

# Deliverable D2.2

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Contributing partners:	STFC, NKI AVL, EMBL, MU, CSIC, CIRMMP, UU, INFN	

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## 1 Executive summary

Identifying problems and gaps in the integrative resources and assisting developers within the consortium and in the extended community to address these issues are core objectives of West-Life. The training events detailed in this report were organised during the reporting period to address developers needs, and to facilitate common understanding and dissemination of technologies.

## 2 Project objectives

With this deliverable, the project has reached or the deliverable has contributed to the following objectives:

No.	Objective	Yes	No
1	Provide analysis solutions for the different Structural Biology approaches		N
2	Provide automated pipelines to handle multi-technique datasets in an integrative manner		N
3	Provide integrated data management for single and multi-technique projects, based on existing e-infrastructure		N
4	Foster best practices, collaboration and training of end users	Y	

## 3 Detailed report on the deliverable

### 3.1 Background

The objective of developer training programme in West-Life is to provide access to expertise, information and guidelines to make their tools available via West-Life platform and/or to exploit the computational resources gathered within the project; with the vision that these events will help expand the reach and availability to users beyond the existing community of tool users. The training events detailed in this report are focussed on developers from partners of the

project as this facilitated common understanding and dissemination of technologies, technical and strategic decisions being taken during the early stages of the project.

## 3.2 Training events

Title	Organiser	Country	Audience	Number of participants	Countries represented
West-Life Hackathon	Luna (Partner 9), STFC (Partner 1)	France	West-Life Developers	10	Czech Republic, France, Italy, Netherlands, Spain, UK
DIRAC Workshop for West-Life	CIRMMP (Partner 6)	Italy	West-Life Developers	12	Czech Republic, Italy, Netherlands, Spain, UK
Hands-On course on Cloud Orchestration	MU (Partner 4)	Czech Republic	Developer community	9	Czech Republic, Germany, Greece, Netherlands, Romania, Spain, UK
Developer conference at Digital Infrastructure for Research September 2016	EGI, EUDAT, RDA, STFC (Partner 1)	Poland	eInfrastructure Developer community	271	European countries

### 3.2.1 West-Life Hackathon, July 2016, Paris

Aim: Enable developers of tools and services across West-Life to modify existing processing portals to fetch and put data to EUDAT B2DROP (<https://eudat.eu/services/b2drop>) folders via WebDAV. These will be using VirtualBox and Vagrant (<https://www.vagrantup.com/>). The hackathon will also introduce developers to the West-Life portal and the new VRE. Participants will be able to clone and create an instance of the VRE for testing. There will be introduction session for Apache Jekyll (<https://jekyllrb.com/>) and further sessions on adding documentation and services contents to the West-Life webpages.

The training event enabled SCIPION portal to use B2DROP. The session also focussed on adding support documentation for the different tools and services offered through West-Life.

These were added to docs.west-life.eu and later migrated to <http://about.west-life.eu/network/west-life/documentation>.

The event was attended by more than 10 developers from different partners of West-Life. The diversity of the participants enabled to tackle development issues of West-Life and also enabled greater foresight into the technical decisions affecting West-Life VRE. One such decision was the introduction of SSO for West-Life partner portals and tools/services. This would enable users to move freely across the different services.

### 3.2.2 DIRAC Workshop for West-Life, January 2017, Florence

Aim: Training for West-Life developers about job submission with DIRAC (<http://diracgrid.org>). DIRAC (Distributed Infrastructure with Remote Agent Control) INTERWARE is a software framework for distributed computing providing a complete solution to one (or more) user community requiring access to distributed resources. DIRAC builds a layer between the users and the resources offering a common interface to a number of heterogeneous providers, integrating them in a seamless manner, providing interoperability, at the same time as an optimised, transparent and reliable usage of the resources. For West-Life, this would enable the tools and services to provide access to grid computing resources for the users, thus assisting in quicker turnaround time for time consuming jobs.

The training workshop was conducted by Andrei Tsaregorodtsev from CNRS and was attended by 12 participants from different partners of West-Life. While few participants already knew about DIRAC and job submission through it, most were new to the concept. The workshop assisted/provided in getting access to virtual organisation infrastructure from either their National Grid Infrastructure (NGI) nodes or through a sample EGI VO. The developers then, were able to install clients and were trained in the basic understanding of different operations of DIRAC and command options to administer job submission.

### 3.2.3 Hands-On course on Cloud Orchestration April 2017, Brno

Aim: Web portals are an emerging approach to enable complex scientific applications, which also require non-trivial use of computing infrastructure, to the end users without the need to deal with technical details of the implementation. On the other hand, the disadvantage of the approach is the lack of control, impossibility to fine-tune the application, and problems with resolving contradicting requirements of different users. Many of those problems can be solved with "portal virtualization". Instead of setting up a single instance of the application portal, a detailed "recipe" to deploy the portal in the cloud environment is provided. Then a group of users with specific needs take this recipe, make minor modifications to it, and execute it using available cloud orchestration services. The result is a customized portal being set up with minimal effort, and the whole process is easily repeatable.

The workshop provided an overview of the infrastructures, tools, and techniques, which are required for efficient web portal virtualization. It was followed by a tutorial using a simple application, and a hands-on session; for the latter one the participants were requested to come

with their applications to be ported to the virtualized environment. The workshop also focused on handling users – authentication and authorisation of virtualised portals with a hands-on session adding these features to a test application. This was a joint workshop organized by MU within West-life, with participation of H2020 INDIGO DataCloud (<https://www.indigo-datacloud.eu>).

