DT4GS

Digital Twins for Green Shipping

D2.6: DT4GS Model Blueprints and Open Model Library v1

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Executive summary

DT4GS Open Model Library is essentially an ecosystem of actors (users, stakeholders, external vendors, etc) that interact through the sharing of data for the purpose of, at company level, optimising operations and, at industry level, facilitating the greening transition. Within the maritime context, the proposed IT infrastructure shall enable services mainly focused on decision - support / decision - making to optimise the management of the ship with respect to the condition of the machinery, and the energy efficiency of ship power plants and voyages. Industrial IoT and data sharing are relatively mature concepts to link embedded engine and hull-monitoring systems with bridge communications in a way that is said to reduce inefficiencies, risks, and overall cost, delivering an internet protocol for proprietary maritime systems to communicate and providing the smart connectivity for those systems.

The main purpose of this document is to describe the Open Model Library and all its components as a result of the discussions held by the consortium partners starting from the first draft solution as described in the Grant Agreement. Starting from the definition of the actors that will actively interact with the Open Model Library (OML) both for configuration tasks and for the actual integration in the broader DT4GS ecosystem, the document presents the requirements that the OML should address to ensure the communication, storage and appropriate deployment of the models outlining the core of the DT4GS frame. The Model Blueprints Template will be responsible to standardise the information describing the models utilising a rule-based programming language. In chapter xx the reader will find a detailed description of the OML ecosystem, comprising SOTA frameworks and services, that aim to efficiently manage the life cycle of models, from initialization and integration to deployment and evaluation. The resources and technological stack adopted to realise the Quantum Analogs of data - driven solutions is thoroughly demonstrated in Chapter 3. Finally, a brief description of a holistic management plan and stakeholders' engagement roadmap for OML is presented.

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Glossary of terms and acronyms used

Table 1 Glossary of acronyms and terms.

Acronym / Term	Description
KG	Knowledge Graph
MBT	Model Blueprint Template
MEE	Model Execution Engine
OML	Open Model Library
UI	User Interface

1 Introduction

As digitalisation in the shipping industry has been maturing over the recent years, DT adoption will be dependent on establishing trusted and convincing DT application exemplars and ensuring that ship operators and other industry stakeholders can set up their own DTs based on their own business models, building their own confidential knowledge at reasonable cost. This requirement is at the heart of the DT4GS approach as illustrated in the figure below.

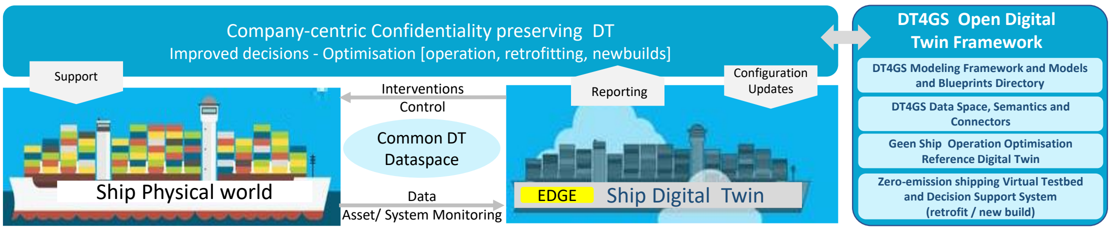

Figure 1 DT4GS approach

DT4GS will provide a virtual representation of ships and physical transport entities with a bi-directional communication links from sensing to actuation/control and data driven simulation and AI based decision support to people who will implement necessary actions. In DT4GS extra emphasis will be given to:

- DT applications on-board the ship utilising advanced IoT and edge computing infrastructure.
- Using labelled data for AI/ML training and to provide the ground truth for accurate predictions (supervised learning), and where there is need to learn from experience to provide the reward function (reinforcement learning).
- Creating a common point of reference in the digital world for shipping vessels, which different stakeholders can access and utilise and adapt in line with their own internal business needs.

To reach its goals DT4GS is divided into 6 WPs each with different goals, tasks, and deliverables.

This Deliverable aims to map the work in progress relative to Work Package 2 and in particular Task 2.4. The task, led by the partner DANAOS Shipping Co., is to define and implement the Open Model Library of the broader DT4GS framework. In particular, the activities are divided into the following sub-tasks, each aimed at implementing the key components for data storage and communication between the various entities and applications making up the DT:

- Specification of DT4GS Model Blueprint Template(s) (T2.4.1)
- Derivation of Quantum Analogues for optimisation and ML models (T2.4.2)
- Open Model Library (T2.4.3)

Given the fact that this deliverable is written during the first part of the project, while the development of the components is still in progress together with the definition of some key aspects for the Model Blueprints and Open Model Library Structure, some information might not be final. However, open topics are underlined in the context of this document will be described in their final implementation in the context of D2.6 “DT4GS Open Model Library v2” due month 34 of the project.

1.1 Mapping DT4GS Outputs

The purpose of this section is to map DT4GS Grant Agreement commitments, both within the formal Deliverable and Task description, against the current document.

Table 2 Adherence to DT4GS Grant Agreement deliverable and work description.

DT4GS GA Component Title	DT4GS GA Component Outline	Respective Document Chapter(s)	Justification
		DELIVERABLE	
D2.6: DT4GS Model Blueprints and Open Model Library v1	Model blueprints template, and optimised models, Open Model Library (OML) prototype. This deliverable includes the outputs of T2.4.	2, 3, 4, 5, 6	*Those chapters describe all the components and technologies to be implemented to develop and manage the first version of the Model Blueprints and Open Model Library*
		TASK	
ST2.4.1	Specification of DT4GS Model Blueprint Template(s) (MBT). Design a suitable blueprint-based description format and language for DT4GS (e.g., the OASIS TOSCA standard specification). This aims to standardise the way the various models in DT4GS, and the data associated with these models, are described. Templates will be produced for DT-driven services, AI/ML models, data processing / analytics applications, and QoS parameters (e.g., deadline, scaling,	3	*This chapter demonstrates the workflow and services adopted in order to realise the first release of MBT as described in the GA. More specifically we describe a variety of standardization techniques and tools exploited to derive the initial description of the model to be used in order to instantiate the its first version in the OML ecosystem. illustrate the streamlined procedure from consuming structured information*

