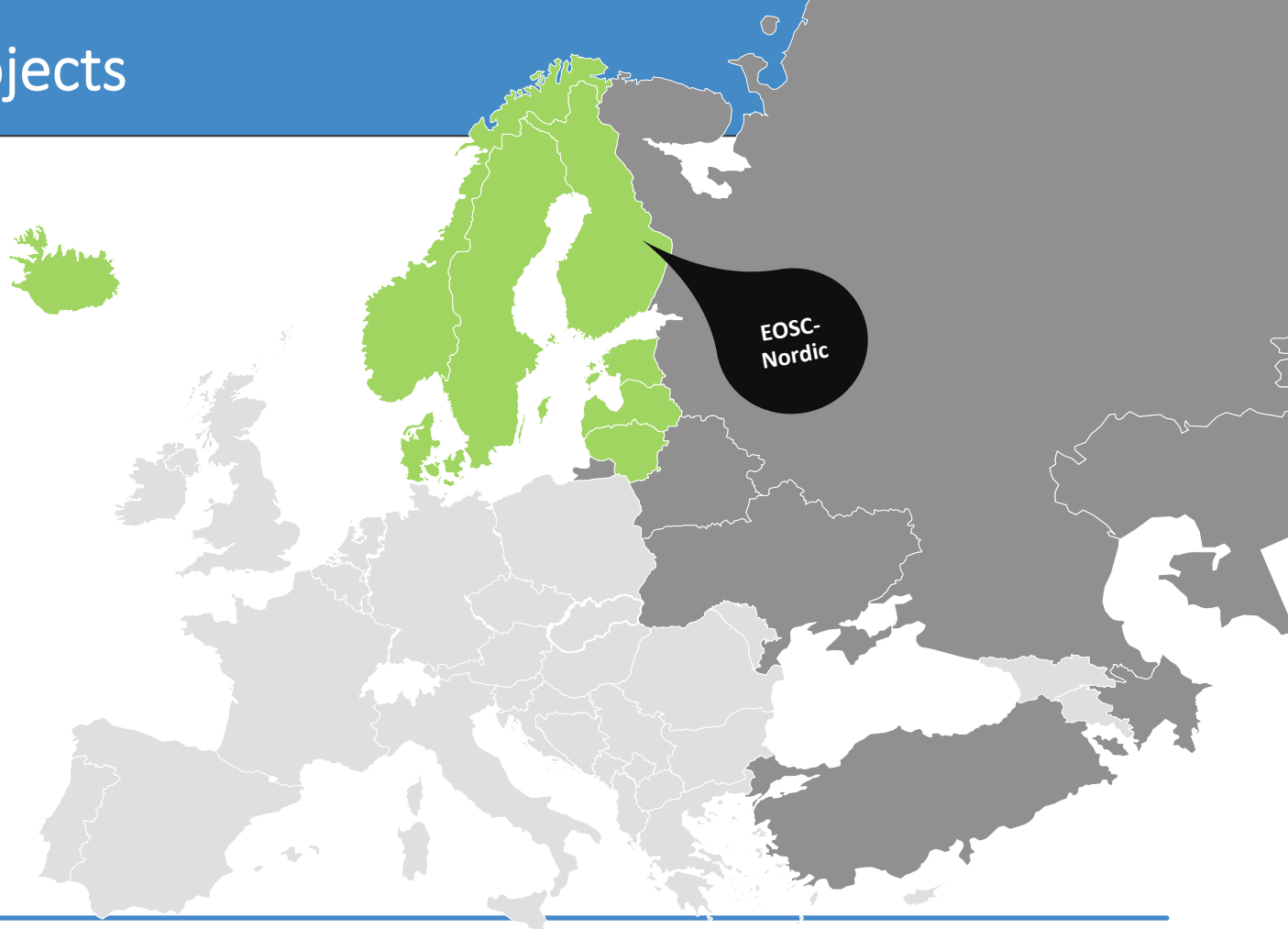
Credits: Federica Tanlongo – GARR
federica.tanlongo@garr.it - EOSC-Pillar