### 3.2.4 Developer conference at Digital Infrastructure for Research September 2016, Krakow

Different partners of West-Life represented the project at the elnfrastructure Developers conference at the DI4R 2016. The partners who represented West-Life were STFC, UU, INFN and Instruct. DI4R was organised by Europe's leading e-infrastructures, EGI, EUDAT, GÉANT, OpenAIRE and the Research Data Alliance (RDA) Europe and was participated by developers and service providers for three days of brainstorming and discussions. Designed with research communities in mind, the Digital Infrastructures for Research 2016 event aims to foster broader adoption of digital infrastructure services and promote user-driven innovation. This event was held at Krakow, Poland from 28<sup>th</sup> to 30<sup>th</sup> September 2016.

Apart from the interaction with developers from different tools and services and West-Life was also represented by three speaking sessions and different posters. The details of the talks are as below:

Speaker	Title
<b>Chris Morris</b>	The Life Cycle of Structural Biology Data: A discipline with a culture of sharing ( <a href="https://www.digitalinfrastructures.eu/content/life-cycle-structural-biology-data-discipline-culture-sharing">https://www.digitalinfrastructures.eu/content/life-cycle-structural-biology-data-discipline-culture-sharing</a> )
<b>Marco Verlato</b>	Federated accelerated computing platforms for EGI ( <a href="https://www.digitalinfrastructures.eu/content/federated-accelerated-computing-platforms-egi">https://www.digitalinfrastructures.eu/content/federated-accelerated-computing-platforms-egi</a> )
<b>Callum Smith</b>	Implementing AAI into existing cross-infrastructure user communities with cloud service offerings: the Instruct use case ( <a href="https://www.digitalinfrastructures.eu/content/implementing-aa-existing-cross-infrastructure-user-communities-cloud-service-offerings">https://www.digitalinfrastructures.eu/content/implementing-aa-existing-cross-infrastructure-user-communities-cloud-service-offerings</a> )

## Appendix 1: West-Life Hackathon

### Course Information

Venue: Luna Technology, 130, rue de Lourmel – 75015, Paris

Date: 19-20 July 2016

Course Organisers:

Francois Ruty, Luna, fruty@luna-technology.com, France

Chris Morris, STFC, chris.morris@stfc.ac.uk, UK

List of participants:

First Name	Last Name	Gender	Country	Institute
Nurul	Nadzirin	Female	UK	EMBL EBI/ PDBe
Jörg	Schaarschmidt	Male	NL	UU
Pablo	Conesa	Male	ES	CSIC
Laura	del Caño	Female	ES	CSIC
François	Ruty	Male	FR	Luna Technology
Matthieu	Reviere	Male	FR	Luna Technology
Chris	Morris	Male	UK	STFC
Tomas	Kulhanek	Male	UK	STFC
Marco	Verlato	Male	IT	INFN
Radim	Pesa	Male	CZ	MU

Course information and notes: [http://internal-wiki.west-life.eu/w/index.php?title=July\\_2016\\_Meeting\\_Minutes\\_\(VRE,\\_virtual\\_folder\\_and\\_AAI\)](http://internal-wiki.west-life.eu/w/index.php?title=July_2016_Meeting_Minutes_(VRE,_virtual_folder_and_AAI))

## Appendix 2: DIRAC Workshop for West-Life

### Course Information

Venue: CERM, Sesto Fiorentino, Italy

Date: 19 Jan 2017

Course Organisers:

Chris Morris, STFC, [chris.morris@stfc.ac.uk](mailto:chris.morris@stfc.ac.uk), UK

List of participants:

First Name	Last Name	Gender	Country	Institute
Jörg	Schaarschmidt	Male	NL	UU
Alexandre	Bonvin	Male	NL	UU
Mikael	Trellet	Male	NL	UU
Pablo	Conesa	Male	ES	CSIC
Laura	del Caño	Female	ES	CSIC
Chris	Morris	Male	UK	STFC
Tomas	Kulhanek	Male	UK	STFC
Marco	Verlato	Male	IT	INFN
Paolo	Andreetto	Male	IT	INFN
Radim	Pesa	Male	CZ	MU
Ales	Krenek	Male	CZ	MU
Narayanan	Krishnan	Male	UK	Instruct





## Appendix 3: Hands-On course on Cloud Orchestration

### Course Information

Venue: Institute of Computer Science, Masaryk University, Brno, Czech Republic

Date: 7 – 8 April 2017

Course Organisers:

Ales Krenek, MU, [ljocha@ics.muni.cz](mailto:ljocha@ics.muni.cz), CZ

Radim Peša, MU, [pesa@ics.muni.cz](mailto:pesa@ics.muni.cz), CZ

List of participants:

First Name	Last Name	Gender	Country	Institute
Jörg	Schaarschmidt	Male	NL	UU
Mikael	Trellet	Male	NL	UU
Ville	Uski	Male	UK	STFC
Alfonso	Perez Gonzales	Male	ES	University of Valencia
Andrea	D'Amato	Male	DE	EMBL
Umut	Oezugurel	Male	DE	EMBL
Nicoleta	Gere	Female	RO	University of Brasov
George	Georgilas	Male	GR	TEI Crete
Jiri	Ketner	Male	CZ	MU

Course material and sample applications: [http://internal-wiki.west-life.eu/w/index.php?title=Cloud\\_Orchestration\\_Training](http://internal-wiki.west-life.eu/w/index.php?title=Cloud_Orchestration_Training)