	security requirements) that govern the execution of the blueprint.		*from the KG (T2.1) to model blueprint generation utilising a rule-based language.*
ST2.4.2	Derive the Quantum Analogues of key DT4GS models for IMCCs. These will be derived using the source models as applicable. The Quantum Analogue models will enable improved performance for said algorithms and models, allowing for quicker execution and / or more accurate results using conventional, easy to access and setup digital infrastructure.	*4*	*A thorough analysis of the available resources and requirements in order to derive the quantum analogues of the data driven models specified in WP1.* A as Dissipative Quantum Neural Networks *(DQNN) was proposed in order to balance the trade-off between computational resources and predictive capabilities of deep neural network models.*
ST2.4.3	An Open Model Library (OML) to support the storage and management of the model blueprints and their quantum analogues and associated data will be developed and deployed. The OML will also keep records of access and modifications to blueprints and will provide DevOps functionality following continuous integration-continuous deployment (CI/CD) for the rapid deployment of up to date DT4GS services in the LLs. The OML will be open to third parties, SMEs, external developers and interested stakeholders - with limited functionality - to promote visibility and innovation outside the consortium.	*3, 5*	*A breakdown analysis of all the appropriate requirements in terms of infrastructure (virtual machines, bare metal provision), resources (memory) and services (SOTA services for scheduling and orchestration & versioning) for the employment of the multitenant architecture of OML. Furthermore, defining roadmaps, validation scenarios and contingency plans for the smooth operation and validation of OML in the context of DT4GS.*

1.2 Deliverable Overview and Report Structure

In this section, provide a description of the Deliverable's Structure outlining the respective Chapters and their content.

Chapter 1: Generic Introduction to the DT4GS ecosystem. Mapping outcomes and results of D2.6 to WP2 tasks.

Chapter 2: Introduction to Management Information Systems in the maritime sector. Demonstration of a thorough gap analysis on pertinent SOTA solutions, for standardising and providing a layer of taxonomy on models and their associated parameters. Motivation and drive for employing a versatile OML incorporating standardisation procedures and techniques.

Chapter 3: Requirements specification. UMLs specifying the inter-linkage between main building blocks of T2.4 and core modules of DT4GS frame. In depth analysis of main building blocks of the envisaged Blueprint Template proposed in the context of the project. Interconnection and dependencies with other core modules of the broader DT4GS frame. A holistic demonstration of the support mechanisms, tools, and services required to realise the first version of the OML.

Chapter 4: Requirements specification in terms of infrastructure and resources for the quantum analogues derivation.

Chapter 5: OML preliminary Management plan initialization.

Chapter 6: Conclusions.

2 Model libraries in the maritime sector

2.1 Introduction

The maritime industry is a vast and complex ecosystem that plays a vital role in global trade, transportation, and resource exploration. As technology continues to advance, the maritime sector has embraced various innovative solutions to enhance efficiency, safety, and sustainability. One such development is the utilisation of model libraries, which have emerged as valuable tools in the maritime domain.

Repositories of models in the maritime sector are comprehensive collections of mathematical and computational models that simulate various aspects of maritime operations, vessel behavior, and environmental conditions. These libraries consist of pre-built models, algorithms, and simulations that can be readily applied to address specific challenges and optimise decision-making processes. The primary objective of model libraries is to assist maritime stakeholders, including shipping companies, port authorities, naval architects, researchers, and policymakers, in better understanding and predicting the behaviour and performance of vessels, marine structures, and oceanographic phenomena. By utilising these models, professionals in the maritime sector can gain valuable insights into vessel design, hydrodynamics, propulsion systems, safety assessments, weather routing, and environmental impacts.

Furthermore, model libraries can incorporate numerical models related to hydrodynamics and ship resistance, allowing naval architects and engineers to evaluate the performance of vessel designs in different operating conditions. These models help in optimizing hull shapes, propulsion systems, and energy efficiency, thereby reducing fuel consumption and environmental footprint.

In addition to vessel-related models, the maritime sector's model libraries may also encompass models that simulate oceanographic phenomena, such as tidal currents, storm surges, and coastal erosion. These models enable coastal planners, port authorities, and offshore operators to assess potential impacts, plan infrastructure developments, and make informed decisions to mitigate risks associated with changing environmental conditions.

The development and maintenance of model libraries in the maritime sector required the collaboration between industry stakeholders, research institutions, and government bodies. These libraries are continuously updated and refined based on new data, research findings, and technological advancements, ensuring their relevance and accuracy over time.

The multitude of data-driven and analytical methods employed in modern Information Systems for vessel monitoring and route optimization available in the literature fuse features from multiple sensors onboard (Filippopoulos et al., 2022). However, there are not many systems available currently in the maritime sector that deal simultaneously with the challenging matter of employing- evaluating and eventually integrating in the workflow, models, in a continuous and automated manner. OML and MBT envisaged ecosystem and support mechanisms will offer a versatile broad range of services employed with SOTA frameworks concerning the CI/CD of models as well as the appropriate communication protocols and virtual/containerized environments for the optimal versioning, storing and deployment of data driven and/or analytical solutions related to operational efficiency, monitoring and environmental compliance.

Through a comprehensive blueprint configuration file, structured information will be generated regarding the architecture, type, purpose and specific mean of deployment for a particular model. MBT will be incorporated in the broader DT4GS frame via the adaptive multipurpose Knowledge Graph implemented in the context of T2.1 by KNT & INLE.

2.2 Related Work & Market Analysis

Management Information Systems is a discipline that involves the use of information technology to support and improve the management and decision-making processes of an organisation. Through the use of various tools and techniques, MIS helps organisations collect, store, and analyse data in order to gain insights and make informed decisions.

In the context of this work, we will set the basis to transcend and extend beyond traditional MIS by introducing automated administrative workflows in the form of structured information (databases, graphs, configuration files, rule-based languages) aiming to create an autonomous, self-sustained repository of the DT4GS models, continuously updated by new batches of data.

Closely related to MIS is the emerging concept of the so-called Digital Twin, first introduced in (Grieves,2014), that represents a virtual representation of a physical system or process that can be used to simulate and analyse its behaviour. A Digital Twin, adapted to the needs of the maritime sector, constitutes a virtual holistic representation of the vessel that spans its life cycle and is updated from near to real-time data, utilising simulation, machine learning and reasoning to help in decision-making, sensing and control actuation. By combining core structural properties of traditional or more sophisticated MIS such as the one proposed in the context of this deliverable, organisations can gain a better insight of their internal operations and pave the way for a fully automated and fault tolerant decision-making procedure, substantially improving their efficiency and effectiveness.

