Assessing Quality Requirements for Onboarding Web Services to the European Open Science Cloud (EOSC): A Case Study of the Gaussian API

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Abstract

The European Open Science Cloud (EOSC) is an initiative by the European Commission to support EU science by establishing a virtual environment for publishing, hosting, and reusing research. It promotes common standards, interoperability, and best practices for sharing and utilizing data and services. The EOSC platform contributes significantly to open science and facilitates transparent and accessible knowledge sharing. The resource onboarding process to the EOSC requires compliance with the established quality criteria. This paper focuses on accessing quality criteria for successful onboarding, including a case study on the RESTful web service for fitting repulsive potentials in density-functional tight-binding with Gaussian process regression - Gaussian API. The onboarding process follows a sequential evaluation of a set of criteria. The examination of The Gaussian API integration into EOSC provides valuable insights for three main aspects: improving service quality, considering the benefits of Open Science, and addressing challenges related to the smooth onboarding process.

Keywords

EOSC, Software quality, Web service, Open science

1. Introduction

Open science can be defined as transparent and accessible knowledge that is shared and developed through collaborative networks. It is an emerging necessity of the 21st century, considering the fact that open data tools, open access platforms, open peer review methods, or public engagement activities are irreversible trends that affect scientific processes and have the potential

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to accelerate the research cycle. Because open science is a fairly new and unexplored field, we can only scratch the surface in revealing its benefits [1].

The European Open Science Cloud (EOSC) [2, 3] is a European Commission initiative from the European Union that aims at supporting EU science by establishing a virtual environment to publish, host, and re-use research such as publications, data, and software. EOSC promotes the development and adoption of common standards, interoperability frameworks, and best practices to ensure that data and services can be easily shared, discovered, and utilized. Furthermore, EOSC also emphasizes the significance of data management, security, and privacy, promoting responsible and ethical practices in handling scientific data.

The EOSC platform consists of many components, including the EOSC Portal, which is a web portal that serves as a universal access channel to the resources of EOSC. The EOSC adapts a common policy framework that enables FAIR (Findable, Accessible, Interoperable, and Reusable) data to be used and shared throughout the entire value chain for scientific, societal, and industrial purposes. Figure 1 shows the six main services of the EOSC portal, which are services, resources, use cases, providers onboarding, policy and funding opportunities.

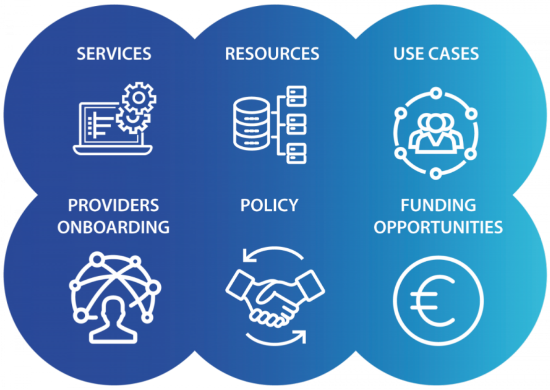

Figure 1: Services of the EOSC Portal. Source: [4].

One of the services present in the EOSC Portal is the onboarding service, which enables collaboration and knowledge sharing among different stakeholders. Through this service, any research data that is submitted must follow the onboarding process. Every submission onto the EOSC Portal goes through the process of onboarding, where it is sequentially checked in various quality criteria set by the EOSC platform, in order to be successfully registered on the EOSC Registry.

The EOSC Portal has clear goals and objectives of simplifying and centralizing access to validated research and data to researchers across Europe. This is done by connecting researchers, disciplinary infrastructures, and service providers via a platform and cultivating structured rules for contribution and collaboration. This way the EOSC portal tackles the challenge of exponential growth of scientific data, enhancing disciplinary, cross-disciplinary, and transnational research. To summarize, EOSC greatly contributes to the growing field of open science. Considering the contribution that the EOSC has brought on to the field of open science in Europe, by offering a centralized platform for validated research, we can state that it acknowledges the potential of open science and the benefit that open science brings to the research community.

