



DOME 4.0

Deliverable D3.7 - Semantic API container component

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Coordinator:	CMCL Innovations	2023.05.30
Dissemination Level:	Public	
Due Date:	M30 (May, 2023)	
Submission Date:	31.May.2023	

Project Profile

Programme	Horizon 2020
Call	H2020-NMBP-TO-IND-2020-twostage
Topic	DT-NMBP-40-2020 Creating an open marketplace for industrial data (RIA)
Project number	953163
Acronym	DOME 4.0
Title	Digital Open Marketplace Ecosystem 4.0
Start Date	December 1 st , 2020
Duration	48 months



This document is part of a project that has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 953163. It is the property of the DOME 4.0 consortium and do not necessarily reflect the views of the European Commission.

Document History

Version	Date	Author	Remarks
v0.1	2023-05-09	Treesa Rose Joseph	Added objective, implementation sections, conclusions
v0.2	2023-05-12	Kristine Wiik	Add screenshots and update introduction
v0.3	2023-05-22	Bjørn Tore Løvfall	Executive summary and lessons learnt; process review feedback
v0.4	2023-05-30	Amit Bhave	Review and minor revisions
v0.5	2023-05-31	Kristine Wiik	Review and minor revisions

Executive Summary

This document is the accompanying document of the tools and services plugin template that can be found on the following GitHub address: <https://github.com/DOME-4-0/Tools-Services-Plugin-Template>. This template can be used as a starting point to create either tools or services that can be registered on the DOME 4.0 platform utilizing compatible data sources in a seamless fashion. We here share the details of how the tools and services will integrate with the rest of the DOME 4.0 platform. One example of how we created and integrated a plugin for an AiiDA lab instance is provided.

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1. Introduction

This document reports on the activities of Task 3.7 of the DOME 4.0 project, named "Interoperability API for Data and Services". The main outcome of this task is the actual semantic API container component that will allow different tools and services to connect to the DOME 4.0 platform. The development of this system builds upon the overall architecture of DOME 4.0 that was portrayed in deliverable D1.3. A relevant subset of this is shown in Figure 1.

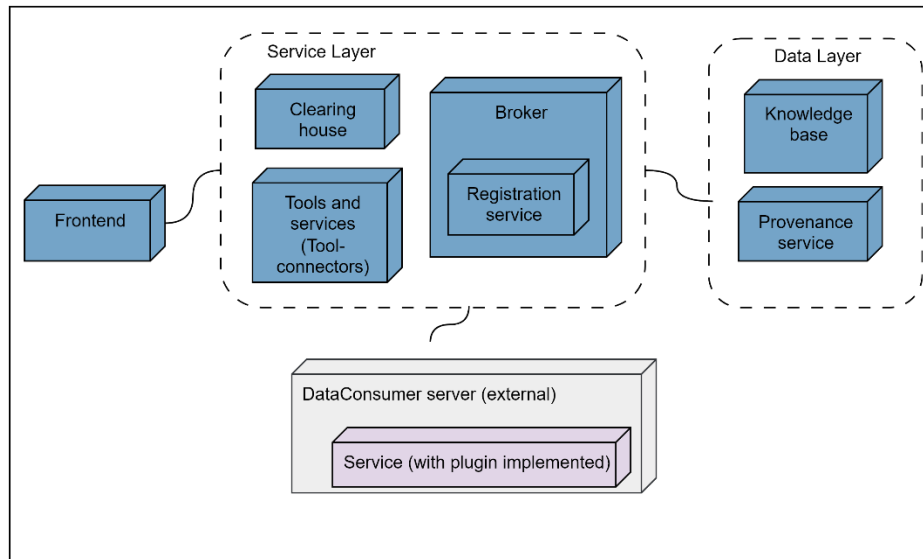


Figure 1: Components involved in the registration of the third party tools/services

1.1 Objective

It is important to ensure that the DOME 4.0 platform provides users with an available list of compatible tools and services that can be used to visualize, process, or modify the data they searched for. This ensures that users can easily identify and select the most suitable tool for their needs, without having to navigate through multiple platforms.

When a user performs a search on the DOME 4.0 platform, the system should display all available tools and services that can be used to work with the data. These tools can include visualization, analysis, data processing, or any other tools registered on the DOME 4.0 platform compatible with that data.

If a user wants to use one of the available tools or services to process or modify the data, the system should allow them easy transfer of the data to the selected tool/service/workflow.

Another requirement is that it should be easy for third parties to add new tools and services to the platform. This can be achieved by providing a reference template with the required APIs that will enable easy implementation of the connection to the platform.