According to a report by Markets and Markets, the global maritime analytics market, which includes fleet management solutions, is expected to grow from USD 534.6 million in 2018 to USD 1,137.9 million by 2023, at a CAGR of 16.7%. This growth is driven by increasing demand for digitalization in the maritime industry, rising adoption of IoT, and increasing need for enhanced operational efficiency and cost savings.

Existing market solutions concerning web-based integrated model repositories in the maritime sector consist mainly of models for new build design and they do not address the full spectrum of operational procedures during the vessels' life.

Some examples of commercialised web-based UI options for open model repositories in the maritime sector are the following:

- Modelica Library for Marine Systems (MLMS): MLMS is a web-based repository of Modelica models for the maritime sector. It includes a user-friendly web interface for searching, browsing, and downloading models, as well as tools for simulation and analysis.

- SimScale: SimScale is a cloud-based platform for simulation and analysis, which can be used for modelling and simulation in the maritime sector. It includes a web-based UI for designing and analysing models, as well as tools for CFD, FEA, and thermal analysis.

- CAESES: CAESES is a web-based platform for parametric modelling and optimization, which can be used for ship design and optimization in the maritime sector. It includes a user-friendly web interface for designing and testing models, as well as tools for CFD and optimization.

- Marine Design Toolkit (MDT): MDT is a web-based platform for ship design and optimization, which includes a range of open-source tools and models for the maritime sector. It includes a web interface for designing and testing models, as well as tools for CFD and optimization.

- OpenVSP: OpenVSP is a web-based tool for conceptual aircraft and vehicle design, which can be used for ship design in the maritime sector. It includes a user-friendly web interface for designing and analyzing models, as well as tools for aerodynamics and stability analysis.

These examples lack the support mechanisms and automation capabilities of a multi-purpose adaptive library of models continuously refined, that spans the vessels lifecycle and addresses not only parametric new build design and retrofitting but also operational optimization and performance monitoring and management.

Multi-tenant web-based architectures as the one proposed in the context of T2.4 can help address some of the key challenges faced by the maritime sector, such as the need for real-time data/model access and processing, model security, and scalability. By providing a shared multi-purpose platform, the cost and complexity of managing multiple applications can be reduced, while enabling collaboration and information sharing among multiple stakeholders/users.

3 Architectural Definition

3.1 Requirements Specification

Open Model Library and generally T2.4 is envisioned as a core module of the broader DT4GS frame that will facilitate the digitization of the maritime sector through a set of SOTA tools and services by employing an ever living continuously refined, through the vessels life, digital replica of the ship. In this context, OML serves as a versatile repository of models addressing each part of the vessel's life from 3D modelling (new build design) and regression formulas for total resistance calculator and emission monitoring, to complex Life Cycle Assessment (LCA) toolkits to assess and evaluate possible alternative solutions towards a carbon neutral operational blueprint. This repository of models adapted to the needs of the waterborne sector, constitutes an ever-growing support mechanism, comprising frameworks for continuous-integration/deployment (CI/CD) of models and their associated parameters. In its simplest form OML is demonstrating an ecosystem of databases, SOTA services for model versioning/deployment and configuration templates that aim to create a standardisation layer outlining the models, their associated parameters and KPIs, etc.

The main drive and motivation behind OML vision was the employment of a holistic and adaptive platform entailing a detailed taxonomy of models that address the vast amount of procedures concerning the vessel’s life cycle. Complemented with a web-based integrated environment for visualisation purposes, this consolidated approach transcends beyond the narrow sectoral boundaries of existing solutions that are outdated and mainly concern only a fraction of the set of procedures comprising the vessel's ecosystem.

Towards this direction the first step was to define a comprehensive list of available models to identify and elicit mandatory requirements to initiate the development and in a later stage realise a prototype version of the OML. An indicative list of models defined in the context of WP1 is depicted in the below diagram.

- Navigation Management (on-going)
- Integrated ship energy production, distribution, recovery & management (on-going)
- Robust fuel consumption and CO2e emission Models (developed)
- Life Cycle Assessment (on-going)

Based on these models we were able to extract the minimum set of requirements that outline the core functionality, architectural definition and necessary resources to realise the first version of OML.

The users of the Open Model Library typically have distinct needs and objectives. Shipping companies, for instance, may seek models that help optimize vessel routing, fuel consumption, and operational costs. Port authorities may require models to assess the impact of infrastructure developments, evaluate navigational safety, and plan for emergency response. Researchers may utilize the library to study vessel behavior, environmental impacts, and contribute to the development of new models. Policymakers may rely on the library to access validated models for regulatory purposes and to support evidence-based decision-making.

Interacting with the Open Model Library involves functionalities such as model insertion and search. Users can contribute to the library by sharing their own models or collaborating on the improvement of existing ones. Inserting a model involves providing relevant documentation, data, and code, ensuring that it meets the library's quality and validation standards. This collaborative aspect fosters knowledge sharing and the continuous growth of the library.

The search functionality within the Open Model Library allows users to explore the available models based on specific criteria. Users can search by keywords, model types, applications, or performance indicators to find the most relevant models for their needs. This feature enables efficient retrieval of information and promotes the reuse of existing models, saving time and resources.

To enhance the user experience, the Open Model Library may offer additional features such as visualization tools, model comparison capabilities, and integration with other software platforms commonly used in the maritime sector. These functionalities enable users to interact with the models more effectively, analyze results, and gain insights to inform their decision-making processes.

In summary, the Open Model Library serves as a collaborative platform that caters to the diverse requirements of maritime stakeholders. Users can interact with the library by contributing models, searching for specific models based on their needs, and providing feedback to improve the quality and applicability of the models. This interactive and community-driven approach ensures that the Open Model Library remains a valuable resource for the maritime sector, promoting innovation, efficiency, and sustainable development.

In the next sections we demonstrate the main components comprising OML as well as a working example, corresponding to a FOC approximation model, that demonstrates the core functionality and applicability of the envisaged platform.

