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Open Model

LOUIS PONET (EPFL)

ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE – EPFL
BATIMENT CE 3316 STATION 1, 1015, LAUSANNE, CH

D7.1- AGREEMENTS ON HPC PLATFORM COOPERATION

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Author(s)	Louis Ponet (EPFL)
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ABSTRACT

The current deliverable D7.1 (Report and agreements on HPC platform cooperation) comprises the work performed from M6 (01.08.2021) to M12 (31.01.2022) in frame of the Task 7.1: Connecting HPC platform- cooperation and practical integration solutions. The task 7.1 is led by EPFL in partnership with SINTEF. The work in Task 7.1 is dedicated to coordinate cooperation with HPC platforms to facilitate execution of OpenModel workflows. The six months work within the Task 7.1 comprised in this report was dedicated in identifying possible HPC cooperation contacts, and when already available to document the technical needs to connect the OpenModel to the respective HPC facilities. In the first six months of the Task 7.1 the following HPC contacts for future connections to OpenModel were identified:

1. The Swiss National Supercomputing Centre – CSCS;
2. Norwegian research infrastructure services - (NRIS);
3. Jülich computer centre;
4. EuroHPC resources through the national EuroCC competence centers;
5. PRACE centres;
6. Connection via VIMMP (integration to HPCs via the VIMMP MarketPlace).

Furthermore, some preliminary explorations of possible communication and scheduling technologies was performed, which may aid in the unification of executing OpenModel workflows on the various HPC centres. Task 7.1 follows the technical developments in the other OpenModel WPs in order to identify the most suitable HPC

connections and respective technical needs to run OpenModel workflows. Further task 7.1 activities will be documented in the deliverable D7.2 (Practical solutions for connecting MarketPlaces to HPC) due on M32 and led by EPFL.

CHANGE HISTORY

Version	Date	Comment
0.1	2022-01-10	First Draft by Welchy L. Cavalcanti (IFAM), template and VIMMP HPC interface.
0.2	2022-01-31	Second draft prepared by Louis Ponet (EPFL).
1.0	2022-02-16	Finalized and submitted.
1.0	2023-01-24	Added request from EC

DISSEMINATION LEVEL

PU	Public	X
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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1 INTRODUCTION

The D7.1 deliverable documents the activities performed in Task 7.1 from M6 to M12. The main objective is to identify HPC platforms to facilitate execution of OpenModel workflows.

Regarding the communication to the HPC services, initially a classical approach relying on SSH will be utilized, but the possibility to communicate with alternative approaches, such as rest-API based services such as Fire-cREST [9] developed by CSCS, or web services as used by e.g. UNICORE (Uniform Interface to Computing Re-sources) [22].

During the first 6 months of the tasks 7.1 work, the following HPC facilities were identified:

1. The Swiss National Supercomputing Centre – CSCS;
2. Norwegian research infrastructure services (NRIS);
3. Jülich computer centre;
4. EuroHPC resource through the national EuroCC competence centers;
5. PRACE centres;
6. Connection via VIMMP (integration to HPCs via the VIMMP MarketPlace).

Due to the multitude of schedulers, and the potential downsides of SSH, two technologies were identified as potential candidates to aid in the unification of the interfaces between OpenModel and each of the centres. WP7 as a whole is dedicated to identify and set up cooperation with diverse projects and European initiatives, future developments in frame of Task 7.1 will be documented within the D7.2 (Practical solutions for connecting OpenModel services to HPC) due M32 and led by EPFL.

2 GENERAL OVERVIEW

2.1 METHODS OF COMMUNICATION

As foreseen by the proposal, AiiDA will initially serve as the main execution engine of the workflows generated by OpenModel. AiiDA currently communicates with HPC services through SSH.

However, recently some of the shortcomings of SSH for this usecase have been brought to light and have prompted many HPC centers to develop alternative methods of communication, usually based around a REST API. This can theoretically allow for more flexibility and more tailored solutions for the specific HPC centres, but also introduce new attack vectors and additional requirements of middleware. The multitude and lack of standards of these solutions makes it potentially difficult from the user's point of view, especially across when interacting with different HPC centers and REST API endpoints.

