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The FOSSR Virtual Research Environment (VRE)

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Alfredo Oliviero

Istituto di Scienza e Tecnologie dell'Informazione (ISTI)
Consiglio Nazionale delle Ricerche (CNR)



FOSSR

Fostering Open Science in Social Science Research
Innovative tools and services to investigate economic and societal change



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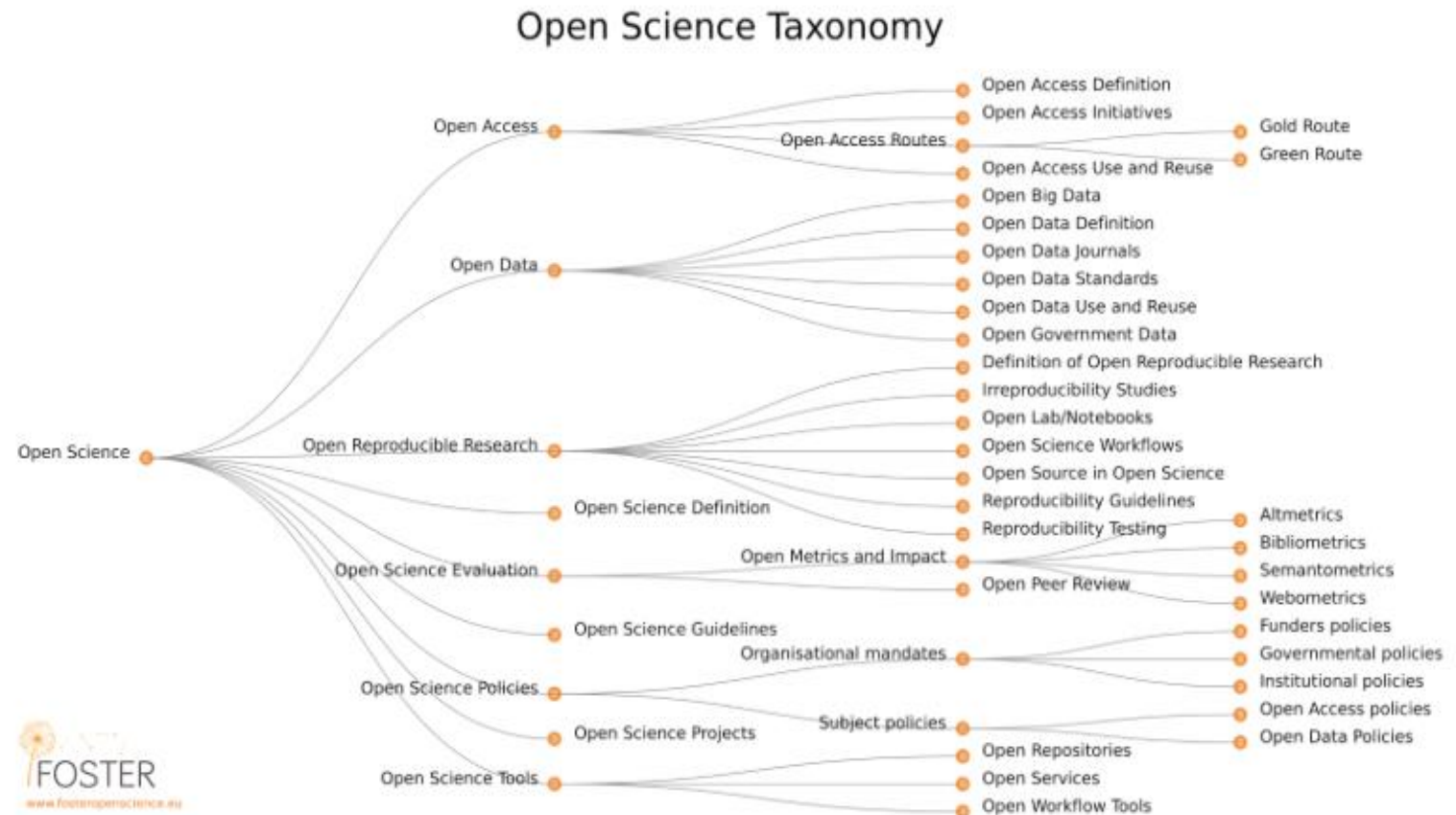


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What is Open Science?

An approach to the scientific process based on cooperative work and ways of disseminating knowledge, improving accessibility to and re-usability of research outputs by using digital technologies and collaborative tools.

SOURCE: COMMISSION RECOMMENDATION
(EU) 2018-790 of 25 April 2018





Open Science Infrastructures

What is an Open science infrastructure?

A shared research infrastructure that support open science and serve the needs of different communities.

It can be physical, digital and hybrid, include publication and data repositories, equipment and other infrastructures for open **sharing**, **evaluation** and **reproducibility**.

Not only Open Access Repositories...

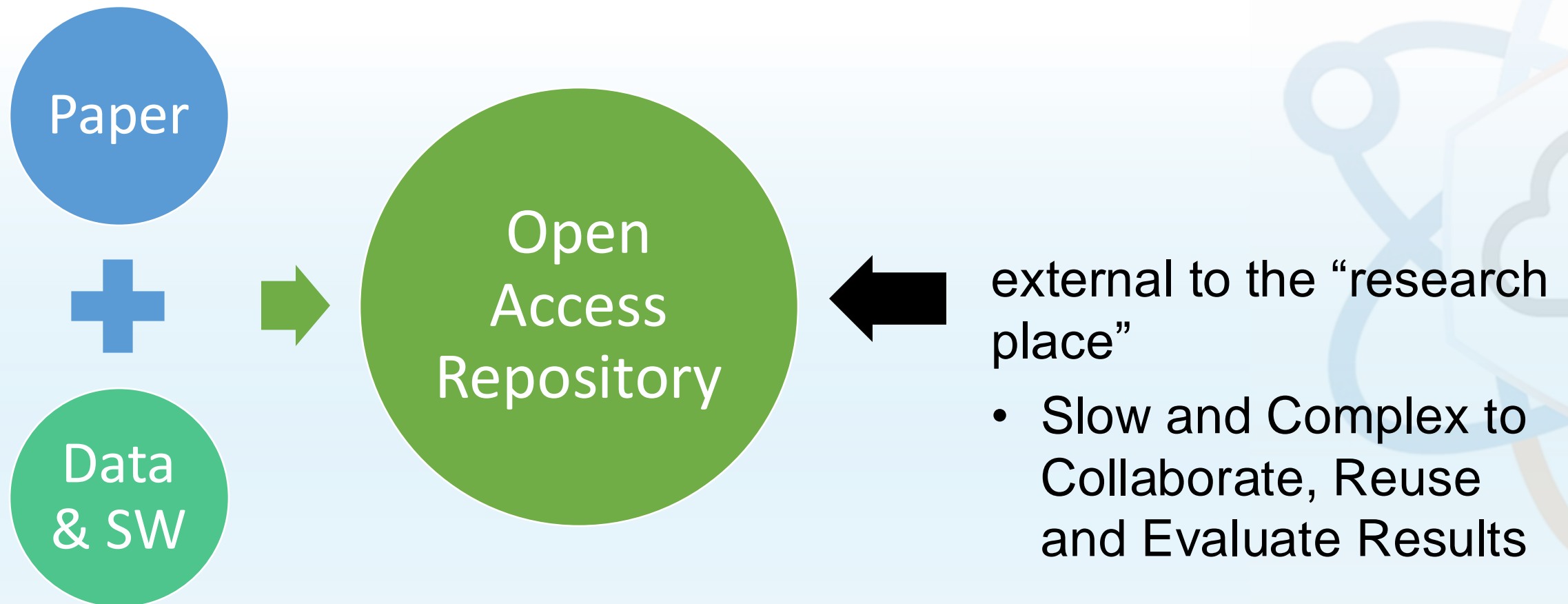
Repositories typically address a specific part of the research workflow, while infrastructures are relevant across the entire research cycle.