3.2 Generic Architectural Definition

In the context of WP2, a Big Data Management Information system adapted to the needs of the maritime sector will be demonstrated. The proposed framework incorporates a variety of state-of-the-art streaming tools for real-time analysis of vessel data as well as tools for continuous integration/deployment (CI/CD) of ML/DL models regarding operational optimization, causal analysis, and event recognition. By utilising DT4GS infrastructure concerning Edge-Headquarter (EDGE-HQ) communication between the vessel and the office, we will incorporate the aforementioned pipeline in a broader data acquisition network in order to aggregate, synchronise and process data coming from the vessel in real-time. The resulting platform (see Figure 2) constitutes a prototype version of a virtual replica of the en-route vessel (Digital Twin framework) that aims to assist shipowners to achieve efficiency in fleet management with tangible benefits in terms of emission reduction, environmental compliance and protection of crew safety onboard.

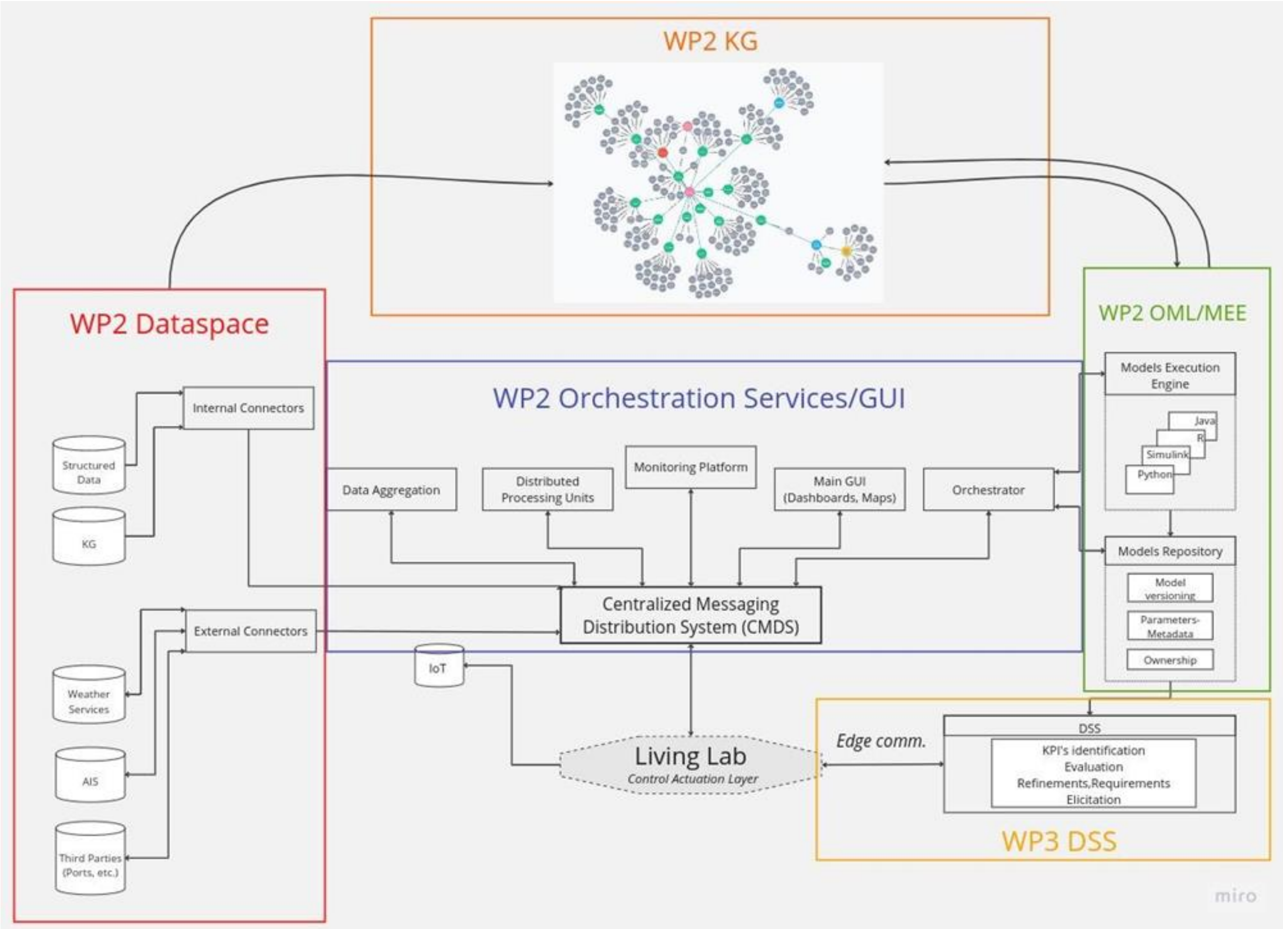

Figure 2: Generic DT4GS frame & OML Placement.

In this deliverable, our efforts and discussion is focused on acquiring and defining all the appropriate resources and requirements to elicit in detail all the information and procedures concerning the integration, training and deployment of the models that were defined in WP1 and may vary from simple regression analysis, to CFD models simulating the added resistance of the vessel on various operating conditions, as well as 3D modelling and simulation modules of integrated machinery equipment (power management, bridge simulators, etc).

In Figure 2 above, we depict a high-level demonstration of the main components constituting T2.4, from acquiring appropriate information utilizing the Knowledge Hub/Knowledge Graph (WP2 & WP3), to employing the Model Blueprint Template (MBT), to the multitenant adaptive realisation of OML.

The Open Model Library will be a collection of open-source models, tools, and data sets that aim to improve decision-making and promote innovation in the maritime industry. This library will contain various models related to vessel performance, safety, and energy efficiency, as well as data sets on weather conditions, ocean currents, and other relevant maritime factors. By providing open access to these models and data sets, the library enables researchers, developers, and stakeholders to collaborate, share knowledge, and develop new solutions that address the complex challenges facing the maritime industry. Ultimately, the Open Model Library seeks to promote sustainability, safety, and efficiency in maritime operations while also fostering innovation and growth in the waterborne sector.

3.3 Model Blueprint Template (MBT)

MBT constitutes the first step towards the model instantiation in the broader OML ecosystem. Utilizing a user defined list of parameters, we construct a structured template in a specific format that in turn is consumed by the Knowledge Graph to generate the appropriate set of nodes outlining the core of the model.