2. Implementation

2.1 Registration of tools and services

To register a data consumer (which can be a tool, service, or workflow), a plugin needs to be developed to enable a seamless connection to the platform. This plugin should be developed by the service provider. A template to create this plugin can be found on GitHub: <https://github.com/DOME-4-0/Tools-Services-Plugin-Template>.

2.1.1 Data model

The data model serves as a blueprint for data integration and sharing. In this context, it helps the DOME platform facilitate the transfer of data from connectors (which retrieve data from various sources) to tools and services that require access to this data. By utilizing a standardized data model, the data can be seamlessly shared and understood by different components within the system. This is the same data model that is shared with the reference connector (T3.5), based on the semantic data exchange ontology developed in T3.1, see D3.1 for more information. This enables developers of new tools or services to take advantage of the semantics embedded in the metadata transferred.

2.1.2 Plugin Template

The plugin template has been developed using the Cookiecutter framework [1] to enable the DOME 4.0 platform to communicate with the tools and services in a uniform manner.

The plugin includes an API *'/fetch-application-output-url'* that facilitates the secure transfer of data from the data catalogue to these tools and services. This must be implemented by the service/tool provider to integrate the dataset coming from the DOME 4.0 platform with their own service. This endpoint is used by DOME to fetch the output URL (download URL or redirect URL depending on functionality) for the service/tool that the user is trying to access. The domain address and other relevant information about the tool/service are obtained by the DOME 4.0 platform when it is registered with DOME. The output URL is then used by the DOME 4.0 platform to either give the end user the modified data or launch a third-party service with the desired dataset already integrated.

To ensure the security of the platform, the plugin has been equipped with authentication and authorization callback APIs used to authenticate the tool or service being used, and APIs to enable the tool or service to check if the users trying to use the tools and services have the relevant roles and data access.

2.1.3 Registration Process

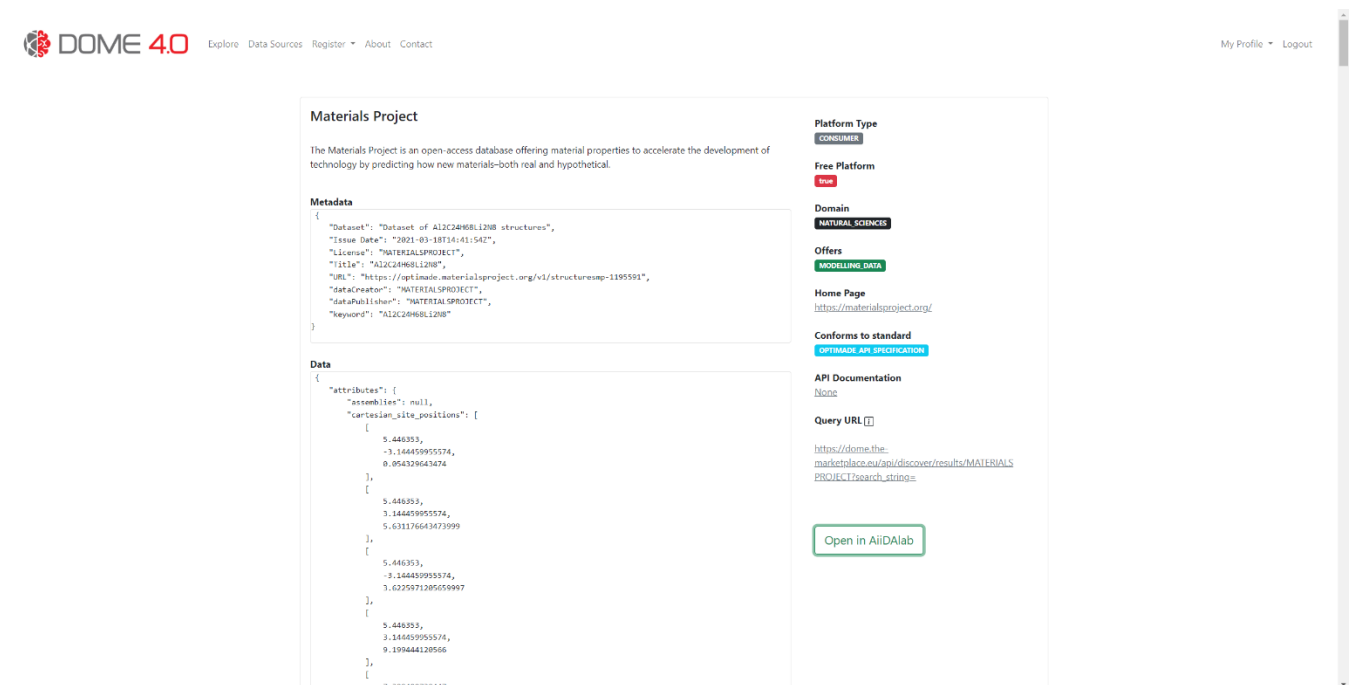
After completing the plugin development process mentioned in the previous section, third-party providers of tools and services who wish to register their service on DOME shall navigate to the registration page on the DOME 4.0 platform. The registration page guides the tools/service providers through the registration process, which involves completing a few forms and documenting key features of their service. These features include information like the type of data and format accepted as inputs, as well as the outputs provided by the service.

