OPEN REPOSITORIES 2020

DOI 10.15161/oar.it/23688

The Reproducibility and Reusability Platform

R. Barbera^[1,2], R. Bruno^[2], M. Fargetta^[2], R. Rotondo^[2], A. Anagnostou^[3], S. J. E. Taylor^[3]

[1] Department of Physics and Astronomy "E. Majorana" of the University of Catania - Italy, [2] Italian National Institute of Nuclear Physics, Division of Catania - Italy, [3] Brunel University London - United Kingdom

Motivations and overview

For Open Science to become a common practice, its enabling technologies must demonstrate to be useful and easy to use. Building and executing software on distributed computing infrastructures (DCIs), with input data related to Open Access publications and coming from FAIR repositories, should hence be as easy as surfing the web. The Reproducibility and Reusability Platform (**RRP**) consists of several interconnected components addressing this.

The <u>INFN Open Access Repository</u> (**OAR**) is based on <u>Invenio</u> and on an enhanced version of the code of <u>Zenodo</u>. It exploits the concept of "communities", which is central in the Zenodo architecture.

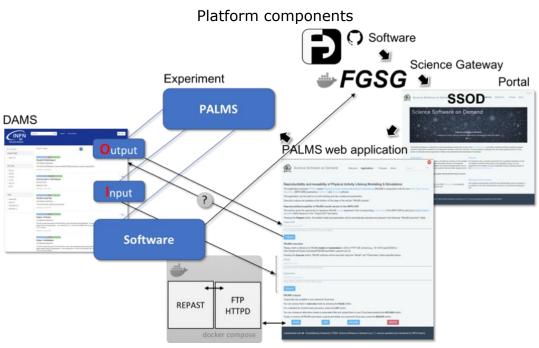
For the RRP, output and input datasets together with the necessary software are published with a registered DOI. Relationships among DOIs allow to reuse or reproduce the experiment results.

Experiment

Physical Activity Lifelong Modelling & Simulations (**PALMS**) is an <u>agent-based</u> simulation application that predicts the lifelong physical activity behaviour of a population considering individual characteristics and their effect on physical activity over time. The model produces individual and aggregated quantitative outputs for quality of life and health conditions related costs.

FGSG + SSOD

The <u>Future Gateway Science Gateway</u> (**FGSG**) is a virtualised environment capable to host one or more Science Gateways exploiting the capabitilies of the <u>FutureGateway Framework</u>. The <u>Science Software on Demand</u> (**SSOD**) is a science gateway running on top of the FGSG infrastructure.



INFN Open Access Repository

<u>INFN</u> adheres to the <u>PlanS</u> initiative since 2018 and the <u>INFN Open Access Repository</u> has born as a demonstrative platform to percept the benefits of Open Access in Science.

DOI 10.15161/oar.it/23572

The repository is open for testing by all INFN staff, associated researchers and people from other organisations are free to use it.

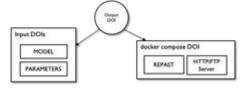


PALMS related artifacts (*papers, reports, datasets, etc.*) are stored in the repository and each content is tagged with a <u>DataCite DOI</u> ensuring that all research outputs are citable, discoverable and, more importantly, linkable to each other to allow complete reproducibility and reusability.



The repository is also integrated with <u>GitHub</u> source code repository so that, input and output datasets together with the necessary software are accessible for reproducibility or using alternative input dataset obtain new results for reusability.

The key element in the repository for the RRP platform is the possibility to establish relationships among registered DOIs.