The focus of this paper is to access the quality criteria for a successful onboarding process onto the EOSC platform. The Gaussian API [5] is a RESTful web service for fitting repulsive potentials in density-functional tight-binding with Gaussian process regression. Considering the fact that The Gaussian API is a web service that has been already approved and published on the EOSC, it is a perfect model for analyzing and describing the quality requirements, as well as elaborating on its successes and failures in terms of EOSC standards.

Section 2 presents the Related work in the field. Section 3 describes and elaborates on the steps and requirements of the onboarding process. The goal of this section is to be familiarized with the terms and the structure put in place by EOSC for the onboarding process, before moving on to the Case Study. Section 4 introduces the Gaussian API RESTful web service. The article then goes into an outline of the best practices and lessons learnt by integrating The Gaussian API into the EOSC platform.

2. Related work

This section provides an overview of existing research studies that describe platforms that support Open Science or/and are similar to EOCS and some research papers that describe the experience of onboarding services to EOSC.

The Australian Research Data Commons (ARDC) [6] is an Australian initiative that supports the management, sharing, and reuse of research data. It offers infrastructure, tools, and services to enable data-intensive research. ARDC shares a similarity with EOSC, in the way that this platform supports service onboarding, allowing researchers to integrate their own services into the platform and make them available to the research community.

A similar concept to EOSC in terms of resource sharing and collaboration is the cloud-based infrastructure, Galaxy Project. The Galaxy Project's public webserver is an open-source collection of bioinformatics tools, used by researchers to analyze large biomedical datasets. The works [7, 8] explore a use-case and provide a discussion on Galaxy Project's functionality.

The European Grid Infrastructure (EGI) is recognized as a key asset for the European Open Science Cloud (EOSC), particularly for the Federating Core. While EGI and EOSC are not identical platforms, they share a common focus on open science and have provided great support to international research across different scientific disciplines [9]. On its own, EGI is an independent, comprehensive, overall hardware and software infrastructure that aims to develop a grid middleware for the needs of the scientific European society, which would allow sharing of data and computational resources, as well as helping to create a more integrated and interconnected research environment in Europe and beyond.

In [10, 11], the authors provide a case-study on the topic of the EOSC Integration of the project NEANIAS. Here, the papers elaborate on their efforts to obtain a FAIR (Findable, Accessible, Interoperable, Reusable) service which is a key requirement for EOSC. In [12], the authors discuss the FAIR principles in the Astrophysics community through a service called ESCAPE. Here, the paper elaborates on ESCAPE's onboarding process, how it has been adapted to FAIR principles, and potential future steps that can be taken toward FAIR maturity.

3. Onboarding to EOSC

The onboarding process in the European Open Science Cloud (EOSC) enables organizations to become service providers, contributing to the advancement of scientific knowledge [13, 14]. This process consists of the request submission, information gathering, validation, and publication stages, each incorporating quality assurance measures to ensure the integrity and reliability of the services offered.

3.1. EOSC onboarding process

This subsection provides a concise overview of the EOSC onboarding process for organizations aspiring to become service providers. It emphasizes the significance of understanding the key stages involved in this process. The EOSC onboarding process is visually represented in Figure 2, providing a clear illustration of the steps involved. These phases and quality assurance techniques, when combined, lay a solid basis for easy integration and assure high-quality services throughout the EOSC ecosystem.