UNESCO, 2023, Open Science Outlook 1

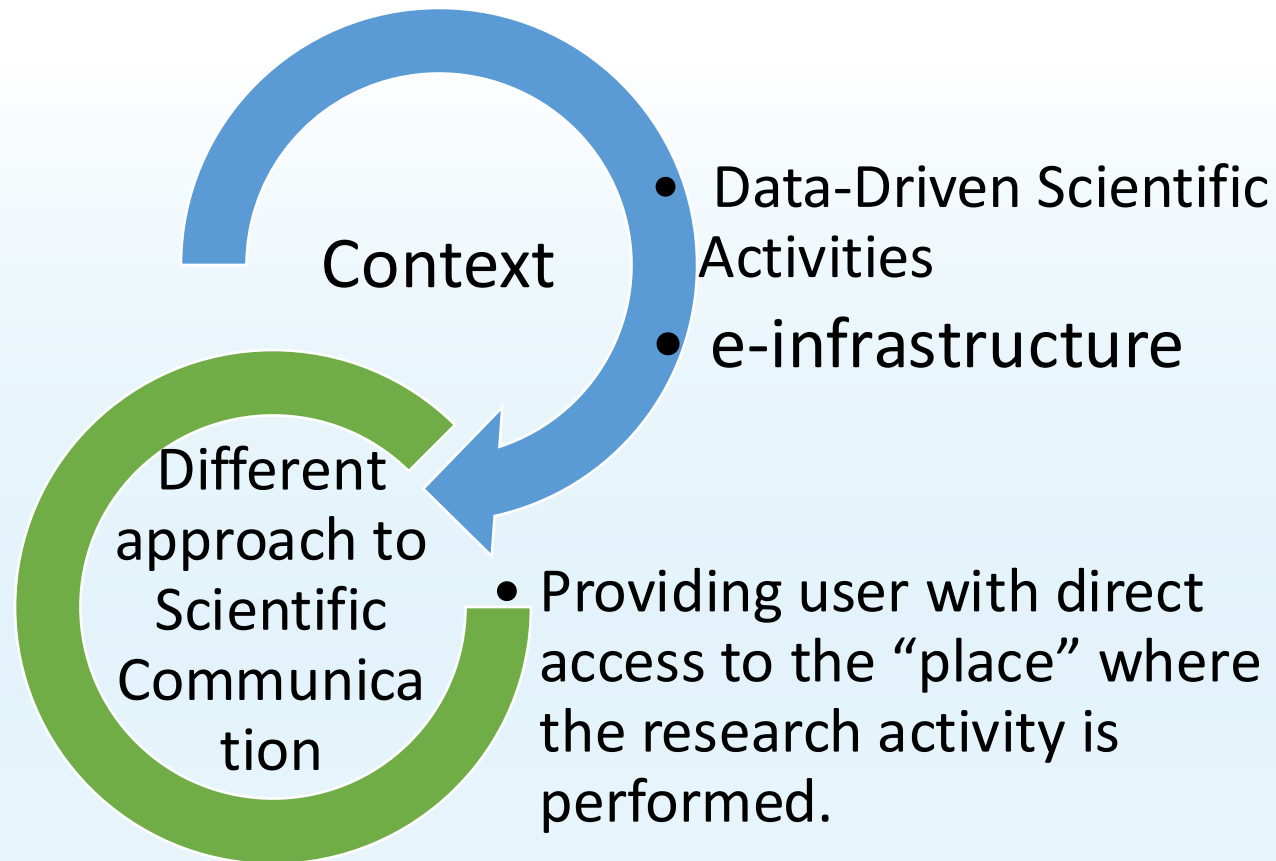


Open Science practices today: Deposit in OA Repo



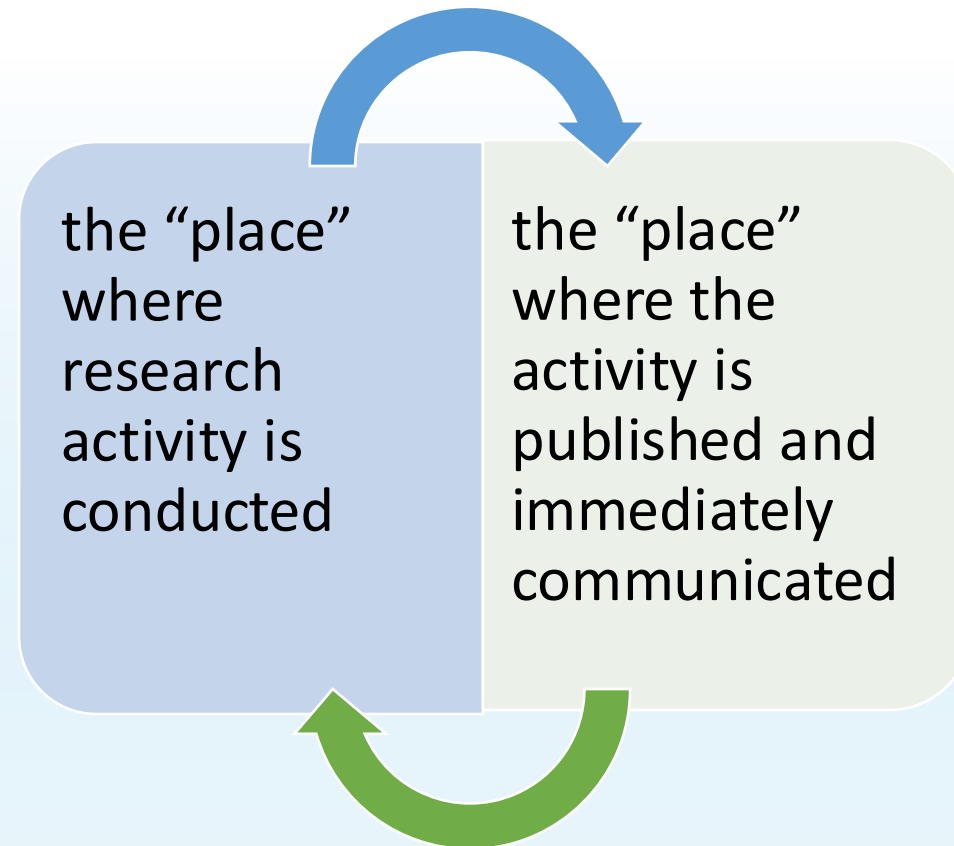


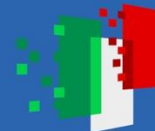
Data Driven and e-infrastructure Research Context



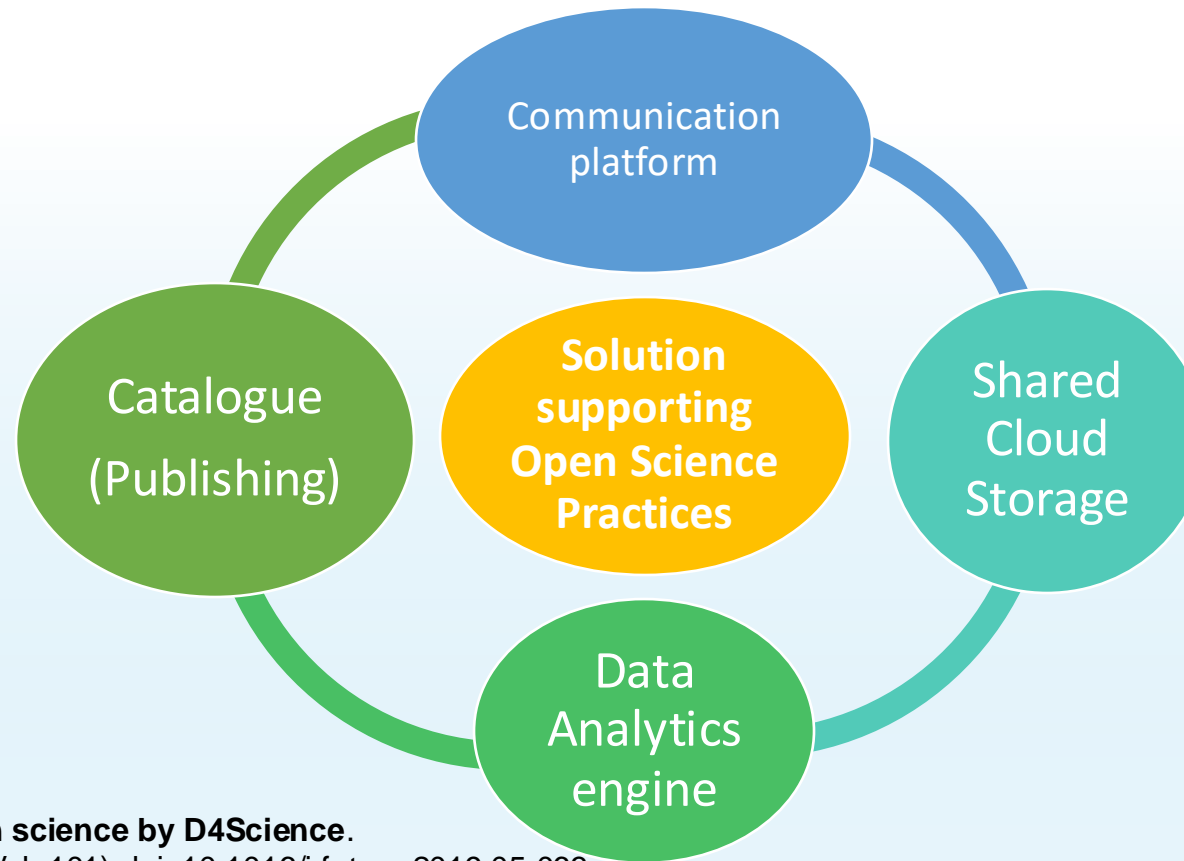


Paradigm shift: coupling of the “place” where research is performed with the “place” where research is communicated