The broader Knowledge Graph employed in WP2, is responsible initially, for providing in high level (use case, data associated, feature set, etc) a preliminary description of the candidate model we want to incorporate in the OML. This information is appropriately decoded and translated, in a later stage, by utilising a rule-based language (PROLOG) to provide a thorough listing of all the parameters describing the model in a structured manner (YAML, JSON, connected acyclic graphs). An example of the parameters describing the model is given below:

- Data class (sensory, telegrams, granularity etc)
- Data processing type (streamlined, custom)
- Model Type / Architecture (regression/ classification deep learning / machine learning, analytical, CFDs, etc.)
- Training Type (continuous etc, one-off)
- Scalability (Eligible for CPU / GPU optimization - QUANTUM ANALOGS)
- Security (certificates, accessibility)
- Minimum resources (OS type, executable format/size, minimum RAM, CPU Hz, etc)
- Integration (topology inside the DT ecosystem)
- Deployment (locally, on edge, as a Web Service (API), as a DLL, as JSON, ONNX, H5, etc.)

Initially, as described above, MBT is constructed by consuming structured information by the end-user. As the model's life cycle progresses the initial instantiation of the model existing in the OML ecosystem as well as in the KG will be adapted and informed accordingly by third party modules (e.g.: Models Execution Engine (MEE)). Utilising a rule-based language we employ the initial model blueprint resembling a configuration file (entry point) of the model in YAML or JSON format.

Representative example of the YAML file constructed by consuming standardised information from the KG is depicted below:

```yaml
artifact_path: keras-foc-model
flavors:
  python_function:
    data: data
    env:
      conda: conda.yaml
      virtualenv: python_env.yaml
    loader_module: mlflow.tensorflow
    python_version: 3.8.10
  tensorflow:
    code: null
    data: data
    keras_version: 2.11.0
    model_type: keras
    save_format: tf
mlflow_version: 2.2.1
model_uuid: 04d84e23a3064bbb9305d5d4ee16ae2b
run_id: 6c3b5ee78db742a282a07990fdb9a335
utc_time_created: '2023-03-09 16:56:30.380113'
```


Figure 3: YAML config file.

The YAML configuration file is consumed by Neo4J (graph database) module, utilising Cypher (query programming language) to construct a preliminary connected acyclic graph depicting the blueprint of the model. This blueprint modelled by the acyclic graph is an adaptive ever-living instance of the model that is updated by core or third-party modules of the broader DT4GS frame that are utilising or altering in a way the models (MEE, OML, KH).

Figure 4: Neo4J snapshot depicting Models Template in the form of connected acyclic graph.

Neo4J enables data retrieval and standardisation of the majority of the information stored in the graph concerning the model with the establishment of an appropriate environment (API). Furthermore, by utilising Neo4j we construct an ever-growing repository/graph database of models that will be utilised appropriately to facilitate in the employment of the actual library of the models (OML) utilising state of the art technologies regarding CI/CD of ML/ analytical models (MlFlow).

Below we depict the end-to-end streamlined procedure, alongside with the architectural definition of each component employed to construct the initial MBT generation procedure, as well as the broader ecosystem comprising T2.4 as a whole.

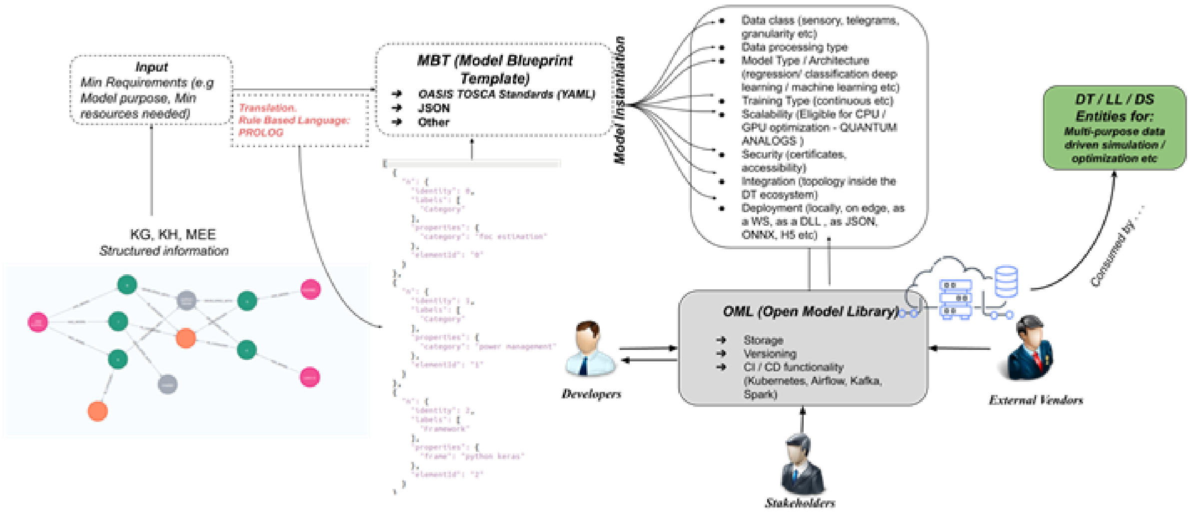

Figure 5: MBT workflow as part of the Internal topology of OML.

In the following sections we describe how the envisaged Open Model Library framework, creates a centralised digital framework to manage efficiently the storing of a variety of simulation models related to ship operations, as well as facilitates the employment of a holistic informed and reasoned decision-making platform.

The main goal of the OML ecosystem is to largely simplify and standardise the way the various tools and services concerning model training and deployment are operating and communicating with each other, following the standards of an ICT (Information Communication Technology) framework. The general streamlined procedure and framework is presented in the next section.

3.4 Model Repository Ecosystem

OML is supported by various SOTA tools and services that aim to vastly standardise and automate the continuous monitoring, integration and versioning of various models developed in the context of DT4GS. These models range from Navigation Management simulation frameworks to optimise the route of the vessel to integrated machinery performance monitoring and assessment, as well as power management and LCA (Life Cycle Assessment) toolkits assessing the financial and environmental possibility of different solutions (retrofitting solutions, operational optimization, new build designs, etc).

In order to be able to successfully integrate and monitor this diverse set of models we will require a versatile ecosystem appropriately orchestrated by a variety of different SOTA services comprising the DT4GS frame.

Furthermore, the proposed scheme should allow the interconnection and communication with a multitude of stakeholders attached to the waterborne sector that have a direct or indirect claim (rear write permission) on the core functionality of the envisaged framework (developers, shipowners, external vendors, suppliers, charterers, etc.).