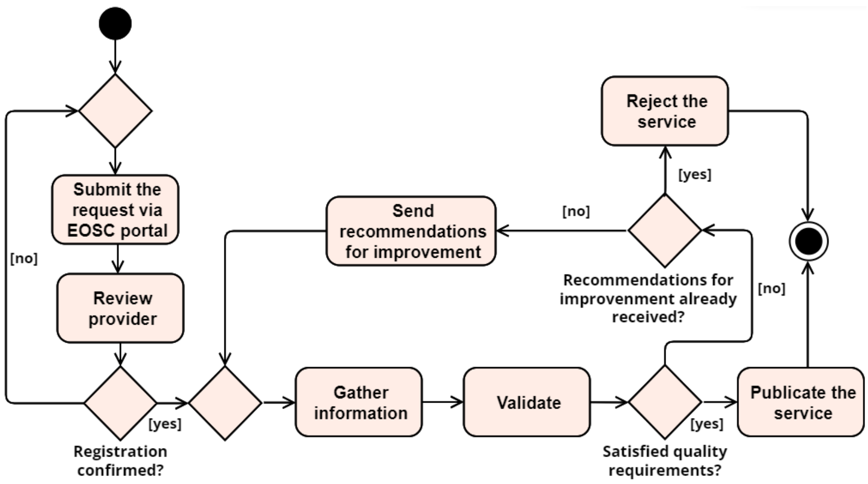

Figure 2: Activity diagram of the EOSC onboarding process. Source: author's contribution.

Submit the request via EOSC Portal.
Organizations can start the onboarding procedure by requesting to become service providers inside the European Open Science Cloud (EOSC) by submitting a request via the EOSC Portal and employing a specific form submission procedure. The details included in the request act as an internal ticket, making it easier to trace and handle the submission. The possibility to join the EOSC ecosystem is available to the organization once it meets the prerequisites for participation. Organizations may get several benefits by joining the EOSC ecosystem, including the growth of their user base, access to insightful data and feedback, active participation in EOSC policy formulation, and contribution to the platform's ongoing improvement.

Information gathering.
During the information-gathering stage of the onboarding process, service providers are

required to complete a service description template, providing comprehensive details about their offerings. The template includes mandatory fields such as service name, service URL, service endpoint, service description, service tagline, and service logo. Additional information fields may be provided for supplementary details. The service's maturity level is also evaluated using TRL criteria to assess its development stage and user validation. By completing the template, service providers contribute essential information for the evaluation and validation of their services within the EOSC ecosystem.

Validation.

The details supplied in the Service Description template are used as the basis for a thorough validation and assessment process that service providers go through. This procedure comprises thorough content checking and the delivery of clarification-related comments. The evaluation addresses a number of crucial factors to guarantee the accuracy, dependability, and compliance of the services provided. After the data has been verified, it is added to the EOSC Service Portfolio, which serves as a repository for services that have been authorized and verified within the EOSC ecosystem. The EOSC user community will only have access to services that adhere to the necessary criteria thanks to this extensive validation and inclusion procedure.

Publication.

The publishing process of a service begins by adding the completed service description template to the EOSC Marketplace on the EOSC Portal. Subsequently, the Marketplace platform requests that service providers create an account. Service providers have the opportunity to review and modify their draft entries. Upon publication, these services become accessible to users, facilitating the progress of scientific knowledge within the EOSC ecosystem.

3.2. EOSC quality requiements

This section stresses the critical role of quality assurance in the onboarding process, emphasizing the precise requirements established by various sources that enterprises must meet at each stage.

Service providers undergo a comprehensive evaluation process based on the [15]. Alignment with EOSC activities is a crucial requirement, ensuring that the service actively contributes to the advancement of Open Science and provides value to users. Service type verification categorizes services into online services and 'human' services, excluding direct onboarding of plain datasets and software artifacts. The evaluation also assesses the service's maturity level, determined by its Technology Readiness Level (TRL). Assessing the Technology Readiness Level (TRL) [16], ranging from 1 to 9, ensures the necessary technological maturity and validation for easy integration into the European Open Science Cloud (EOSC) ecosystem. Meeting a minimum requirement of TRL 7 indicates successful usage by early adopter scientists. The details about the required TRL levels and their corresponding characteristics can be found in Table 1 [17].

The EOSC portal [2] specifies additional prerequisites that providers must fulfill to be listed on the platform. Firstly, accessibility is emphasized, aiming to extend the service's availability to users beyond its original community and enabling a broader range of users to benefit from its functionalities.