The VRE makes it possible to do more, supporting the entire (data-driven) research lifecycle

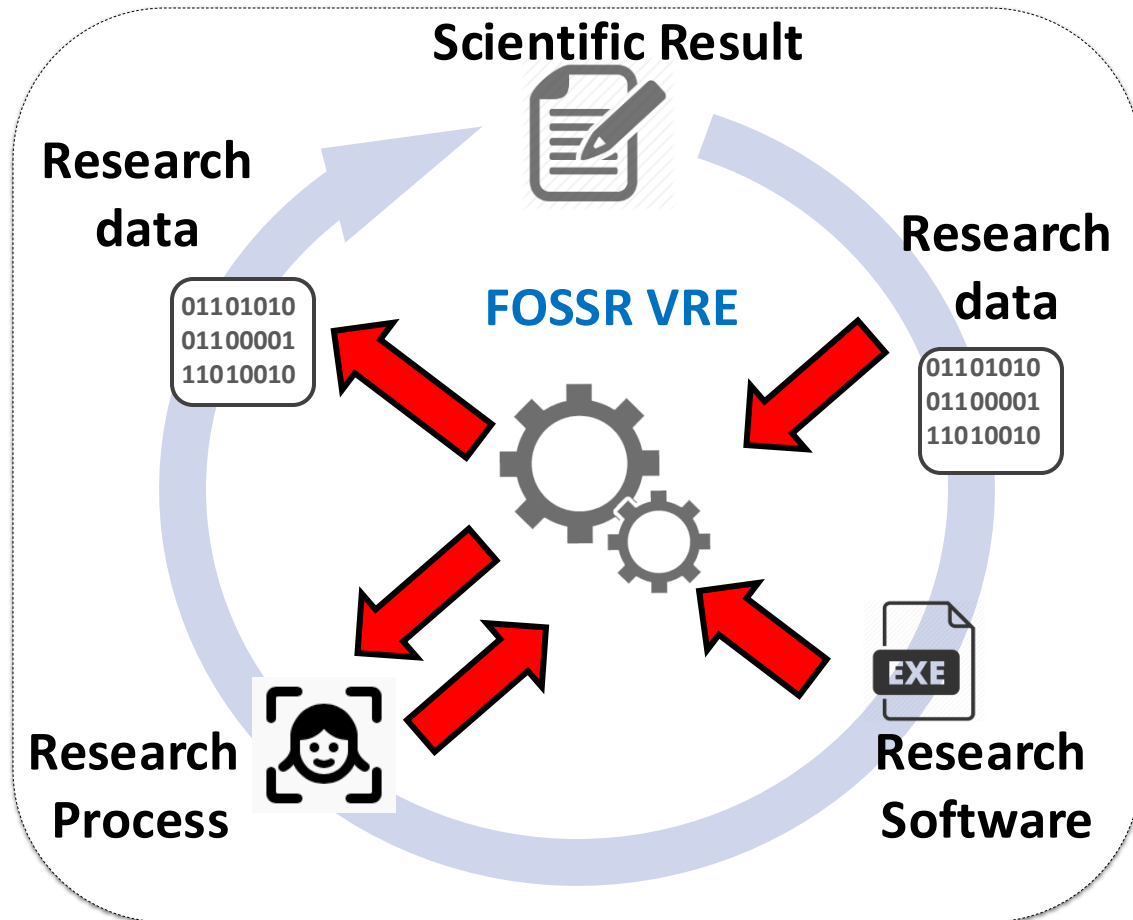


M. Assante, et al. (2019) **Enacting open science by D4Science**.
Future Generation Computer Systems (Vol. 101) [doi: 10.1016/j.future.2019.05.063](https://doi.org/10.1016/j.future.2019.05.063)

M. Assante et al. (2023) **Virtual research environments co-creation: The D4Science experience**.
Concurrency Computat Pract Exper. 2023; 35(18):e6925. [doi:10.1002/cpe.6925](https://doi.org/10.1002/cpe.6925)



FOSSR VRE as a platform to support and promote Open Science practices



Enable

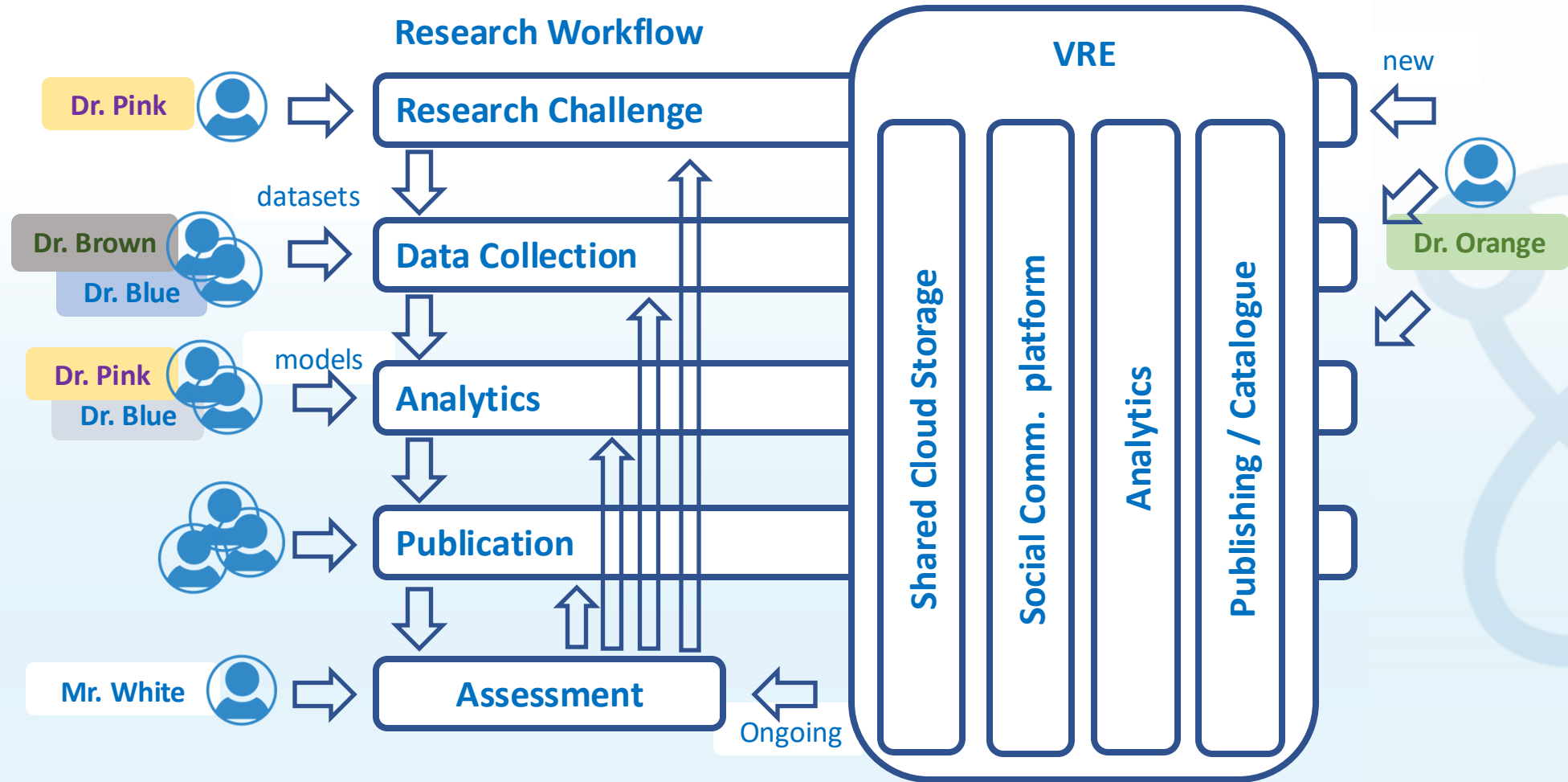
- Reproduce, Reuse, Evaluate
- Active collaboration
- Effective sharing
- Provenance and attribution

Adopt

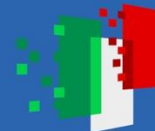
- As-a-service approach
- Standards
- Economy-of-scale to reduce operational costs