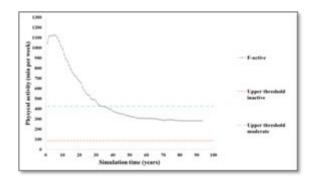


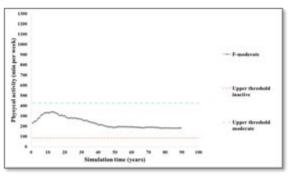
Physical Activity Lifelong Modeling System

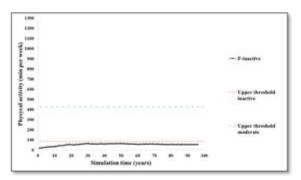
PALMS is a micro-simulation that predicts the lifelong physical activity behaviour of a population taking into account individual characteristics and their effect on physical activity over time. The model produces individual and aggregated quantitative outputs for quality of life and health conditions related costs.

The simulation software uses <u>REPAST</u> an open source agent-based modeling. For it a specific <u>docker-hub</u> <u>image</u> exists for PALMS executions. Each run requires two inputs, a model file for REPAST and a parameters' file. Both elements are registered into the INFN Open Access repository.

Graphs below represent the minutes spent for physical activity over time of three different kind of female profiles: Active, Moderate and Inactive.







The FutureGateway Framework

The **FutureGateway** is an INFN <u>software project</u> aiming to to build reliable and secure <u>Science Gateways</u>.

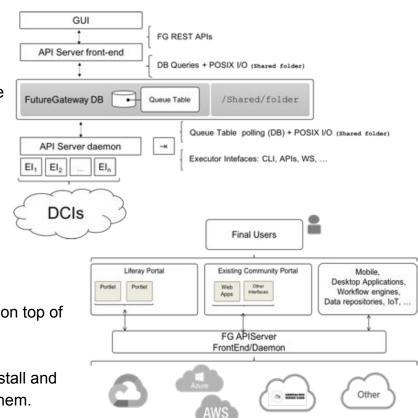
Science Gateways are today one of the most satisfying answers to execute software on top of distributed computing infrastructures by wide communities. This kind of platforms are normally requiring a non common set of experience and technical skills, often unavailable inside communities such as: Biomedicine, Chemistry, ...

FG is a mature product essentially providing a set of RESTful APIs to interact with one or more DCIs using a pluggable set of components called 'Executor Interfaces'.

The FG has three components:

- An API front-end to process incoming REST APIs from GUIs
- A database + a folder belonging to a sharable file system
- A daemon polling a queue table responsible to target execution on top of DCI using the correct EI

The FG is a complete framework, providing: APIs, scripts, tools to install and manage a Science Gateway and easily develop user interfaces for them.

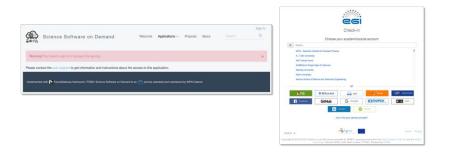


The **FGSG** and the egi.eu **SSOD** service

The FGSG consists of a platform capable to host one or more Science Gateways using the FGF and totally based on Docker containers. This solution guarantees a rapid SG development and a secure and high scalable solution thanks to the adoption of Docker compose and Docker Swarm.

One of the available Science Gateways is the: 'Science Software on Demand' (SSOD), a general purposes SG having principally disseminative scopes, developed in the context of the EOSC-hub project.

The SSOD service is integrated with the <u>EGI</u> Authentication and Authorisation Infrastructure (<u>EGI Checkin</u>). Only authorised users can access the portal and use their applications.





The **RRP** use case with **PALMS**

The SSOD has a section dedicated to the OpenScience' Reproducibility and Reusability platform that currently contains the PALMS experiment.

The application allows to retrieve the necessary inputs to reproduce a given output referenced in the form of a DOI.

- To "reproduce" a given output, its DOI is 'solved' querying the INFN Open Access Repository, then the interface places the related input file references, still in the form of DOIs, in the execution input form below.
- The execution input form accepts also HTTP based URLs to input files.
- Once the input fields have been filled, it will be possible to execute the PALMS simulation reproducing the given output.
- Generated output files will be available in a special area dedicated
 to the Science Gateway user allowing IO operations, thus opening
 the way to the "reusability".