As of today, most of these solutions are at a beta stage in the most progressed cases, most are still in their infancy. If they become more widely used and relied upon by the HPC centres we will, together with the AiiDA team, develop plugins that will abstract away the methods of communication from the end user.

2.1.1 SSH

SSH does not warrant further introduction. It is ubiquitous and very well established, adhering to the latest security developments. In light of simplicity, this will initially remain the preferred method of communication.

2.1.2 FIRECREST [9]

One of the recently developed and promising communication methods, used mainly by CSCS, is the FirecREST software. It abstracts away the

2.2 SCHEDULERS

The situation on the level of the job schedulers that are in use by the HPC centres is very similar to the method of communication, albeit more progressed. A single defining method of job scheduling similar to SSH for communication never really existed. This meant that, similar to the development of centre-specific communication tools, different scheduling tools were developed and are used by different HPC centres. From the point of view of OpenModel this is not an issue, since AiiDA already interfaces with most of them.
See [5] for a detailed list.

However, the project and AiiDA team recognize the need to unify the scheduler interface and currently no standalone library offer such functionality. Previously, libsubmit offered parts of this, but this was embedded in the Parsl suite. The project will back any efforts that pursue a unifications and establishment of a stand alone library to interact with schedulers of different types.

2.2.1 LIBSUBMIT [1]

Libsubmit was developed as part of the parsl workflow execution suite as an abstraction layer between the software and the various schedulers.

3 SWISS NATIONAL SUPERCOMPUTING CENTRE – CSCS [28]

3.1 OVERVIEW [26]

CSCS develops and operates cutting-edge high-performance computing systems as an essential service facility for Swiss researchers. These computing systems are used by scientists for a diverse range of purposes – from high-resolution simulations to the analysis of complex data.

CSCS has a strong track record in supporting the processing, analysis and storage of scientific data, and is investing heavily in new tools and computing systems to support data science applications. For more than a decade, CSCS has been involved in the analysis of the many petabytes of data produced by scientific instruments such as the Large Hadron Collider (LHC) at CERN. Supporting scientists in extracting knowledge from structured and unstructured data is a key priority for CSCS.

3.1.1 USER LAB

On behalf of the Swiss Confederation, CSCS runs a User Lab [30], where researchers in Switzerland can apply for computational resources that are free at the point of use. A transparent review process by independent experts ensures that all deserving projects receive the computing resources they need to accomplish their aims.

3.1.2 COMPUTATIONAL SERVICES FOR SCIENCE

Swiss scientists, research institutions and projects with their own funding can access the computational resources at CSCS as contractual partners. The environment provided is either shared with the User Lab, or a dedicated solution can be deployed, depending on specific needs.

Examples of services provided by CSCS to contractual partners [27] are the analysis of data from the Large Hadron Collider (LHC) at CERN, the archiving of data from the X-ray laser SwissFEL for the Paul Scherrer Institute and the provision of computational resources for the numerical weather forecasts of MeteoSwiss.

3.2 SERVICES

3.2.1 SERVICE CATALOG [31]

CSCS provides a wide range of service which can be found in the Service Catalog [31] ranging from Compute and Storage Resources, to Interaction and Worfklow Tools and many Science and Informatics related Software packages.

3.2.2 COMPUTERS [29]

CSCS hosts many compute facilities, mostly based on Cray servers. These include both hybrid solutions (with GPU accelerators) and standard CPU-only nodes. For the full list see [29].

3.3 CONTACT

Email: info@cscs.ch
Phone: +41 91 610 82 11
Fax: +41 91 610 82 82

4 NORWEGIAN RESEARCH INFRASTRUCTURE SERVICES [35]

4.1 OVERVIEW

An important foundation for the successful collaboration on e-infrastructure in Norway is NRIS - a collaboration of five organisations to pool competencies, resources and services. The collaboration was until recently known as "the Metacenter".

NRIS consists of highly qualified IT staff at the four universities NTNU, the Universities of Bergen, Oslo and Tromsø and employees at Sigma2, counting almost 50 people.

The purpose is a geographically distributed competence network that ensures that all researchers who use the national e-infrastructure have quick and easy access to domain-specific support close to the user.