A prototypical and simplified scientific workflow enacted by these components



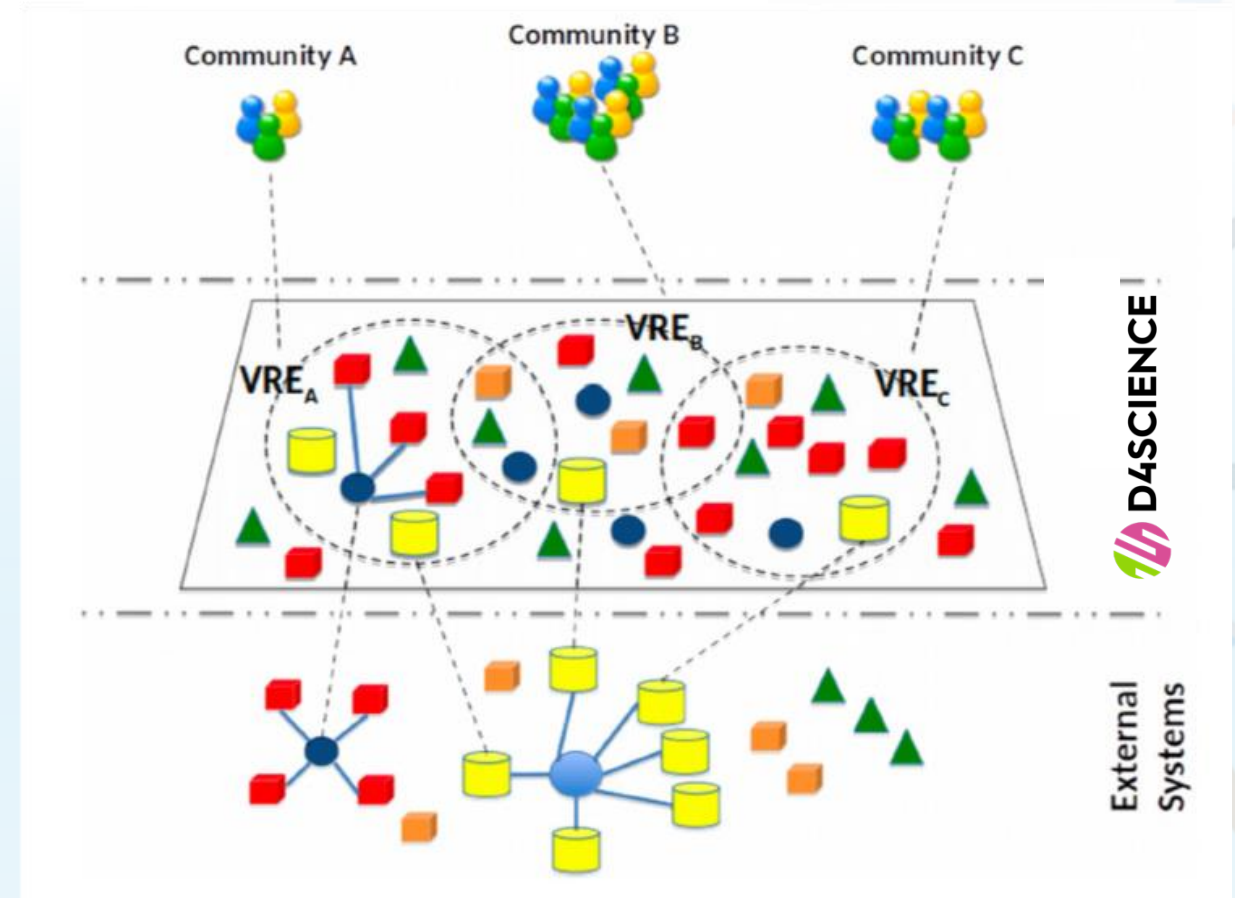
All of this happens well before their paper is published!



FOSSR VRE platform based on D4Science Infra Services

 **D4SCIENCE** promotes Open Science practices through the operation of a Data Infrastructure service

- leverage **external systems** (e.g. data, storage services, computational resources, cloud computing infrastructures)
- by exposing them as a **common unified space of resources**
- to serve **diverse community of researchers**
- via the **provision of tailored services and sharing tools**
- made accessible through a flexible, web-based and on-demand environments called **Virtual Labs**

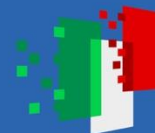




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2008 -2012



2014



2014-2020



Today

Evolution

D4Science is a federated
digital infrastructure
promoting Open Science

- 4 sites (1 Pisa, 3 @ GARR)
- 6.900 CPUs core
- 29 TB RAM
- 1.400 TB Storage

D4Science is owned and managed by CNR (ISTI)

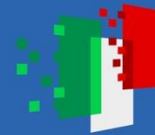
It supports ESFRI RIs, national and European
projects, national and international initiatives



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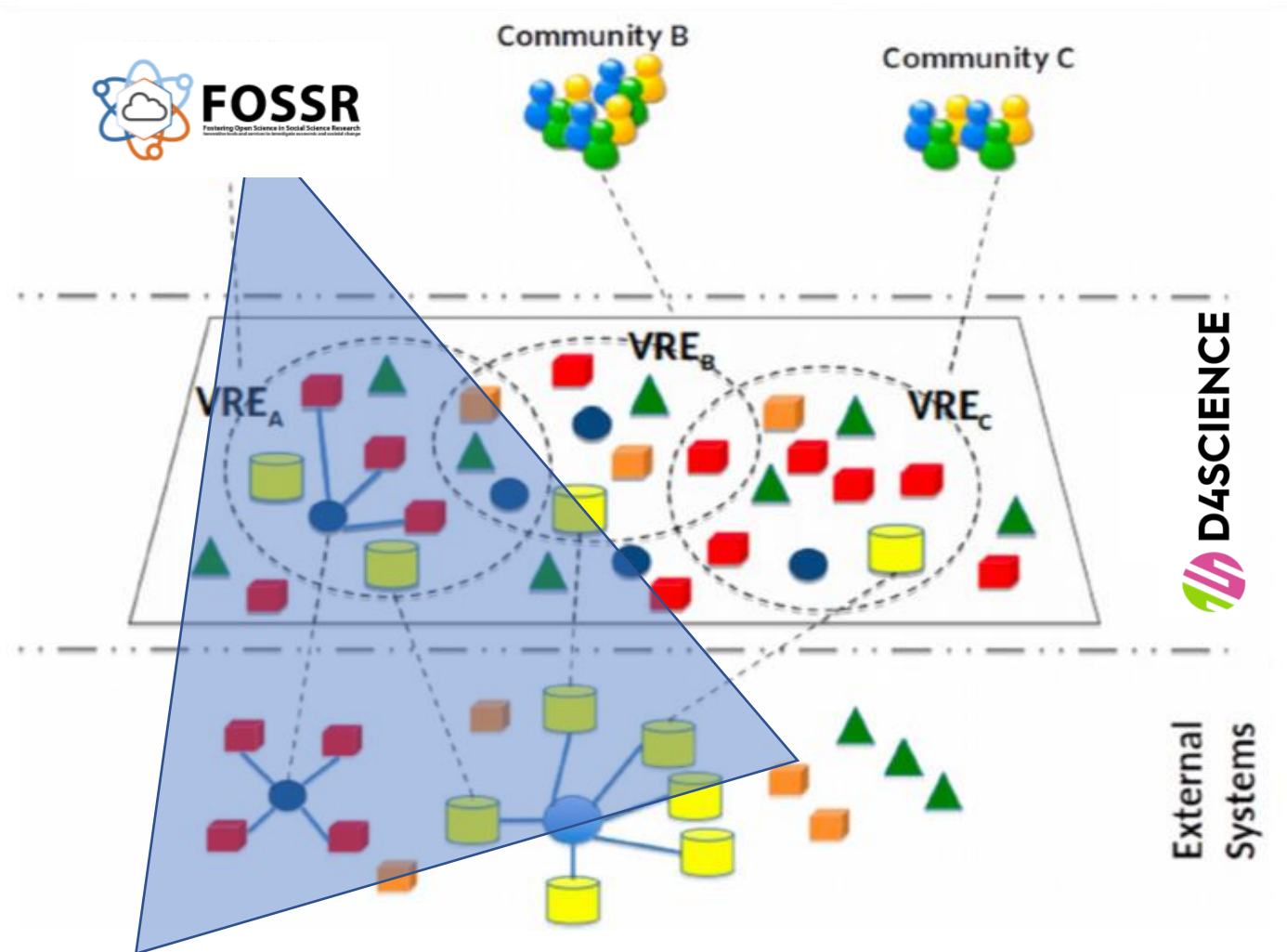