This multitenant architecture is realised with the appropriate orchestration of a versatile SaaS (System as a Service) ecosystem consisting of various microservices encapsulated on different virtual machines (docker-containers) that offer the possibility to different users to exploit core functionalities of the platform. By utilising different microservices for a set of different purposes, OML realises a fault tolerant, secure, reusable and technology-agnostic library of models.

Containers offer the advantage of running in isolated processes within a given user space, which significantly reduces the resources required compared to virtual machines that require their own operating system. Consequently, running an application as a container is much cheaper than running it on a virtual machine.

This technology plays a central role in the microservices revolution in software development, owing to the small footprint of containers that enables easy running of multiple self-contained and isolated applications. Containers also allow for running small microservices alongside one another, and orchestration tools such as Kubernetes which simplify upgrading unique microservices without causing any downtime.

Another advantage of using containers is their ephemeral nature, whereby restarting a container brings it back to its previous state, ensuring consistent application performance. This is particularly useful for software developers running tests on their system, as the test run starts afresh each time without any previous data. However, preserving data becomes challenging when running a container for a database, as any changes made while it is running get lost upon restarting. In such instances, mounting a volume accessible from the container becomes necessary, with tools like Kubernetes facilitating container management and operators aiding in setting up persistent volumes.

In high level the multitenant architecture of the OML is depicted in Figure below. With dashed lines the containerized services are depicted, while with red colour we depict the services/repositories comprising explicitly T2.4. Containerized services are communicating with each other via a dedicated network protocol, bridging the services via a secure gateway.

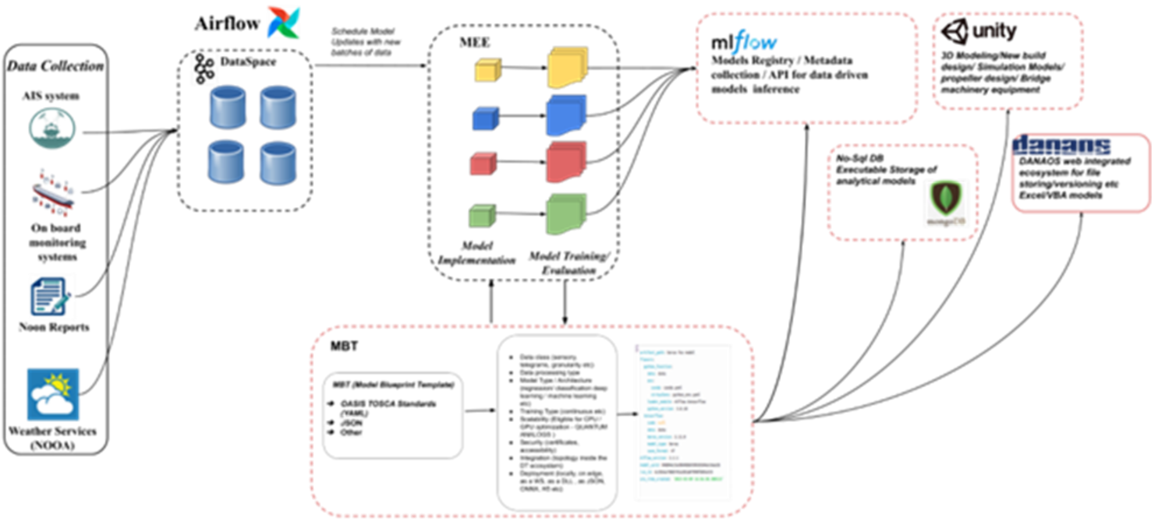

Figure 6: OML architectural definition and dependencies with other core modules of the DT4GS frame.

3.4.1 Model Versioning

Mlflow is a SOTA platform with a web integrated GUI as well as an interoperable dedicated API that manages the lifecycle of ML models from initialization and training, up until the stages of versioning and deployment. As showcased in Figure 8 MlFlow constitutes a core component of OML and manages the life cycle of models. It offers a versatile set of functionalities that aim to automate the way data driven models are described. The main functionality includes: 1) tracking experiments to record and compare parameters and results (MLflow Tracking), 2) wrapping ML code in a reusable, reproducible form in order to share with other internal or external users (MLflow Projects), 3)managing and deploying models from a variety of ML libraries to a variety of model serving and inference platforms (MLflow Models), 4) providing a central model store to collaboratively manage the full lifecycle of an MLflow Model, including model versioning, stage transitions, and annotations (MLflow Model Registry).

- The maritime sector deals with a wide range of tasks, such as ship navigation, port operations, logistics, safety, and security. Machine learning can be used to optimize these tasks and improve the overall efficiency of the sector. As described below, MlFlow can be used to develop and deploy machine learning models in the maritime sector to optimize: Ship Navigation: Machine learning models can be trained on historical data to predict weather patterns, ocean currents, and other environmental factors that impact ship navigation. These models can be used to optimize ship routes and reduce fuel consumption.
- Port Operations: Machine learning models can be used to predict vessel arrival times and optimize berth allocation. These models can help reduce congestion in ports and improve the overall efficiency of cargo handling.
- Safety and Security: Machine learning models can be trained to detect anomalies in vessel behavior and identify potential security threats. These models can be used to improve maritime surveillance and enhance security measures.

MlFlow can be used to manage the entire machine learning lifecycle in these applications. Data scientists can use MlFlow to track experiments, manage data, package code into reproducible runs, and share and deploy models. MlFlow can also be integrated with other tools and platforms commonly used in the maritime sector, such as GIS software and maritime databases, to streamline the machine learning workflow.

In the following we depict a set of screenshots utilising MlFlow functionality to manage the early stages of a data-driven model concerning FOC approximation for one vessel.

In Figure 7 below we can observe the MLFlow Model Registry for one vessel regarding FOC approximation. We also depict (Figures 8, 9) how different parameters of the model are tagged and logged in the web-based GUI as well as the automated metadata collection (performance, batches of data used for training, etc.) for a particular version of the model in the following figures.