The Norwegian national e-infrastructures for research encompasses equipment, operations and related services for high-performance computing, data storage, software systems and high-capacity networks, as well as tools for efficient workflows and software for simulations and analysis of data. In addition, one of the members of NRIS, Sigma2 is a partner in the EuroCC competence center in Norway, where the research institutes NORCE and SINTEF is also partners. Domain specific knowledge is then also available on requests and particularly relevant, knowledge that sits in the border between IT and the respective domains are available as a resource.

4.2 SERVICES

NRIS offers a wide array of different services. Please have a look at the Service Catalog [53]. In addition, the national EuroCC competence center is available for additional competence needs [54]. Services at NRIS is also available to the industry and public sector.

4.3 CONTACT

Sigma2 AS
Org. no.: 814 864 332
E-mail: contact@sigma2.no
Mail: Postboks 4769 Torgard,
7465 Trondheim
Norway
Invoice: regnskap@sigma2.no
Visit: Abels gate 5
7030 Trondheim
Norway

5 JÜLICH COMPUTER CENTRE [16]

5.1 OVERVIEW [12]

The Jülich Supercomputing Centre at Forschungszentrum Jülich has been operating the first German supercomputing centre since 1987, and with the Jülich Institute for Advanced Simulation it is continuing the long tradition of scientific computing at Jülich. Computing time at the highest performance level is made available to researchers in Germany and Europe by means of an independent peer-review process. At the time being, JSC operates one of the most powerful supercomputers in Europe, JUWELS.

About 200 experts and contacts for all aspects of supercomputing and simulation sciences work in JSC. JSC's research and development concentrates on mathematical modelling and numerical, especially parallel algorithms for quantum chemistry, molecular dynamics and Monte-Carlo simulations. The focus in the computer sciences is on cluster computing, performance analysis of parallel programs, visualization, computational steering and federated data services.

In cooperations with renowned hardware and software vendors like IBM, Intel and ParTec, JSC meets the challenges that arise from the development of exaflop systems - the computers of the next supercomputer generation. As a member of the German Gauss Centre for Supercomputing, the Jülich Supercomputing Centre has coordinated the construction of the European research infrastructure "PRACE - Partnership for Advanced Computing in Europe" since 2008.

5.2 INDUSTRY RELATIONS [11]

The Industry Relations Team of the Jülich Supercomputing Centre

- manages industry-related research projects
- channels commissioned work to experts in the HPC centre
- provides the contact for the provision of computing time to industry.

It serves as a head office for industry outreach by advertising the expertise of the JSC provided by the Simulation Laboratories and Cross-Sectional Teams to industrial companies in the fields of engineering, biology, medicine, and physics. Thereby, the team aims at establishing new industrial collaborations based on both commercial and third-party funded relations.

5.2.1 SERVICES

- Provision of tailor-made computing solutions for the industry
- Knowledge transfer and consulting in high performance computing and associated research fields (engineering, biology, medicine, and physics), see Simulation Labs [13]
- Analysis of simulation code performance and optimization, see Cross-Sectional Team Performance Analysis [47]
- Consulting in hardware suitability - which hardware fits to your simulation problem?
- Porting of simulation codes to different architectures (GPU, accelerators, etc.)
- Computing time on HPC resources at JSC

- Big data analytics [10]
- Training and education (e.g. Python, MPI, …), see courses [15]

5.2.2 COMPETENCES

- Shared and distributed memory parallelization of complex simulation codes
- Simulation code performance analysis
- Single-core and multi-core performance optimization of simulation codes
- High-performance parallel I/O
- GPU and accelerator programming
- Specific field-related expertises as provided by the Simulation Laboratories
- Decades of experience in running supercomputers and supporting users with highly complex simulation problems

5.3 CONTACT

- Dr. Hartmut Fischer (modes of cooperation and contractual affairs including price information):
  - Phone: +49 2461 61-8808
  - email: ha.fischer@fz-juelich.de
- Dr. Andreas Lintermann (research-related simulation problems)
  - Phone: +49 2461 61 1754
  - email: a.lintermann@fz-juelich.de
- Dr. Daniel Rohe (usage of HPC resources):
  - Phone: +49 2461 61-8846
  - email: d.rohe@fz-juelich.de

5.4 COMPUTERS

The Jülich Supercomputing Centre operates two big supercomputers, JUWELS [17] and JURECA [14].

For the full system specification of JUWELS, see [3].

For the full system specification of JURECA, see [2].