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FOSSR VRE on D4Science





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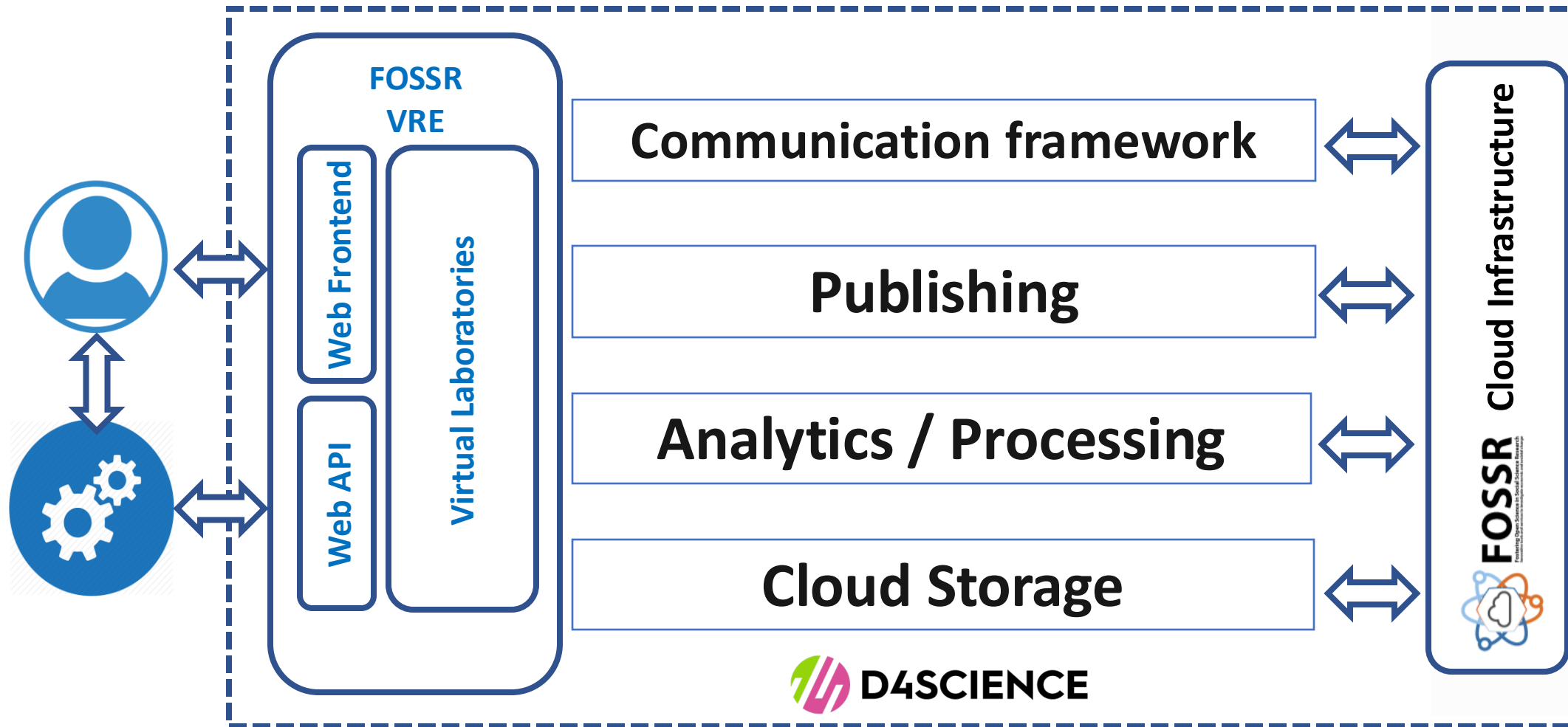


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FOSSR VRE Open Science Services for Virtual Lab tools





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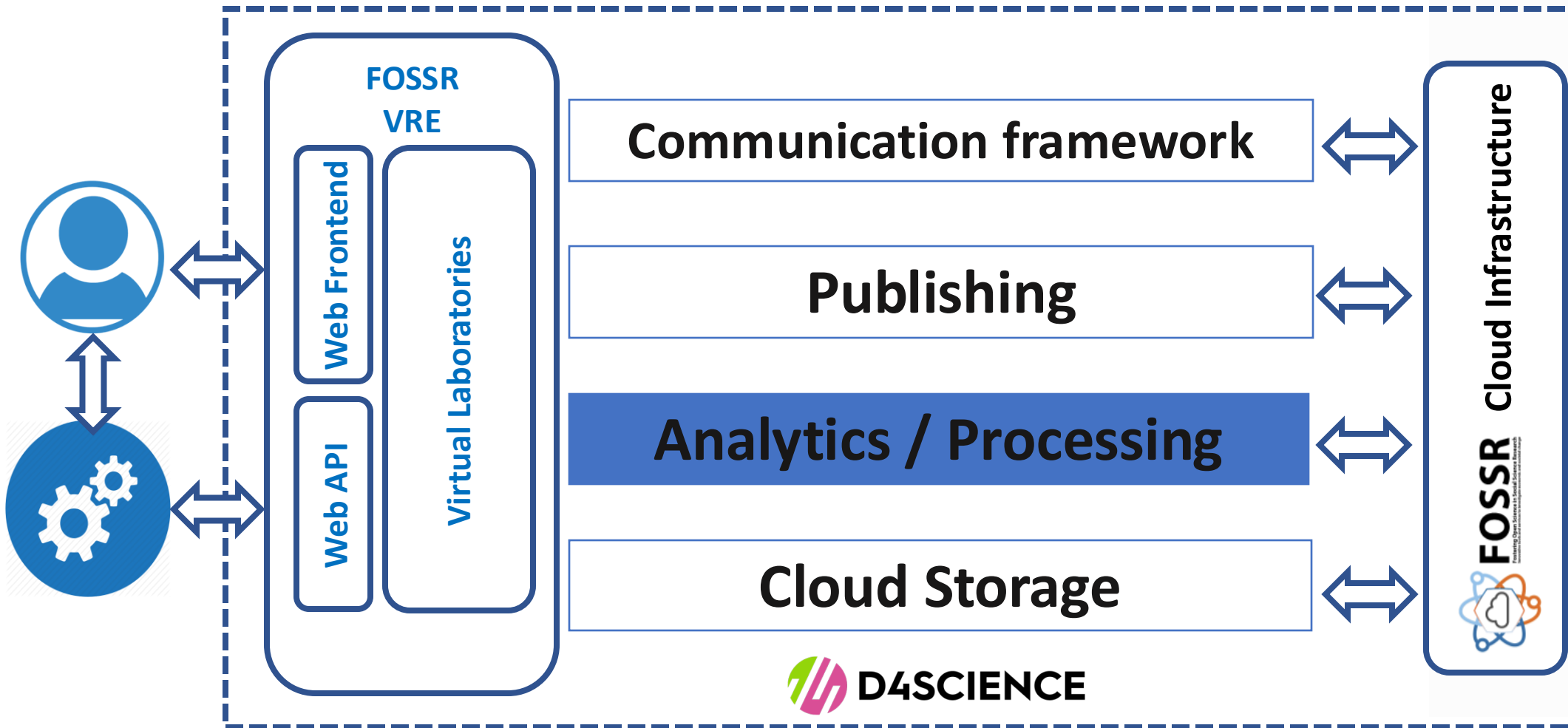


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FOSSR VRE Open Science Services for Virtual Lab tools

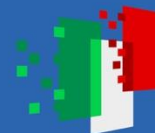




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From theory to practice, where is the FOSSR VRE? -> <https://fossr.d4science.org>

← → ↻ 🏠 🔒 https://fossr.d4science.org ⚙️ ☆ 📧 🔍 Cerca ↺ 🖨️ 📄 ☰

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Home Sign In

FOSSR VRE
Fostering Open Science in Social Science Research
Virtual Research Environment

FOSSR VRE Gateway

Collaboration and innovation to enhance social research through accessible data sharing, development of innovative tools, and investment in advanced training

Sign In Register

Terms of Use Cookies Policy Privacy Policy

Powered by **D4SCIENCE** Cookie Settings

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PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) MISSIONE 4, COMPONENTE 2, INVESTIMENTO 3.1 "Fondo per la realizzazione di un sistema integrato di infrastrutture di ricerca e innovazione"

This work was supported by FOSSR (Fostering Open Science in Social Science Research), funded by the European Union - NextGenerationEU

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Federated Identity and Access Management Service: Academic Login

https://accounts.d4science.org/auth/realms/d4science/protocol/openid-connect/auth? ... Cerca

Fossr **D4SCIENCE** English ▾

Sign in to your account

Username or email

Password

☐ Remember me [Forgot Password?](#)

Sign In

Or sign in with

Academic / other LinkedIn

Google Twitter

GitHub CNR-ISTI

New user? [Register](#)

[Terms of Use](#) | [Cookies Policy](#) | [Privacy Policy](#)

egi **EUROPEAN OPEN SCIENCE CLOUD**

Check-in

Choose your academic/social account

Q CNR

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- [CNR Institute of Clinical Physiology](#)
- [CNR Institute of Informatics and Telematics](#)
- [CNRS - Units staff](#)
- [CNRST](#)
- [National Research Council \(CNR\)](#)

or

Bitbucket D4SCIENCE SSO LOG-IN

Choose your academic/social ac

Q Search...