Based on the information given in the registration process, the semantic broker will be able to match relevant data sources with relevant tools or services, to automatically provide the user with easy access to relevant tools and services.

The User interface and the specific APIs to register the tools and services are not yet available and will be developed as part of T1.4 and T3.3 respectively, but to demonstrate how this will be once all is in place, we currently have registered the AiiDALab instance with a few hardcoded details to ensure and demonstrate that the communication with the tool works.

2.1.4 Example

An example of a registered tool/service is the AiiDALab, which is a web platform that enables computational scientists to package scientific workflows and computational environments and share them with their collaborators and peers. AiiDALab is now registered with the DOME platform. When data that is compatible with the AiiDALab is accessed, the user is presented with an option to open it in AiiDALab (Figure 2). Upon selecting this option, the user is navigated to the deployed, registered AiiDALab page, as illustrated in Figure 3 below. Under the hood, the DOME platform sends the URL of the search result that the user has chosen to visualise, to the AiiDALab's endpoint.



The screenshot shows the DOME 4.0 interface. At the top, there is a navigation bar with the DOME 4.0 logo, links for 'Explore', 'Data Sources', 'Register', 'About', and 'Contact', and a user profile section with 'My Profile' and 'Logout'.

The main content area displays a data instance for 'Materials Project'. The title is 'Materials Project' and the description is 'The Materials Project is an open-access database offering material properties to accelerate the development of technology by predicting how new materials—both real and hypothetical.'.

The 'Metadata' section shows a JSON object with the following fields:

```

{
  "Dataset": "Dataset of A12C24H6BLI2NB structures",
  "Issue Date": "2021-03-18T14:41:54Z",
  "License": "MATERIALSPROJECT",
  "Title": "A12C24H6BLI2NB",
  "URL": "https://optlmade.materialsproject.org/v1/structuremp-1195591",
  "DataCreator": "MATERIALSPROJECT",
  "DataPublisher": "MATERIALSPROJECT",
  "keyword": "A12C24H6BLI2NB"
}

```

The 'Data' section shows a JSON object with the following fields:

```

{
  "attributes": {
    "submission": null,
    "cartesian_site_positions": [
      [
        5.44833,
        -3.14445995574,
        0.054329643674
      ],
      [
        5.44833,
        3.14445995574,
        5.631176643673999
      ],
      [
        5.44833,
        -3.02445995574,
        3.622571285559997
      ],
      [
        5.44833,
        3.14445995574,
        9.199444128566
      ],
      [
        7.199609791647
      ]
    ]
  }
}

```

On the right side, there is a 'Platform Type' section with 'CONSUMER' selected. Below it, 'Free Platform' is 'True', 'Domain' is 'NATURAL SCIENCES', 'Offers' is 'MODELLING DATA', 'Home Page' is 'https://materialsproject.org/', 'Conforms to standard' is 'OPTIMADE API SPECIFICATION', 'API Documentation' is 'None', and 'Query URL' is 'https://dome-the-marketplace.eu/api/discover/results/MATERIALSPROJECT?search_string='. At the bottom right, there is a green button labeled 'Open in AiiDALab'.

Figure 2: Page showing a data instance and its metadata. The "Open in AiiDALab" button on the right shows that the data is compatible with AiiDALab.