6 EUROHPC [18]

6.1 OVERVIEW [7]

The European High Performance Computing Joint Undertaking (EuroHPC JU) is a legal and funding entity, created in 2018 and located in Luxembourg.

The EuroHPC JU allows the European Union and the EuroHPC JU participating countries to coordinate their efforts and pool their resources to make Europe a world leader in supercomputing. This will boost Europe's scientific excellence and industrial strength, support the digital transformation of its economy while ensuring its technological sovereignty.

More precisely, the EuroHPC JU aims to:

- develop, deploy, extend, and maintain a world-leading supercomputing and data infrastructure in Europe. The objective is to reach exascale capabilities by 2022/2024. Exascale supercomputers are capable of more than a billion billion operations per second (when compared to ten billion operations per second of an ordinary laptop device). Another objective is to build 'hybrid' machines that blend the best of quantum and classical HPC technologies with the first state-of-the-art pilot quantum computers by 2025.
- support the development and uptake of innovative and competitive supercomputing technologies and applications based on a supply chain that will reduce Europe's dependency on foreign computing technology. A specific focus will be given to greener and energy-efficient HPC technologies. Synergies with broader technology sectors and markets, such as autonomous vehicles, extreme-scale, big data, and applications based on edge computing or artificial intelligence will be encouraged.
- widen the use of HPC infrastructures to a large number of public and private users wherever they are located in Europe and support the development of key HPC skills, education and training for European science and industry. One of the objective is to create a network of national HPC Competence Centres to ease access to European HPC opportunities in different industrial sectors and deliver tailored solutions. Another iconic objective will be to set up the first pan-European Master of Science programme for HPC to develop HPC talents in Europe.

The EuroHPC Joint Undertaking is composed of public and private members:

Public members:

- the European Union (represented by the Commission),
- Member States and Associated Countries that have chosen to become members of the Joint Undertaking: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, the Netherlands, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden and Turkey.

Private members:

- representatives from the three participating private partners, the European Technology Platform for High Performance Computing (ETP4HPC) [33], the Big Data Value Association (BDVA) [25] and the European Quantum Industry Consortium (QuIC) [48].

Of particular importance is the focus of developing and sustaining competence in EuroHPC. Specifically, the EuroCC project. Within the EuroCC project under the European Union's Horizon 2020 (H2020), participating countries are tasked with establishing a single National Competence Centre (NCC) in the area of high-performance computing (HPC) in their respective countries. These NCCs will coordinate activities in all HPC-related fields at the national level and serve as a contact point for customers from industry, science, (future) HPC experts, and the general public alike. This is of particular value to the HPC interaction and the long-term efforts related to improvements on this arena.

6.2 COMPUTERS

Today the EuroHPC JU has procured seven supercomputers, located across Europe: LUMI [20] in Finland, Leonardo [19] in Italy, MeluXina [21] in Luxembourg, Vega [23] in Slovenia, Karolina [50] in the Czech Republic, Discoverer [8] in Bulgaria and Deucalion [6] in Portugal.

6.3 ACCESS/CONTACT [4]

E-mail: info@eurohpc-ju.europa.eu

7 PRACE CENTRES [45]

7.1 OVERVIEW [36]

The mission of PRACE (Partnership for Advanced Computing in Europe) is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. PRACE seeks to realise this mission by offering world class computing and data management resources and services through a peer review process [39].

PRACE also seeks to strengthen the European users of HPC in industry through various initiatives. PRACE has a strong interest in improving energy efficiency of computing systems and reducing their environmental impact.

PRACE is established as an international not-for-profit association (aisbl) with its seat in Brussels. It has 26 member countries [43] whose representative organisations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level. To find out more about the PRACE organisation go here [46].

7.2 COMPUTERS [44]

The computer systems and their operations accessible through PRACE are provided by 5 PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). Four hosting members (France, Germany, Italy, and Spain) secured funding for the initial period from 2010 to 2015. In 2016 a fifth Hosting Member, ETH Zurich/CSCS (Switzerland) opened its system via the PRACE Peer Review Process to researchers from academia and industry. In pace with the needs of the scientific communities and technical developments, systems deployed by PRACE are continuously updated and upgraded to be at the apex of HPC technology. To find out more about these systems, go here [42].