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FOSSR VRE Gateway – Dashboard page (landing page)

Massi's home ★ VREs [🔗](#)


Name	Owner	Last modified
This folder is empty		

Previous

Show [▼](#)

Showing 0 to 0 of 0 entries

Virtual Labs

 **FOSSR Virtual Lab** 🔒 open


This Virtual Lab comprises a suite of services promoting Open Science practices and designed to foster collaboration and enhance interaction among diverse research audiences. Specifically:
Shared Cloud Storage: An intuitive application for ...
[Read More »](#)

My Virtual Labs

You are not subscribed to any environment, please begin by [joining](#) one.

[Explore](#) the Virtual Research Environments available in the infrastructure.

Request a Virtual Lab





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FOSSR VLab Home

FOSSR

Go to 0 Massi Testing

[FOSSR-Lab](#) [JupyterLab](#) [RStudio](#) [Analytics Engine](#) [Catalogue](#) [How-to](#)

FOSSR
Fostering Open Science in Social Science Research
Innovative tools and services to investigate economic and social change

This Virtual Lab comprises a suite of services designed to promote Open Science practices, foster collaboration and interaction among diverse research communities. Specifically:

- Shared Cloud Storage: An intuitive application for storing both private and shared data.
- Open Data Analytics Platform: A computational environment for dataset exploration and validation ...

[See more](#)

[Other options ...](#)

[Invite Members](#)

Post a message

Share an update or a link, use "@" to mention and "#" to add a topic

Members: OFF ☐ ON

[Share](#)

Show sorted by: newest Post

Massimiliano Assante
July 11, 2:26 PM

Dear participants,
welcome to FOSSR-Lab #VRE. This environment is equipped with the following:

- * Analytics Framework: JupyterLab, RStudio, Analytics Engines
- * Workspace cloud storage: for sharing files and folders on the cloud, where you will also find the presentations
- * Catalogue: for publishing research products
- * Docs / how tos

[Reply](#) - [Like](#)

Shared Folder

FOSSR-Lab [Recent](#)

Name	Owner	Last modified
Datasets	MA	22 Jul 15:58 24
Presentations	MA	22 Jul 15:58 24
FOSSR-Logo.jpg	MA	04 Jul 18:54 24

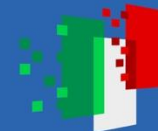
[Previous](#) 1 [Next](#)

Show entries

1 to 3 of 3 items

[Go to shared workspace](#)

JupyterLab



FOSSR VLab – Jupyter Lab (highly customisable)

Jupyter Notebook is a web-based tool that lets you write and run code, display data, and add documentation in an integrated format.

The screenshot displays the FOSSR VLab Jupyter Lab interface. On the left, a sidebar shows 'Server Options' with three choices: 'Default Large - 4 Cores / 8G RAM', 'Default Medium - 4 Cores / 4G RAM', and 'VRE Training server - 8 Cores / 64G RAM'. A blue arrow points from the 'VRE Training server' option to the main interface. The main interface shows a file explorer with a directory structure including 'Phytoplankton_EOV/Chla_Product/Programs'. Below the file explorer, a grid of application icons is visible, including Python 3, Clojure, Julia 1.5.0, Kotlin, and SQL. Another blue arrow points from this grid to the right, where a Jupyter Notebook is open. The notebook contains text about 'Notebook 1.2.' and 'Files for input:', followed by two code blocks. The first code block uses 'bash' and 'grep' to process 'SMAGs_v1_concat.faa'. The second code block uses 'bash' and 'prodigal' to detect genes and translate them on the server. The third code block shows commands to create a protein database adapted to a specific directory.

FOSSR VLab – Jupyter Lab (highly customisable)

Jupyter Notebook is a web-based tool that lets you write and run code, display data, and add documentation in an integrated format.

Server Options

- Default Large - 4 Cores / 8G RAM**
The Default notebook server includes Python, R, Julia, Octave and Java kernels and libraries preinstalled for Python.
- Default Medium - 4 Cores / 4G RAM**
The Default notebook server includes Python, R, Julia, Octave and Java kernels and libraries preinstalled for Python.
- VRE Training server - 8 Cores / 64G RAM**
This notebook server includes a set of Python libraries preinstalled for Python.

Start

Phytoplankton_EOV/Chla_Product/Programs

Notebook

Python 3, Clojure, Clojure [conda env:root] *, Julia 1.5.0 [conda], Kotlin, Kotlin [conda env:root] *, Python [conda env:root] *, SQL, SQL [conda env:root] *

Notebook 1.2. allows for the creation of p
derived from Metagenomic or Metatrans
annotated as well as unknown sequences

Files for input:

Data available from: Tara Oceans Eukaryotic Genomes (the "SMAGs")
manually curated SMAGs (Single amplified genomes and metagenomes)

```
%%bash
grep -c ">" SMAGs_v1_concat.faa
```

Use Prodigal to detect genes and translate them (on server)

```
%%bash
for file in TARA*; do prodigal -i "$file" -o "$file.co
```

Create a protein database adapted to di

```
%%bash
cat *.protein.faa >> Euk_prot.faa
cut -d " " -f 1 Euk_prot.faa > Euk_prot_shortheader.faa
cat Euk_prot_shortheader.faa SMAGs_v1_concat.faa > Euk
```



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FOSSR VLab – Rstudio 4+

RStudio is an integrated development environment (IDE) for R, a programming language used for statistical computing and graphics

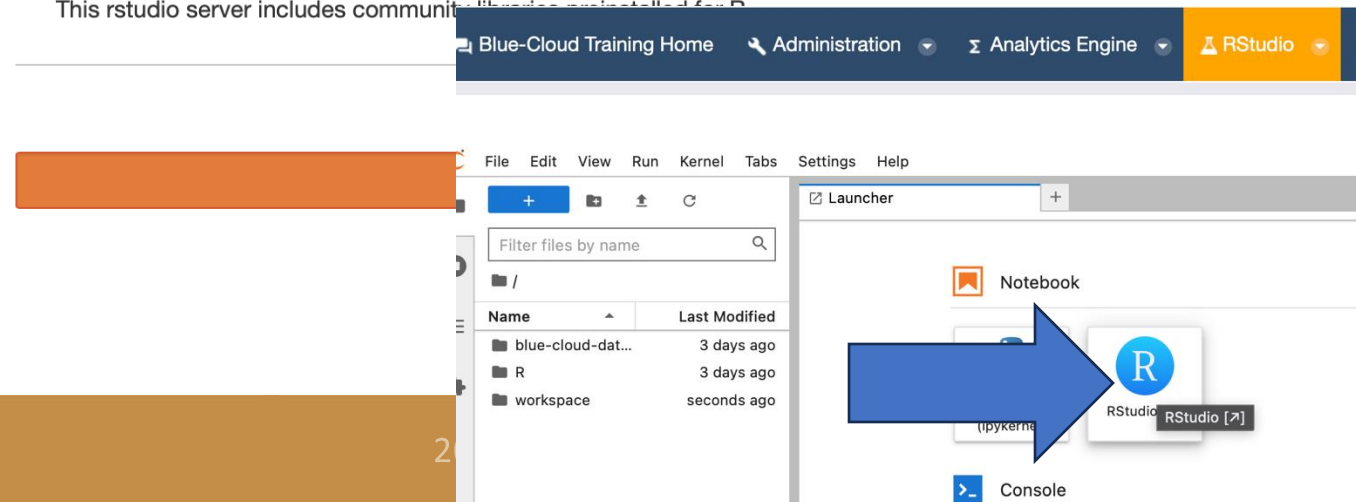
Server Options

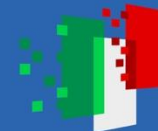
- **RStudio v4 Large - 8 Cores / 32G RAM**