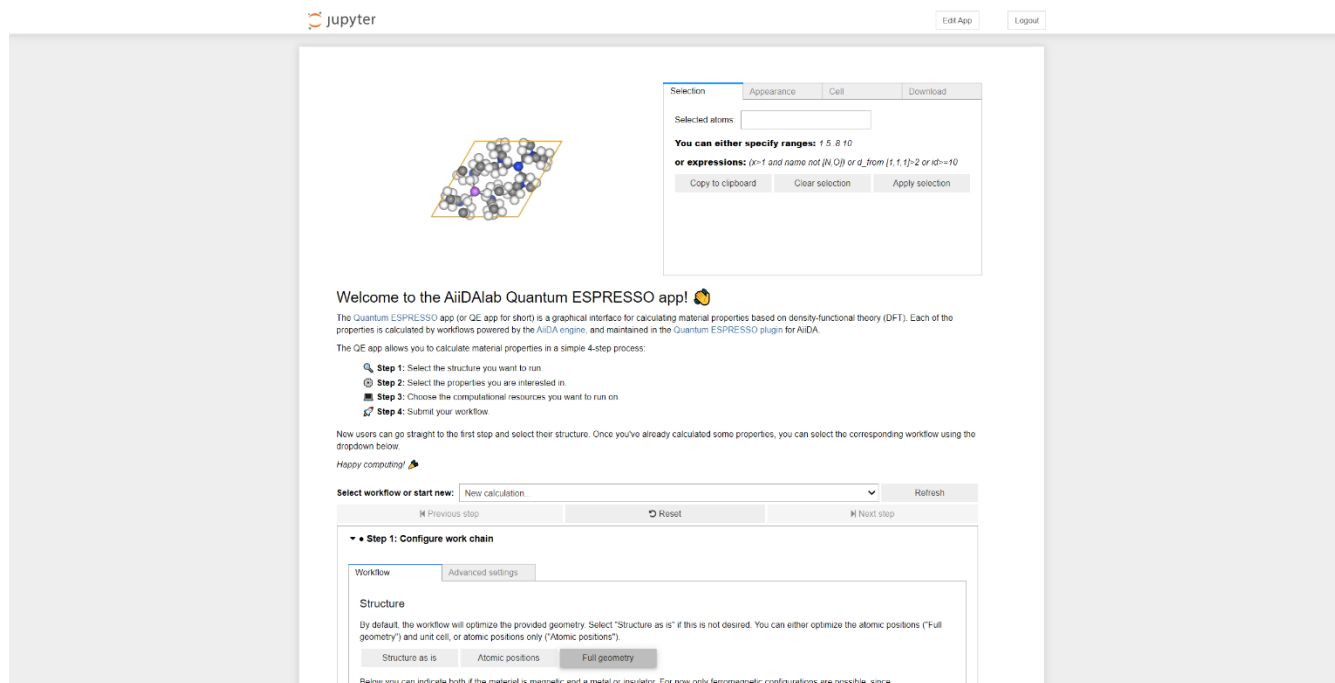


Figure 3: The AiiDALab Quantum ESPRESSO app, here visualizing the data instance, opened by clicking the "Open in AiiDALab" button in Figure 2.

2.2 Connecting to the registered tools/services

When a user searches for a particular datum, the knowledge base retrieves a list of registered compatible tools/services/workflows that can be used with the datum. This list is based on the type and format of the data/data provider.

When the user selects a tool or service from the list, the tool-connector module enables the connection between the chosen tool or service and the data. This module acts as a bridge between the tool/service and the data and handles the transfer of data to the tool or service as shown in Figure 4.

The tool-connector module works by utilizing integration points or APIs provided by the various tools and services. These integration points allow transfer of data to the tools and services as shown in Figure 5.

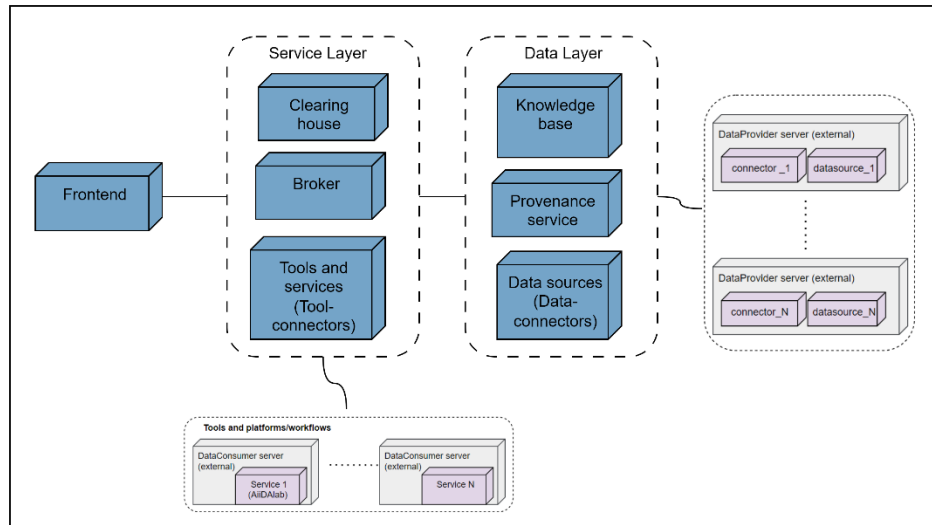


Figure 4: Components of involved in the flow of data to the consumer services (Tools, services, and workflows)