Regional projects



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Regional projects



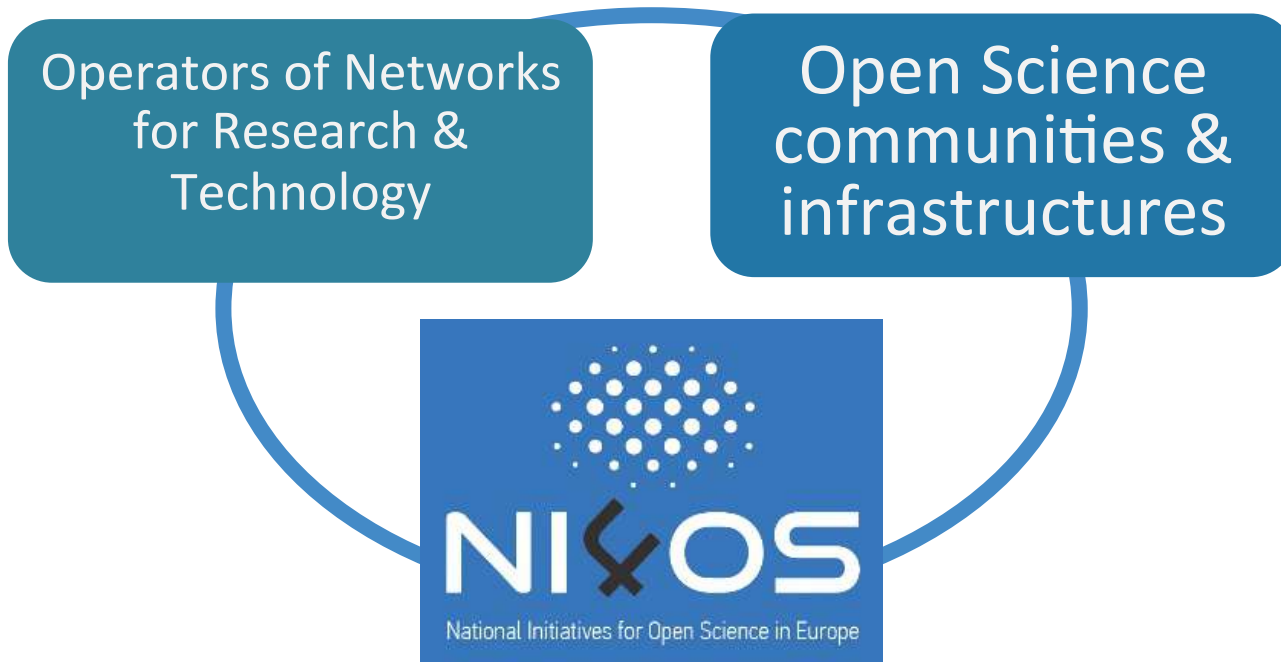
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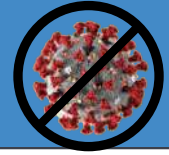
Regional projects

Greece
Cyprus
Bulgaria
Croatia
Serbia
Slovenia
Hungary
Romania
Albania
Bosnia-Herzegovina
North Macedonia
Montenegro
Moldova
Armenia
Georgia



Credits: Federica Tanlongo – GARR
federica.tanlongo@garr.it - EOOSC-Pillar



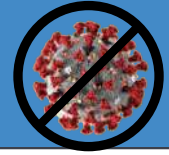


□ NI4OS-Europe takes action in the fight against COVID-19:

- NI4OS-Europe opens a fast track access channel to its
 - Generic services -computational (HPC, Cloud)
 - Data Analyzing tools
 - Storage services
 - Thematic Services related to covid-19
 - For scientific communities that perform extensive research to tackle the COVID-19.

□ APPLY and gain Fast Track Access to NI4OS-Europe resources:

- Are you a researcher, contributing in the fight against COVID-19?
- Seize the opportunity and make use of NI4OS Fast Access Channel!
- Contact us at: ni4os-europe-covid19@ni4os-europe.eu



□ The initiation procedure to the fast access channel is as follows:

- Contact NI4OS-Europe fast access channel at ni4os-europe-covid19@ni4os-europe.eu and express your need by briefly describing:
 - Area of research,
 - Estimated overall computational load and usage pattern in the near future,
 - Execution environment (programming language, libraries),
 - Parallelization requirements, if any,
 - Data exchange, etc.
- Needs will be matched against the available resources and you will be responded soon.
- An online meeting might be arranged so that the needs of the project are discussed.
- You will be provided details on how to access the resources.

- **CPUs, GPUs, Phi-cards available.**

Computational Resources Available

- **Computational resources have already been allocated to:**
 - The Bioinformatics European Research Era Chair and the Bioinformatics Group at the Cyprus Institute of Neurology and Genetics.
 - **“Network-based multiomics integration boosts drug repurposing against COVID-19.”**

Our in-house drug discovery software tools

ChemBioServer

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

Filtering, clustering & visualization of compounds for drug discovery



The screenshot shows the ChemBioServer web interface. It features a navigation menu on the left with options like 'Basic Search', 'Filtering', 'Advanced Filtering', 'Clustering', 'Customize Pipeline', and 'Visualize Compounds Properties'. The main content area displays 'Welcome to ChemBioServer' and provides information about the server's purpose, system requirements, and services. The footer includes the year 2011 and the affiliation 'BioAcademy | Home | BioAcademy | Biomedical Research Foundation Academy of Athens'.