7.3 HPC ACCESS [40]

PRACE systems are available to scientists and researchers from academia and industry from around the world through the following forms of access:

- **Preparatory Access** is intended for short-term access to resources, for code-enabling and porting, required to prepare proposals for Project Access and to demonstrate the scalability of codes. Applications for Preparatory Access are accepted at any time, with a cut-off date every 3 months.
- The PRACE SME HPC Adoption Programme in Europe (SHAPE) [38] provides support to SMEs to include HPC in their business model.

- The **Distributed European Computing Initiative (DECI)** which is designed for projects requiring access to resources not currently available in the PI's own country and whose projects do not require resources on the very largest (Tier-0) European Supercomputers or very large computational allocations.
- **Project Access** is intended for individual researchers and research groups including multi-national research groups and can be used for 1-year production runs, as well as for 2-year or 3-year (**Multi-Year Access**) production runs.

Project Access is subject to the PRACE Peer Review Process [39], which includes technical and scientific review. Technical experts and leading scientists evaluate the proposals submitted in response to the bi-annual calls. Applications for Preparatory Access undergo technical review only.

For more information on how to apply for access to PRACE resources, go here [41].

Special rules apply to applications from industry. Please refer to the Terms of Reference for each Call for Proposals here [40].

7.4 INDUSTRY ACCESS [37]

Like similar programs running in the USA or Japan, the PRACE Open Research Model now allows European companies access to world-class HPC resources and services in order to increase their competitiveness by reducing the time-to-market, improving reliability and safety of their products, and developing innovative industrial processes.

In this business model industrial users may only use the facilities and services provided by the infrastructure for basic research and development purposes. The condition associated with this free access is for the industrial user to publish all results obtained at the end of the grant period.

8 USING HPC FACILITIES VIA VIMMP

Virtual Materials Market Place (VIMMP) is an European Union's Horizon 2020 research and innovation programme project under the grant agreement No 760907 [53]. VIMMP was approved under the call H2020 (NMBP-25-2017). Within the main objectives of OpenModel WP7 it is included to collaborate with Materials Modelling Marketplace projects such as VIMMP. Thus, in OpenModel one possibility to facilitate Connecting to HPC platforms can be via the VIMMP project.

In addition to the Core Services, VIMMP Marketplace provides users with means to execute simulation workflows created on the VIMMP Marketplace on external HPC resources [24, 32, 49, 51, 52]. Figure 1 [24] illustrates the relationship between the VIMMP Marketplace and external HPC resources. The latter are viewed by the VIMMP as a particular type of services provided on the Market Place by HPC providers.

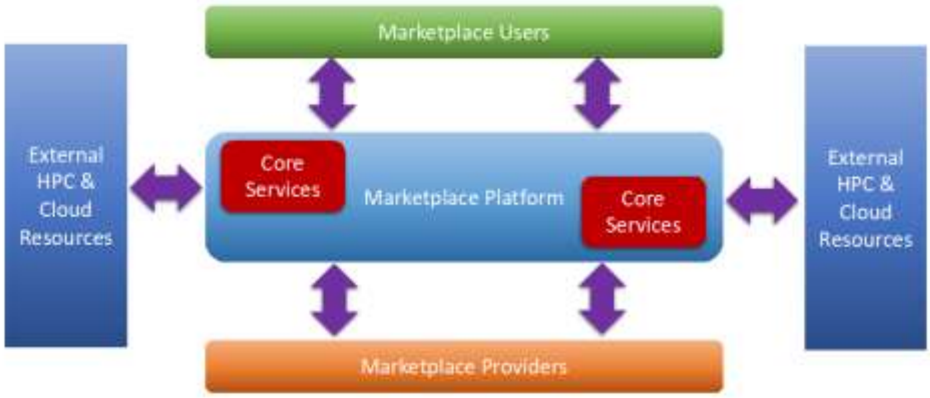

Figure 1: Marketplace Core Services and external HPC resources [24].

The diagram in Figure 2 [49] demonstrates from a high-level perspective the system scope of the VIMMP Platform. In this concept, users are abstracted to either potential providers or consumers of business objects who can use the VIMMP interface to achieve their purposes. They can ingest, search and retrieve data based on the metadata available for business objects on the platform. Moreover, External Data Providers may deliver new business objects via an API and External services such as the Translation Router, an application developed by IFAM, can use the Search API to query the system for information. An example use case is related to definitions and code lists stored as metadata for all business objects. These metadata can be loaded by external services and used for ingesting and searching the system again.