Providers are expected to describe their service using a standardized template that highlights its value proposition and functional capabilities. Completing all mandatory fields in the service

Table 1
Technology Readiness Level

TRL Scale	Description
TRL 7	A critical stage in technology development where a system prototype is demonstrated in an operational environment. The software is stable and reliable, having undergone validation by target users. Documentation includes comprehensive functionality requirements and plans to handle system load during production.
TRL 8	The system is complete and qualified for practical use. Real users rely on the service for their work. To ensure adoption and user satisfaction, the service is supported by comprehensive end-user documentation, an acceptable use policy, and service-level agreements (SLAs). Incident response and problem management mechanisms are established to promptly address issues and provide effective user support.
TRL 9	The technology reaches its highest level of maturity, representing an actual system that has proven its worth in an operational environment. It has fulfilled all the requirements of TRL 8 and has been successfully serving users for a minimum duration of one year. Feedback from customers is actively collected and documented, contributing to ongoing improvements. Additionally, the service must demonstrate quntitative outputs resulting from its usage.

description template is crucial to provide comprehensive insights into the service's features, functionalities, and benefits.

Operational readiness, with at least one instance of the service required to be operational in a production environment, actively serving the user community. Additionally, adherence to the FAIR principles for research data is emphasized, ensuring that data is easily findable, accessible, interoperable, and reusable for maximum impact. Thorough documentation, including release notes and instructional materials, is essential to keep users informed about updates, changes, and usage guidelines.

Lastly, providers must establish effective support and feedback channels, such as helpdesks, to assist users, address issues, and gather valuable feedback.

To ensure smooth integration and optimal user experience, providers are required to register their services in an EOSC-compliant or compatible catalogue for global visibility.

Interoperability and simplified service discovery are facilitated through machine-readable service descriptions with common and persistent identification methods. Portability of data and services is encouraged whenever possible. Clear and transparent Terms of Use, encompassing access policies and data handling guidelines, provide users with a comprehensive understanding of the services. Furthermore, providers have the flexibility to customize services based on user-specific needs. Effective integration within the EOSC ecosystem relies on describing accessibility and interoperability measures such as metadata practices, APIs, and protocols. Adhering to quality guidelines, including Technology Readiness Level assessments and certifications, promotes reliability and performance [13].

Non-compliance with the requirements during the Portal Onboarding process can result in various actions, including requesting amendments to the resource description, participation in information/training sessions, or rejection of the resource. Failure to address the deficiencies or update the resource may lead to rejection and potential suspension of the provider from the platform [18].

4. Case study: Onboarding the Gaussian API

4.1. Gaussian API service

The Gaussian API [5] is a RESTful web service intended for fitting repulsive potentials in density functional tight-binding with Gaussian process regression. DFTB is comprised of a sequence of models obtained through a Taylor series expansion of the total energy within the KS-DFT framework.[19] The source code is based on the idea and code presented in [20], but it is made as REST API, the whole process is automated and additional code adaptations and modifications are made. The primary reason for making it a RESTful API is to enable integration and interoperability between different software systems.

Due to its popularity in computational chemistry, physics, and other sciences, Gaussian regression (GPR) combined with molecular dynamics simulations has shown to be useful for the prediction of various molecular and materials' properties and functionalities. Additionally, these approaches can be used to tune the parametrization in approximate computational techniques in a bias-free way. A good and useful approximate technique is the Density functional tight binding method (DFTB), which aims to approximate the Density functional theory approach while giving comparable accuracy at only a fraction of its computational time. Moreover, DFT simulations that have been unfeasible in computational time can now be implemented using DFTB.

A great advantage of DFTB is that it allows for direct access to electronic properties. However, the aforementioned advantages come at the expense of the introduction of empirical parameters, reducing their transferability. The electronic structure component of DFTB enables the creation of workflows for transferable parametrization. However, dealing with the repulsive potential (Vrep) in this context poses challenges. A recent study [20] introduced an approach to fit the Vrep using the GPR method. DFT-DFTB energy or force residues can serve as training data for this purpose. The approach described in the reference allows for simultaneous application to multiple elements, like C, H, and O, in molecules with diverse organic components. With some adjustments, this approach can be easily adapted to other computational tasks. Because of the complexity of DFTB repulsive potentials, there exists no simple functional form. Thus, fitting the Vrep to DFT poses the greatest challenge in the parametrization workflow. Consequently, the Vrep in the GPR method is represented as a linear combination of kernel functions:

$$V_{\text{rep}}(R) = \sum_{i,j \in \{X\}} \alpha_{ij} k(R, R_{ij}) \tag{1}$$

where α_{ij} represents the regression coefficients whose summation is carried over all the atomic pairs within X. The idea is to minimize the difference between the DFTB model and the DFT reference forces. This is done using a loss function with the form:

$$L = \sum_{i,j \in \{X\}} (t_{ij} - V_{\text{rep}}(R_{ij}))^2 + \sigma_n \|\alpha\|^2 \tag{2}$$

where t_{ij} represents the repulsive potential values alongside σ_n as a regularization parameter. Their main role is to provide a level of uncertainty in the calculation. Finally, the regression coefficients are calculated as follows:

$$\alpha = (K + \sigma_n I)^{-1} y \tag{3}$$

where K represents the covariance matrix for all atom pairs in X.

The usage of the API revolves around making an HTTP request to a designated endpoint. The service provides two methods, POST and GET requests. The POST method, called **GPrep**, takes in several parameters including a file from the local device that contains the relevant forces and distances. On the other hand, the **GPrepRemote** is a GET method that works similarly to the POST method, with the exception that instead of an input file it takes a public URL where a data file resides.

To invoke the API call, there is a set of necessary parameters that need to be provided as seen in Figure 3: **file** that contains the forces and the pair distances; **sigma** which is the standard deviation for the data noise; **delta**, the standard deviation of the latent function; **theta**, which symbolizes the length scale of the latent function; **beta**, the exponential damping factor which allows for a smooth decay of the function; **d**, the cutoff transition which characterizes the damping function; and **N**, the total data points.

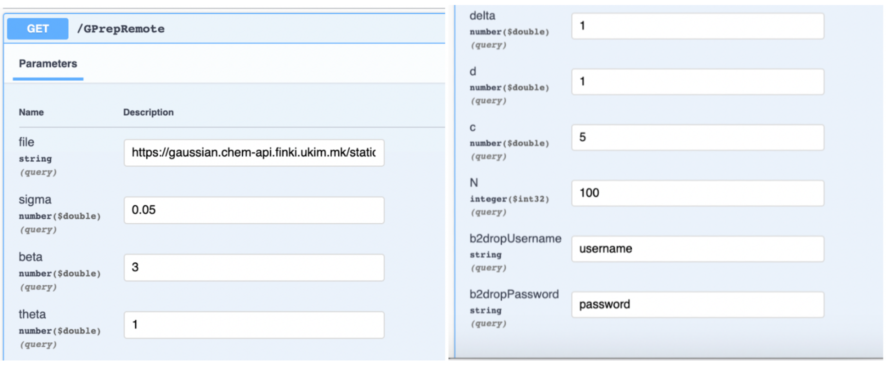

Figure 3: HTTP form for the GET method GPrepRemote. Source: author's contribution.

The API is integrated with the well-known scientific data storage service B2DROP [21], where the output Slater-Koster [22] files will be saved if the calculation is successful. To access the B2DROP service the user needs to provide their username and password as the last 2 parameters to the API call.

4.2. The onboadring story

The onboarding process of the Gaussian API service is shown in Figure 4. As a first step, the onboarding process was initiated by the NI4OS project [23] operational team by providing a dedicated form and submitting a request to the EOSC.

Upon submitting the request, relevant information regarding the service was provided using the NI4OS project service portfolio. These include service description, technology readiness level, domain, target users, access type and mode, as well as links to the user manual and user support. In order to register the service, the services portfolio management tool - AGORA [24] was used. The basic information such as the organization, name, location, and relevant background details were specified. Furthermore, the research field domain in which the service relates to aiding users in finding relevant services was selected. In addition, a logo, a description, and contact information were entered.

Then, the resource was integrated within the NI4OS pre-production environment where it was additionally validated by tools from the environment. The next step in the onboarding process was the definition of policies. These include the user policy, terms of use, access policy, and privacy policy. Additionally, a user manual describing the usage of the service was crafted. For a deeper understanding of the service usage, a training course on a dedicated training platform was published [25]. The integration with the pre-production environment included providing user support via the helpdesk system, as well as monitoring the health, status, availability, and reliability through the ARGO monitoring system [26]. The integration with the accounting system provided utilization data for different time periods.