This rstudio server includes community libraries preinstalled for R

- **RStudio v4 Standard - 4 Cores / 8G RAM**

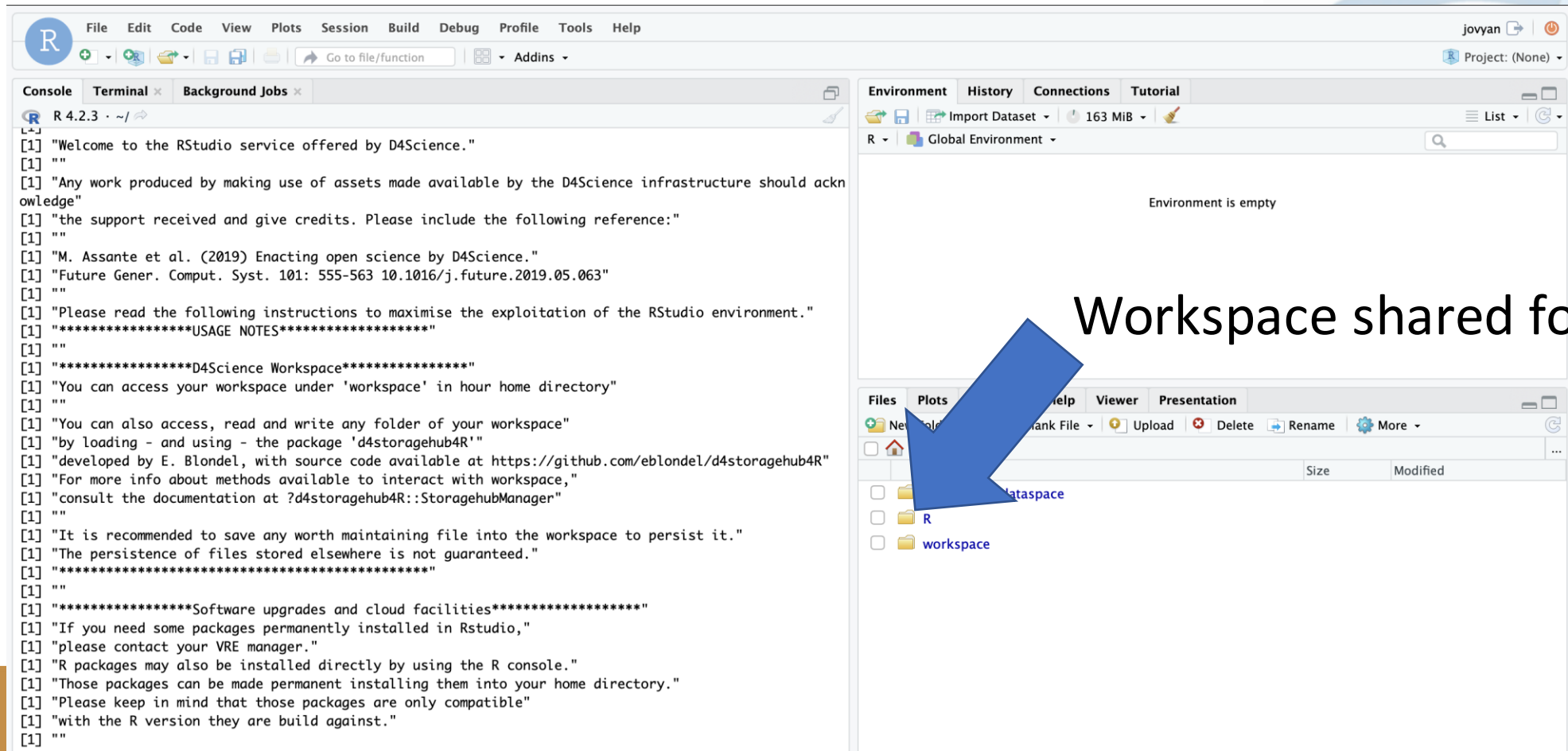
This rstudio server includes community libraries preinstalled for R





FOSSR VLab – Rstudio 4+

RStudio is an integrated development environment (IDE) for R, a programming language used for statistical computing and graphics





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Analytics Engine – Cloud Computing Platform



Analytics Engine (CCP)

Run your Methods/Algorithms on the Cloud [Learn more](#)

Methods

Search

Uncategorised

Image Classifier

Geospatial Processing

Archaeological_Text_Processing

Ariadne English Archaeology Named Entity Recognizer 1.0.0 Marco Lettere

Identifies terms and phrases in English for analysing archaeological text. The method delivers named entities of archaeological context, physical object, material, time appellation and structure, linked to concept labels of the National Cultural Heritage Thesauri (UK). This method was supplied by the Ariadne Infrastructure that integrates archaeological research data across Europe - for full details see <https://cloud.gate.ac.uk/shopfront/displayItem/archaeology-ner-en>

gatecloud

D4Science development Infrastructure

D4Science production Infrastructure

Ariadne English Dendrochronology Entity

Method execution form

Advanced WordCloud

[Clone of] word cloud generator. rif https://github.com/amueller/word_cloud

Inputs

* Runtime

The image of the runtime to use for method execution. This depends on the infrastructure specific protocol for interacting with registries.

python:3.9.19

* file

file of words to build the word cloud

Sfoglia... Nessun file selezionato.

* Image width

output image width

600

* height

output image height

400

blacklist

specify file of stopwords (containing one word per line) to remove from the

Execution Monitor

Search

Live executions Archived executions

Image Classifier

1.0.2 running

Accepted 9/10/2024 @ 18:44:47.

Last update 9/10/2024 @ 18:46:01: Deploying and executing on 'D4Science production Infrastructure'.

D4Science production Infrastructure

nubisware/simpleimageclassifier:latest

```
create-entrypoint ... ok. Initialization completed.
Starting deployment...
Ensuring absence of stack ... ok
Ensuring absence of tmp folder ... ok
Create tmp folder ... ok
Create env ... ok
Create compose file ... ok
Create entrypoint ... ok. Initialization completed.
Starting deployment...
Stack deployment ... ok. Waiting for termination...
Stack terminated. Checking outcome ...
Stack terminated.
```

Generate code for Python 3

Direct link



CCP main features

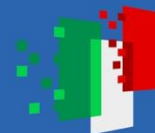
Per-method Web UI and REST API access
via Standard (OGC API – Processes)

Method import support via a dedicated tool supporting
any prog. language

“out-of-the-box” methods **as-a-Service** and automatic
code generation for Python, R, Julia, IPy notebooks

Provenance management

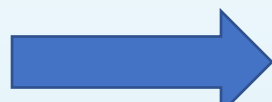




*Method:
Script, Algorithm
Software*



Importing phase



METHOD
EDITOR

Resulting Web UI & Web API

SimpleImageClassifier 1.0.1 Marco Lettore

A simple image classifier with parametrizable url to input picture compatible with the D4Science infrastructure

Inputs

* Runtime ?
rubiware/simpleimageclassifier:latest

Annotations for execution ?

* Input picture ?
https://as1.ftcdn.net/v2/jpg/00/85/32/68/1000_F_85326806_k3nKFIDnL7BKZZpgpIil

Outputs

☒ Input image ☒ Output image

Execute

Generate code for: Python 3

Execution Monitor

Search

SimpleImageClassifier

1.0.1 running

Accepted 05/03/2024 @ 13:54:48.

Last update 05/03/2024 @ 13:58:33: Execution completed: Initialization completed

D4Science production Infrastructure rubiware/simpleimageclassifier:latest

```
__init__.py
simpleimageclassifier
main.py
simpleimageclassifier
@132n[03/05 12:58:06 detection2]: @0Arguments:
Namespace(confidence_threshold=0.2,
config_file='/usr/local/lib/python3.8/dist-
packages/simpleimageclassifier/configs/COCO-
InstanceSegmentation/mask_rcnn_R_50_FPN_3x-vgan1', input=
'/ccp_data/output/canegatto.jpg'), opts=['MODEL.DEVICE', 'cpu',
'MODEL.WEIGHTS', 'detection2//COCO-
InstanceSegmentation/mask_rcnn_R_50_FPN_3x/137849600/model_final_f10217.p
```

outputs/output.zip

Generate code for: Python 3

1.0.1 running

Accepted 01/03/2024 @ 15:19:26.

Last update 01/03/2024 @ 15:22:33: Execution completed: Initialization completed

METHOD EXECUTIONS

CCP, Methods and Method Executions in the Cloud Storage (Workspace)

Web UI / Web API

SimpleImageClassifier 1.0.1 Marco Lettore

A simple image classifier with parametrizable url to input picture compatible with the D4Science infrastructure

Inputs

* Runtime ?

nubisware/simpleimageclassifier:latest

Annotations for execution ?