VIMMP also provides an interface to external HPC providers. This interface, the Job API, enables external HPC Facilities or cloud providers to offer their computing power on the marketplace. Finally, the translation service is envisioned as a tool for translators to combine workflows in an automated-fashion. This component is not developed within the scope of the VIMMP project, but it was identified as a service that, if developed in a future project, could enable translators to combine workflows and reduce the related human effort. The Translation Service represented in this diagram (Figure 2) is seen as an opportunity for future projects and still needs to be better understood in terms of requirements with the help of the translator´s community.

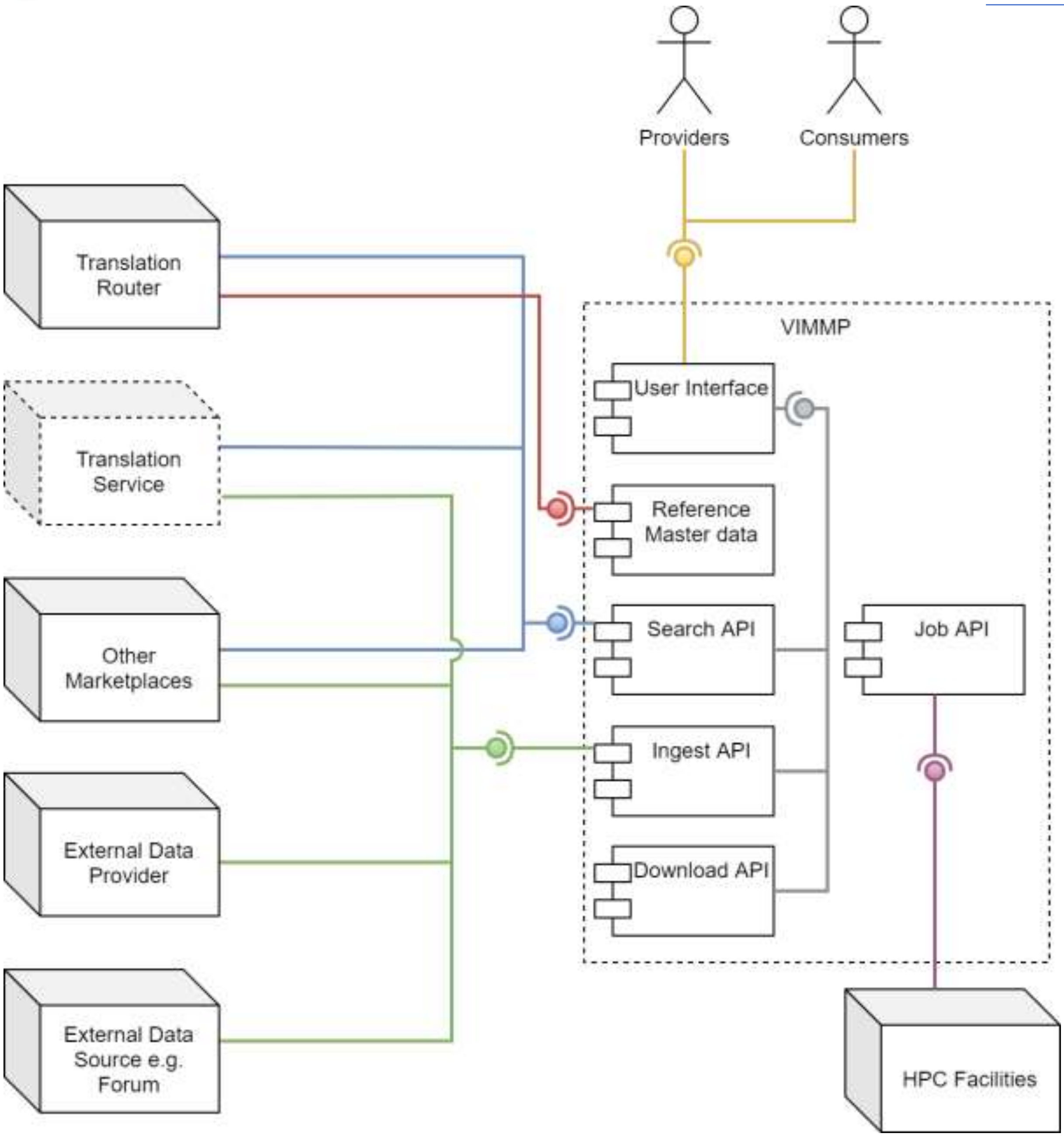

Figure 2: System scope of the VIMMP Platform [49].