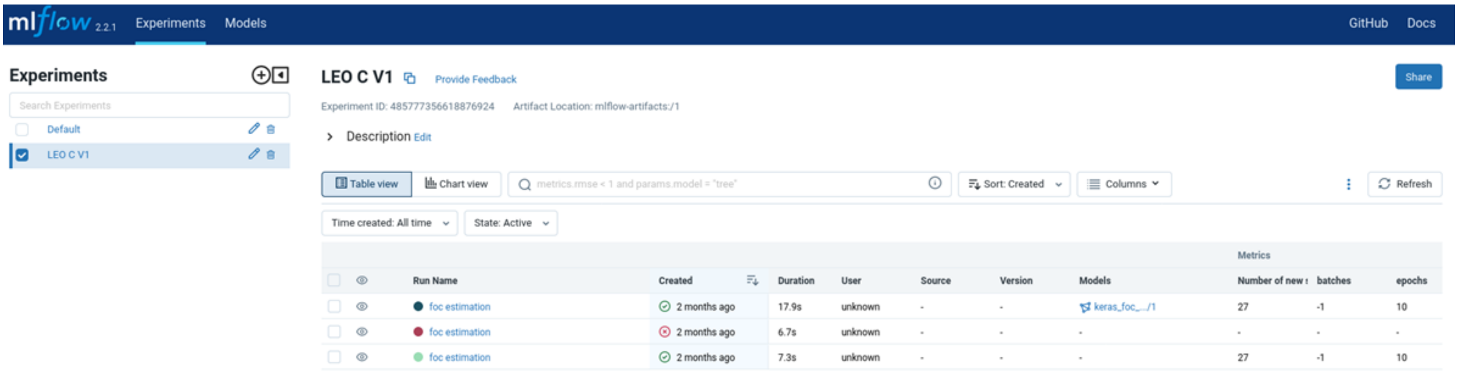

Figure 7: MLflow snapshot (experiment for one vessel for FOC approximation).

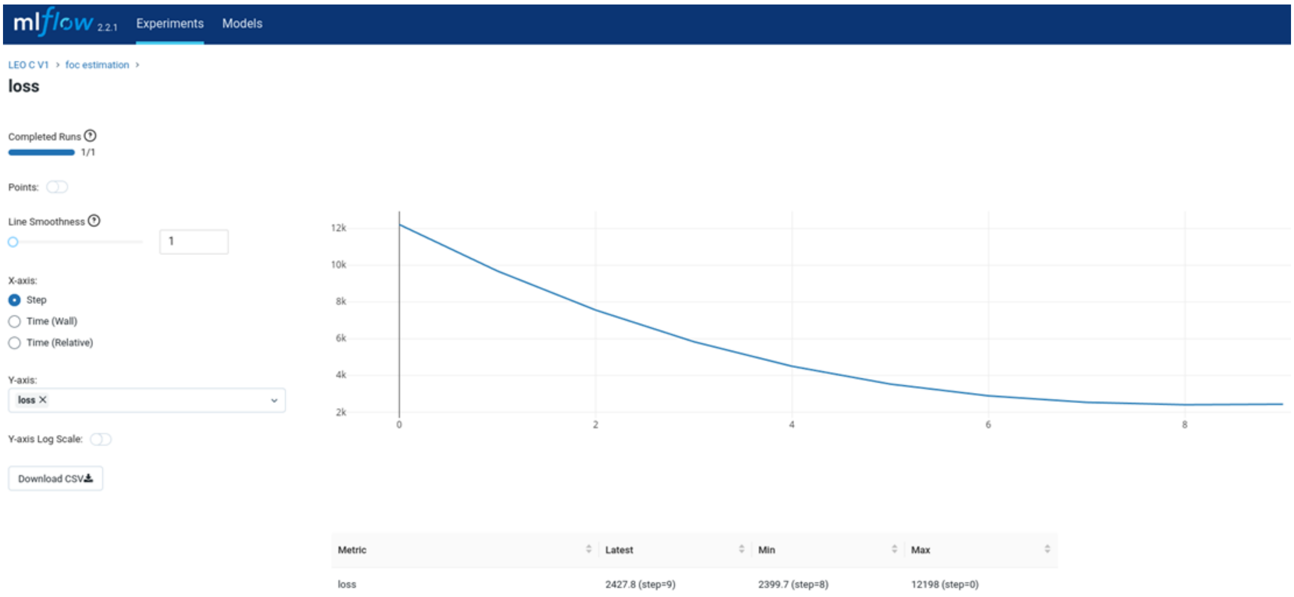

Figure 8: MLflow snapshot (dedicated UI for models performance visualisation).

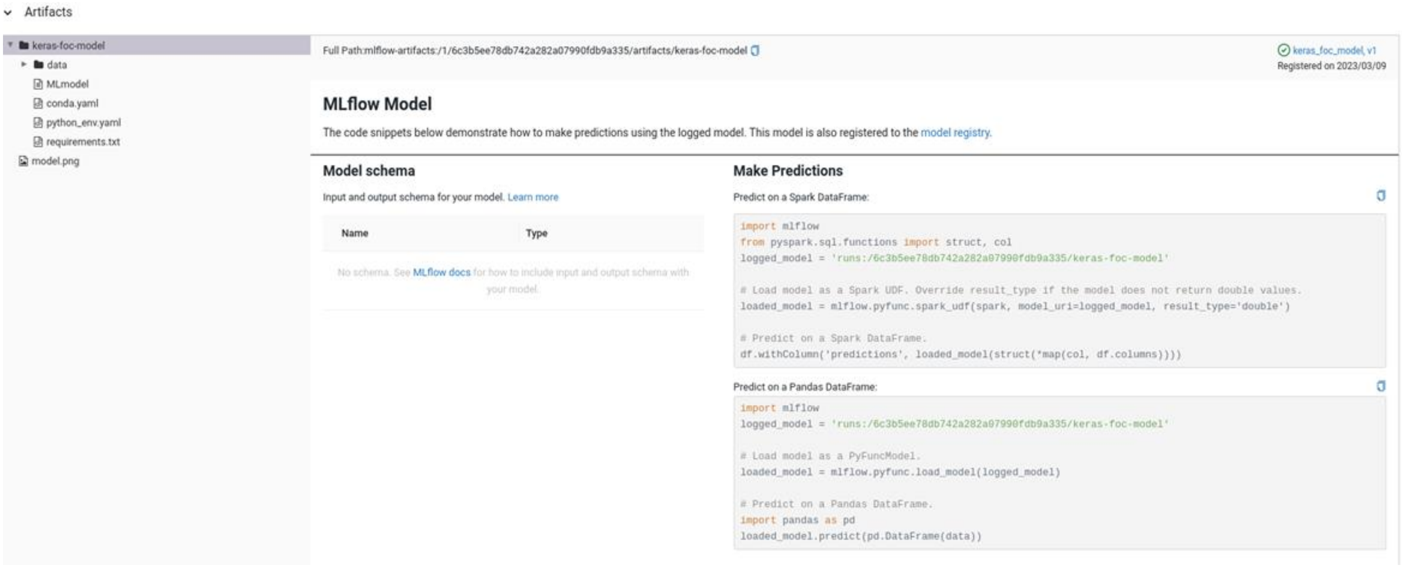

Figure 9: MLflow snapshot (dedicated UI for metadata collection & model inference).