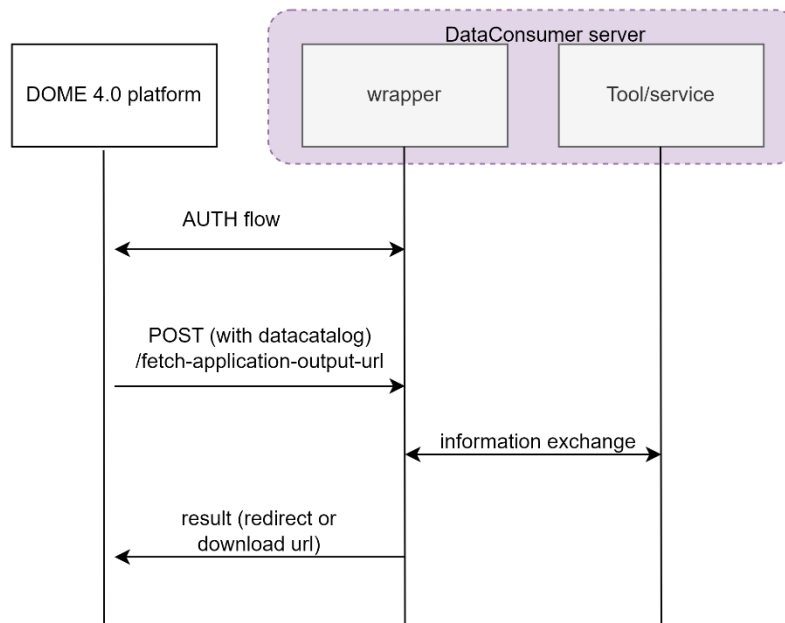


Figure 5: Interaction between DOME 4.0 platform, wrapper and consumer services (Tools, services, and workflows)

3. Conclusions / Next steps

As part of this task, we have developed a plugin template that helps communication between the DOME 4.0 platform and the third-party tools and services that need to be registered. We currently have registered the AiiDALab instance with a few hardcoded details to ensure that the communication with the tool works.

Next steps:

- As part of T3.3, we further develop the registration service, which is part of the broker, to create APIs to register new tools and services.
- As part of T1.4, we develop a user interface i.e., add another consumer registration page to ease the registration process of third-party tools and services.

4. Lessons learnt

Making a template for all possible tools and services is very challenging, and to be able to capture as many tools and services as possible we decided to create a relatively generic template which utilizes the data set ontology from D3.1. Having a hard coded version of AiiDALab instance early on proved useful in developing the final template.

5. Deviations from Annex 1

In the task description, it is mentioned that the Semantic API for this task should be based on the OSP API. None of the showcases can leverage any of the benefits of using OSP. We therefore decided to implement something that is simpler and more generic. It would be possible to use the template created in this task to interface with the OSP API, should we need to do so in the future.

6. References

- [1] "Cookiecutter," 10 May 2023. [Online]. Available: <http://www.cookiecutter.io>.

7. Acknowledgement

The author(s) would like to thank the partners in the project for their valuable comments on previous drafts and for performing the review.

Project partners:

#	Type	Partner	Partner full name
1	SME	CMCL	Computational Modelling Cambridge Limited
2	Research	FHG	Fraunhofer Gesellschaft zur Förderung der Angewandten Forschung E.V.
3	Research	INTRA	Intrasoft International SA
4	University	UNIBO	Alma Mater Studiorum – Università di Bologna
5	University	EPFL	Ecole Polytechnique Federale de Lausanne
6	Research	UKRI	United Kingdom Research and Innovation
7	Large Industry	SISW	Siemens Industry Software NV
8	Large Industry	BOSCH	Robert Bosch GmbH
9	SME	UNR	Uniresearch B.V.
10	Research	SINTEF	SINTEF AS
11	SME	CNT	Cambridge Nanomaterials Technology LTD
12	University	UCL	University College London



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8. Table of Abbreviations

Abbreviation	Explanation
API	Application programming interface
URL	Uniform resource locator
UI	User interface