Figure 3 [24] gives more details about VIMMP-HPC Integration, which is based on the concept of a *VIMMP Job* that submits VIMMP Marketplace workflows with accompanying data to HPC resources and retrieves results back to the VIMMP Marketplace.

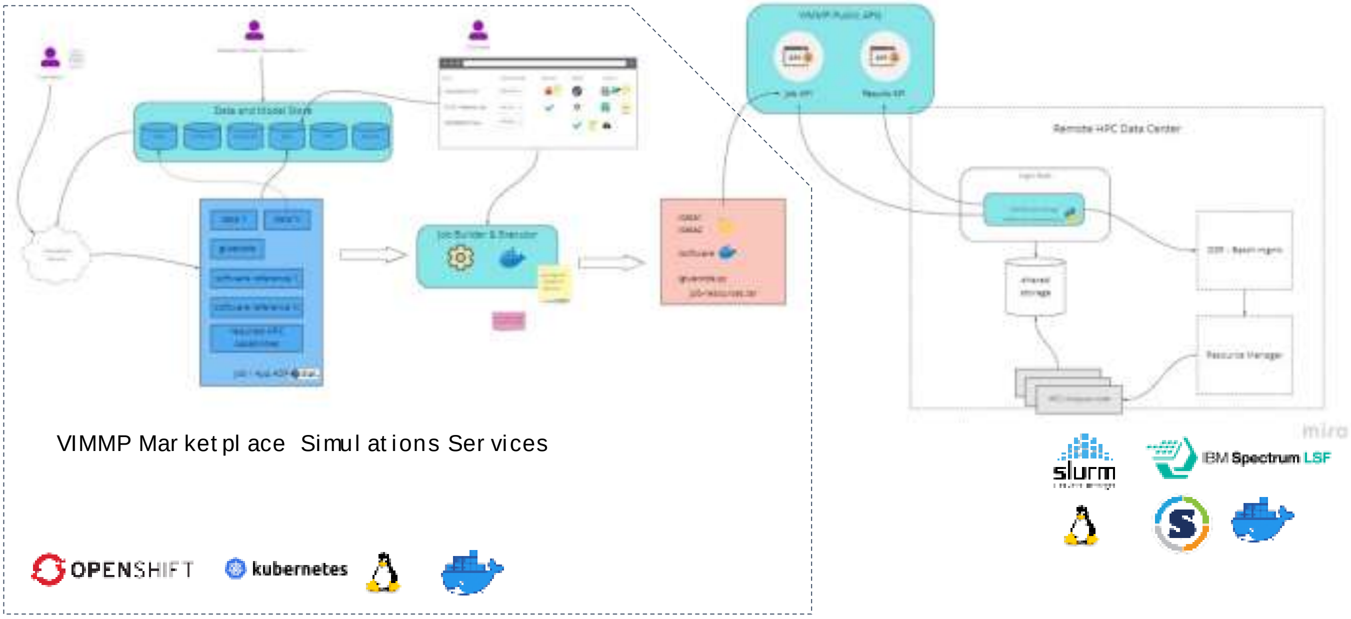

Figure 3: VIMMP-HPC Integration Architecture. VIMMP Job Service is one of the Marketplace core services responsible for VIMMP-HPC interactions [24].

Thus, the VIMMP-HPC integration is using a so-called VIMMP Job Service, which is responsible for creating jobs containing simulation workflows and corresponding data and forwarding them to HPC systems. The VIMMP job Service contains two major components, one acting in the VIMMP Marketplace and another one acting on a HPC system [24]. In VIMMP the OSP implemented is from the partner EDF and it is called SALOME (https://www.salome-platform.org/). The prototype of the VIMMP job Service has been developed in VIMMP by the VIMMP partners IBM UK in collaboration with OSTHUS and named a `job-executor.py`. Its purpose is to initiate workflow execution by taking a suitably packaged set of input files containing workflow inputs, SALOME job services definition and a Docker image containing workflow components.