Next, the service was uploaded to the NI4OS service catalog, and later, the resource was published in the EOSC marketplace.

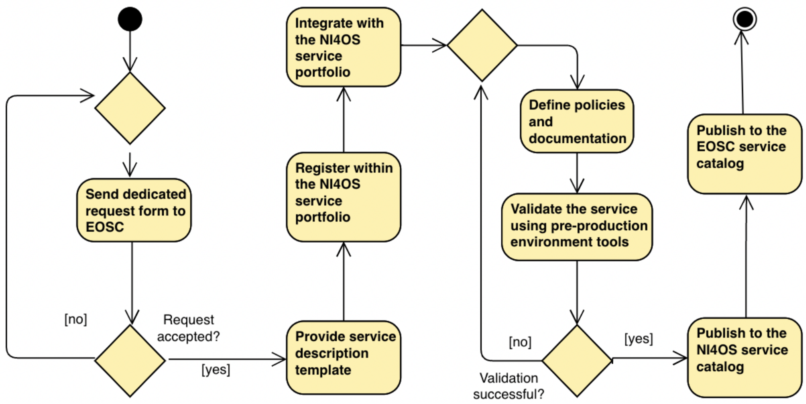

Figure 4: An activity diagram of the onboarding process of Gaussian API to the EOCS portal. Source: author's contribution.

4.3. Lessons learned

During the onboarding process we have learned important lessons and identified best practices for service providers to successfully onboard their services to the European Open Science Cloud (EOSC) platform.

Interoperability. Interoperability is crucial for services in the EOSC. It means they can easily communicate, share data, and collaborate with other EOSC components. Interoperability ensures efficient resource integration, supports interdisciplinary research, and encourages data and service sharing.

Data Management and FAIR Principles. Service providers should support effective data management practices aligned with the FAIR principles—Findability, Accessibility, Interoperability, and Reusability.

Accessibility and Availability. Services should be accessible to users beyond their original community. This involves making services available to diverse user groups, regardless of their technical background or geographic location. Ensuring availability ensures uninterrupted access to services at all times.

Security and Privacy. Services must prioritize the security and privacy of user data. Compliance with data protection regulations, and privacy-enhancing technologies are essential to establish trust and protect sensitive information.

Quality Assurance and Testing. Service providers must prioritize quality assurance and testing to ensure reliable and high-quality services. This involves implementing testing frameworks, conducting regular quality checks, and promptly addressing any identified issues.

Support and Documentation. Service providers should offer comprehensive support and documentation to assist users in using their services effectively. This includes providing clear and up-to-date documentation, FAQs, tutorials, and user forums. Service providers should provide user guides, tutorials, and training materials. These resources improve the user experience and help users resolve any issues or questions they may have.

Collaboration and EOSC Community Engagement. Service providers should actively engage with the EOSC community, collaborate with other service providers, and participate in relevant working groups or initiatives. This promotes knowledge sharing and the development of interoperable services.

Continuous Improvement. Service providers should continuously improve their services by actively seeking user feedback, analyzing usage data, and conducting assessments. This iterative process allows for service improvements and ensures that the user needs are addressed.

5. Conclusion

The European Open Science Cloud (EOSC) gives academics, institutions, and service providers a huge chance to contribute to open science. This paper explained the process of onboarding services to the EOSC, highlighting essential factors and best practices.

Several important lessons have been learned during the onboarding process, and these lessons have identified best practices for service providers to successfully onboard their services to the EOSC platform. The way that service providers develop and onboard their resources must be consistent with the core principles of the EOSC. Adhering to the FAIR guiding principles, considering interoperability, implementing user-centric design, providing documentation and metadata, providing service availability, and continually improving services based on user feedback are a few of these.

For the purpose of offering dependable and high-quality services, quality assurance and testing are essential. Organizations that prioritize quality assurance demonstrate their dedication to providing great services that conform to the highest standards of dependability, compliance, and user satisfaction.

By following these practices, service providers may help the EOSC develop and succeed while giving researchers access to a variety of tools and data sources that support their research. The EOSC has the ability to transform the research environment by promoting cooperation and open science.

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