Annotations for execution

* Input picture ?

https://as1.ftcdn.net/v2/jpg/00/85/32/68/1000_F_85326806_k3nKFdNtL7BKZZpgpIil

Outputs

☒ Input image ☒ Output image

Execute

Generate code for:

Python 3

Execution Monitor

Search

SimpleImageClassifier

1.0.1 running

Accepted 05/03/2024 @ 13:54:48.

Last update 05/03/2024 @ 13:58:33: Execution completed: Initialization completed

D4Science production infrastructure nubisware/simpleimageclassifier:latest

```

_init__py
simpleimageclassifier
_main__py
simpleimageclassifier
@132a[03/05 12:58:06 detection2]: @1[Arguments:
namespace(confidence_threshold=0.5,
config_files=[/usr/local/lib/python3.8/dist-packages/simpleimageclassifier/configs/COCO-
InstanceSegmentation/mask_rcnn_50_FPN_3x.yaml], input=
'/ccp_data/output/camegatto.jpg'], opts=[MODEL.DEVICE, 'cpu',
'MODEL.WEIGHTS, 'detection2://COCO-
InstanceSegmentation/mask_rcnn_50_FPN_3x/137849600/model_final_f18217.p
outputs/output.zip

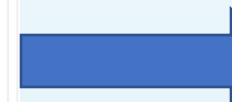
```

Generate code for: Python 3

1.0.1 running

Accepted 01/03/2024 @ 15:19:26.

Last update 01/03/2024 @ 15:22:33: Execution completed: Initialization completed



Workspace > CCP > executions > SimpleImageClassifier_1.0.1_2024-03-26T07-56_f07872aa-b783-4b4e-8512-95545

Andrea's workspace

- VRE Folders
- _shared attachments
- _uploaded_forms
- CCP
 - executions
 - SimpleImageClassifier_1.0.1_2024-03-26T07-56_f07872aa-b783-4b4e-8512-95545
- DataMiner
- DCF-RDB-RECOFI-andrea.rossi
- My Methods
- Notebooks
- OpenvinoCourse

Name	Owner	Type
ccp-entrypoint.sh	Andrea Rossi	application/x-sh
ccpenv	Andrea Rossi	text/plain
method.yaml	Andrea Rossi	text/x-yaml
output	Andrea Rossi	Folder
stderr.0flq2hacvtxu.txt	Andrea Rossi	text/plain
stdout.0flq2hacvtxu.txt	Andrea Rossi	text/plain

METHOD EXECUTIONS



Launch Method Execs programmatically, automatic code generation

The screenshot shows the SoBigData Lab Method Development interface. The left sidebar displays a file explorer for the project 'sobigdata-dataspace / GRETEL /'. The main area shows a code editor with a Python script named 'main.py'. The code is as follows:

```
1 import os
2 import torch
3 #torch.manual_seed(5)#3,5
4 import random
5 #random.seed(0)
6 import numpy as np
7 #np.random.seed(0)
8
9 '''os.environ["OMP_NUM_THREADS"] = "4" # export OMP_NUM_THREADS=1
10 os.environ["OPENBLAS_NUM_THREADS"] = "4" # export OPENBLAS_NUM_THREADS=1
11 os.environ["MKL_NUM_THREADS"] = "4" # export MKL_NUM_THREADS=1
12 os.environ["VECLIB_MAXIMUM_THREADS"] = "4" # export VECLIB_MAXIMUM_THREADS=1
13 os.environ["NUMEXPR_NUM_THREADS"] = "4" # export NUMEXPR_NUM_THREADS=1'''
14
15 from src.evaluation.evaluator_manager import EvaluatorManager
16 from src.evaluation.evaluator_manager_do import EvaluatorManager as PairedEvaluatorManager
17
18 from src.utils.context import Context
19 import sys
20
21 if __name__ == "__main__":
22     print(f"Generating context for: {sys.argv[1]}")
23     context = Context.get_context(sys.argv[1])
24     context.run_number = int(sys.argv[2]) if len(sys.argv) == 3 else -1
25
26     '''if torch.backends.mps.is_available():
27         context.logger.info(f"MP5 support founded switch to torch.set_default_dtype(torch.
28         context.logger.info(f"Clean the cache if torch.float64 where used before")
29         torch.set_default_dtype(torch.float32)'''
30
31     context.logger.info(f"Executing: {context.config_file} Run: {context.run_number}")
32     context.logger.info(
33         "Creating the evaluation manager..."
```

The screenshot shows the SimpleImageClassifier method execution interface. It includes a section for 'Inputs' with a 'Runtime' field set to 'nubisware/simpleimageclassifier:latest'. There is a section for 'Annotations for execution' and a section for 'Input picture' with a URL. The 'Outputs' section shows 'Input image' and 'Output image' checkboxes. A large blue arrow points from the 'main.py' code editor to the 'Input picture' field.

The screenshot shows the Execution Monitor for the SimpleImageClassifier method. It displays the execution status as 'running' and 'Accepted 05/03/2024 @ 13:54:48'. The last update is '05/03/2024 @ 13:58:33: Execution completed: Initialization completed'. The output section shows the generated code for Python 3, which is a shell script for running the method.

Automatic
code generation:

- ✓ Python 3
- R
- Jupyter Python3
- Julia 1.9.0
- Bash (curl)
- Bash (wget)
- Galaxy CCP request (preview)
- Galaxy tool (preview)

METHOD
EXECUTIONS



- Provenance plays an important role in Data Science;
 - Experiments are often developed iteratively involving multiple executions with different versions of data sources, accessing multiple applications and infrastructure services;
- CCP adopts the ***the PROV Ontology (PROV-O)*** expresses the PROV Data Model using the OWL2 Web Ontology Language (OWL2).

“Provenance is information about entities, activities, and people involved in producing a piece of data or thing, which can be used to form assessments about its quality, reliability or trustworthiness.”

W3C Recommendation <https://www.w3.org/TR/prov-dm/>

```

1 <prov:document
2   xmlns:prov="http://www.w3.org/ns/prov#"
3   xmlns:d4s="http://d4science.org/#"
4   xmlns:xsd="http://www.w3.org/2001/XMLSchema"
5   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
6 <prov:activity id="activity-f07872aa-b783-4b4e-8512-95545aec7a94">
7   <prov:startTime>2024-03-26T07:53:17.376Z</prov:startTime>
8   <prov:endTime>2024-03-26T07:56:03.306Z</prov:endTime>
9   <prov:type xsi:type="xsd:QName">d4s:computation</prov:type>
10  <prov:softwareAgent prov:id="d4s:sobigdata.d4science.org"/>
11  <prov:person prov:id="d4s:andrea.rossi"/>
12  <prov:entity prov:id="d4s:operator_name">
13    <prov:value xsi:type="xsd:string">SimpleImageClassifier</prov:value>
14  </prov:entity>
15  <prov:entity prov:id="d4s:operator_version">
16    <prov:value xsi:type="xsd:string">1.0.1</prov:value>
17  </prov:entity>
18  <prov:entity prov:id="d4s:operator_description">
19    <prov:value xsi:type="xsd:string">A simple image classifier with parametrizable url to input pi
20  </prov:entity>
21  <prov:entity prov:id="d4s:VRE">

```




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LIVE DEMO TIME





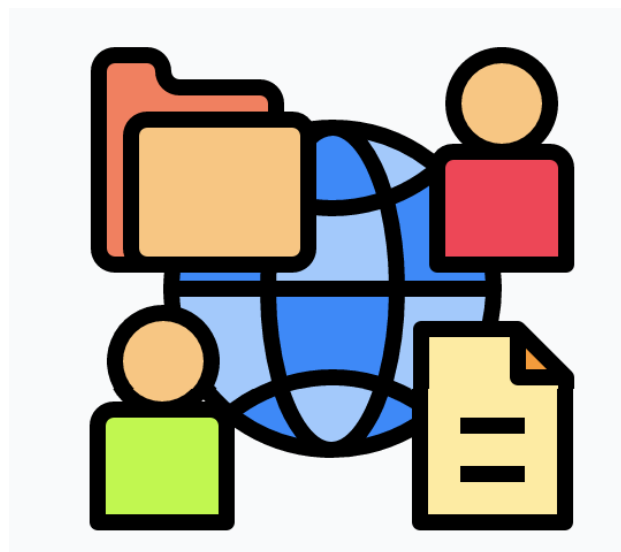
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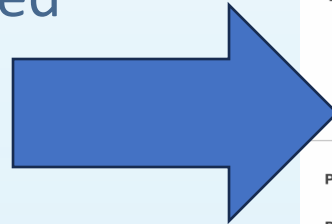
FOSSR VRE promotes technologies enabling the
sharing of datasets and methods

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- Publishing any research product:
 - Community-defined type-specific metadata (metadata profiles)
- ... making it **FAIR**
 - human- and machine-based exploitation



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