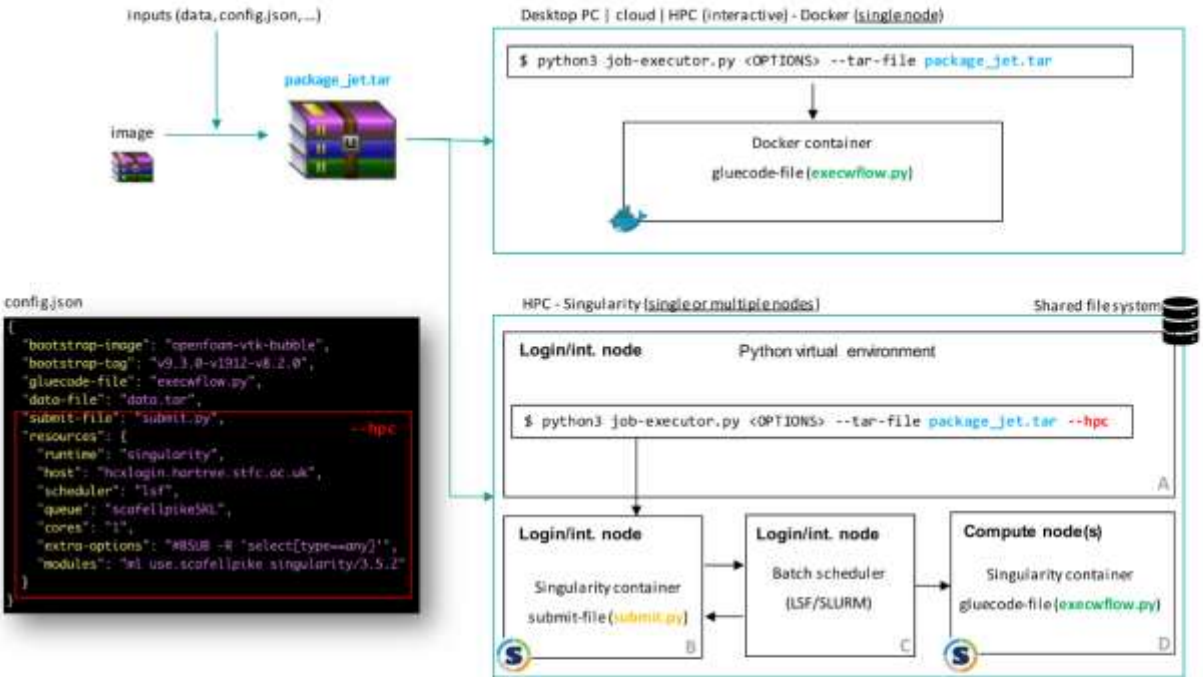

Figure 4: Comparison of control flow of `job-executor.py` script for a workstation and HPC installation [24].

8.1 USING SSH TUNNELING FOR DATA TRANSFERS [51]

It is often the case that on premises HPC systems are configured to not allow data transfers to the outside world. Download of data from the HPC is usually allowed, usually by mean of the scp command.

In this case one can still initiate data transfer from the HPC system using SSH reverse tunneling [24].

Assuming that hostA is the host outside of the HPC system and hostB belongs to HPC system (usually a login node) the respective configuration to enable reverse tunneling can looks like this:

HostA, $HOME/.ssh/config file

```
Host hostA
        User userb
        HostName hostB

        RemoteForward 9998 hostA:22
```

HostB, $HOME/.ssh/config file

```
Host hostA
    User usera
    Hostname localhost
    Port 9998
```

Data transfer then cab done as follows:

```
hostA> ssh hostB

hostB> scp myfile hostA:~/myfile
```

8.2 VIMMP CONTACTS

VIMMP main contact related to the above content:

Fraunhofer IFAM - VIMMP project coordinator – (contact via welchy.leite.cavalcanti@ifam.fraunhofer.de)

OSTHUS GmbH and IBM UK – responsible partners to implement connection of VIMMP to HPC facilities.

OSTHUS GmbH is part of the external advisory board in Open Model project.

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