FEPrepare

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

Automates lead optimization



AFMM

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

Automatic parameterization for small molecules

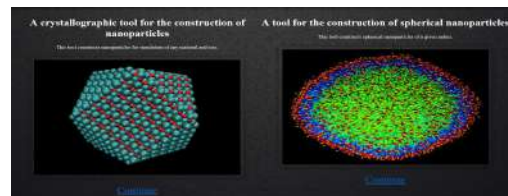


The screenshot shows the AFMM web interface. It features a navigation menu on the left with options like 'Home', 'About', 'FAQ', 'Contact', and 'Help'. The main content area displays 'AFMM - A Neutronic Molecular Force Field Parameterization Program' and provides information about the program's purpose, system requirements, and services. The footer includes the year 2011 and the affiliation 'BioAcademy | Home | BioAcademy | Biomedical Research Foundation Academy of Athens'.

Nano-Crystal

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

Creates nanoparticles for simulations



Subtract

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

Calculates the volume of protein cavities



The screenshot shows the Subtract web interface. It features a navigation menu on the left with options like 'Home', 'About', 'FAQ', 'Contact', and 'Help'. The main content area displays 'Welcome to Subtract Server!' and provides information about the server's purpose, system requirements, and services. The footer includes the year 2011 and the affiliation 'BioAcademy | Home | BioAcademy | Biomedical Research Foundation Academy of Athens'.



**EUROPEAN OPEN
SCIENCE CLOUD**

<https://www.eosc-portal.eu/>



NETWORKING



COMPUTE



STORAGE



SHARING & DISCOVERY



DATA MANAGEMENT



PROCESSING & ANALYSIS



SECURITY & OPERATIONS



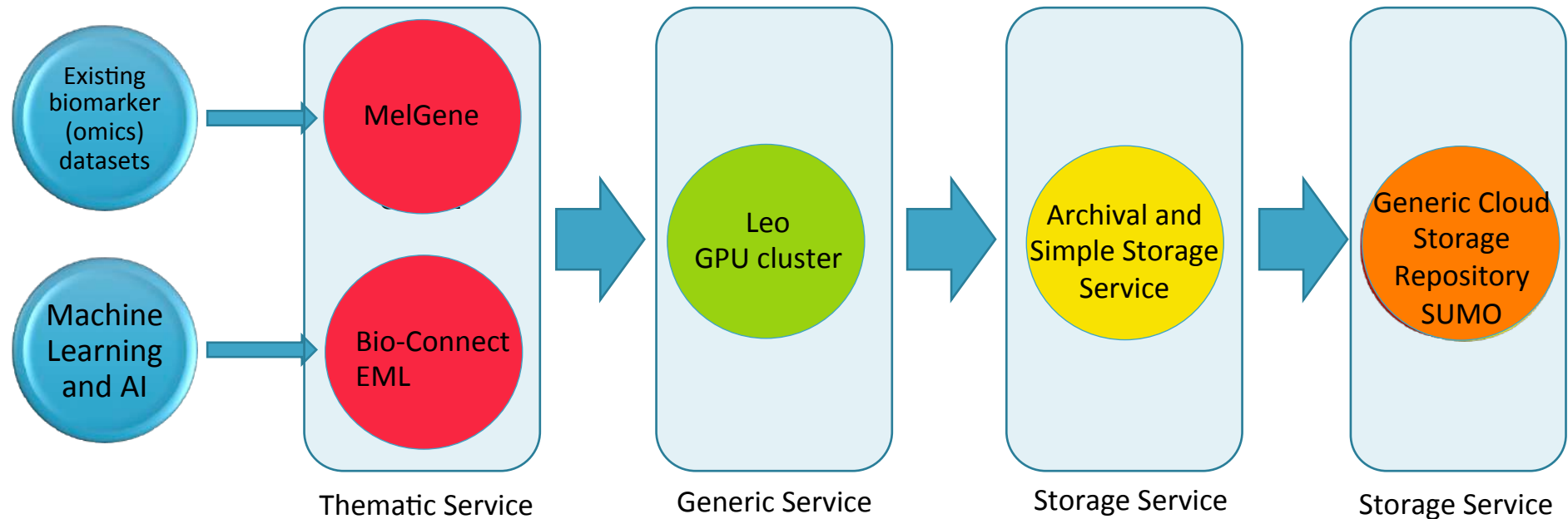
TRAINING & SUPPORT

Use Case Example: Extracting correlations for patient stratification using machine learning



Extracting correlations for patient stratification using machine learning

- Stratifying patients for COVID-19 response based on existing data



Global Open Science as a driver for enabling a new paradigm of transparent, data-driven science as well as accelerating innovation



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



https://twitter.com/NI4OS_eu



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

zcournia@bioacademy.gr