3.4.2 OML Support Services (GUI & MongoDB Repository)

Implementing a web-based UI for an open model repository in the maritime sector can involve several steps. Here is an outline of the process that DT4GS adopted:

1. Defined requirements: The first step is to define the requirements for the web-based UI, including the types of models that will be stored in the repository, the desired features and functionalities of the UI, and the target audience.
2. Choose a web development framework: There are several web development frameworks available, such as Angular, React, and Vue.js. (**Angular JS**)
3. Design the UI: The UI should be designed based on the requirements and target audience, using wireframes and mockups. The design should be intuitive, user-friendly, and responsive.
4. Choose a database: The database should be chosen based on the requirements of the project and the expertise of the development team. (**MongoDB**)
5. Implement the UI: The UI should be implemented using the chosen web development framework, along with HTML, CSS, and JavaScript. The UI should be tested and refined based on user feedback.
6. Implement the backend: The backend should be implemented using the chosen programming language and database and should include the necessary APIs for accessing and manipulating the models in the repository. (**Python, Jenkins, Flask**)
7. Test and deploy: The web-based UI should be thoroughly tested and debugged, and then deployed to a web server or cloud platform. The deployment process should be automated, using tools such as Docker and Kubernetes. (**Docker**)
8. Maintain and update: The web-based UI should be maintained and updated over time.

Overall, implementing a web-based UI for an open model repository in the maritime sector can be a complex process that requires careful planning, design, and implementation. However, with the right tools and expertise, it can be a powerful tool for sharing and accessing models.

In the figures below we demonstrate an ongoing implementation concerning the OML GUI consisting mainly of components regarding model performance visualisation model repository as well as providing a dedicated environment on how to appropriately query the models.

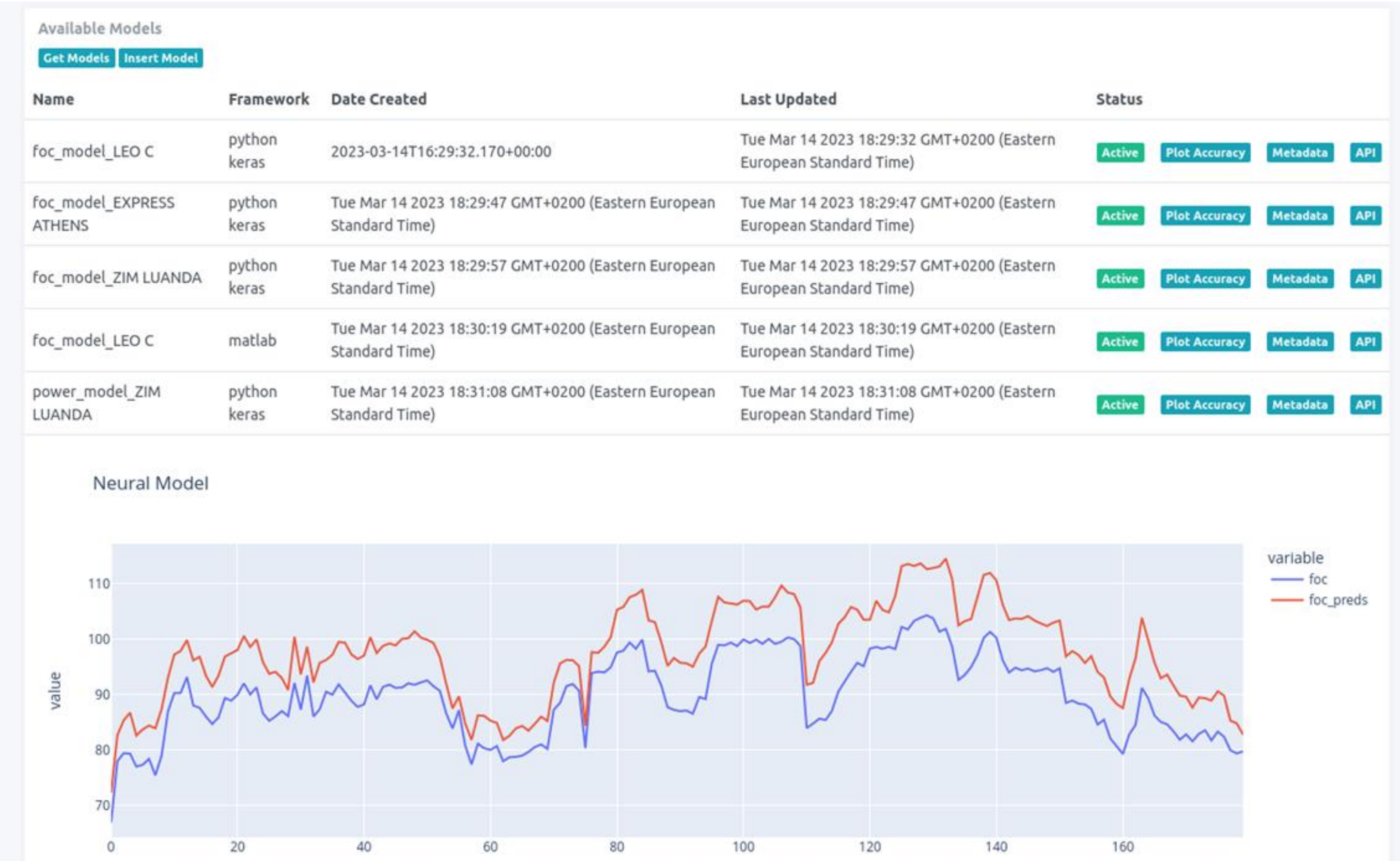

Figure 10: OML GUI. Model collection / performance visualisation / metadata acquisition.

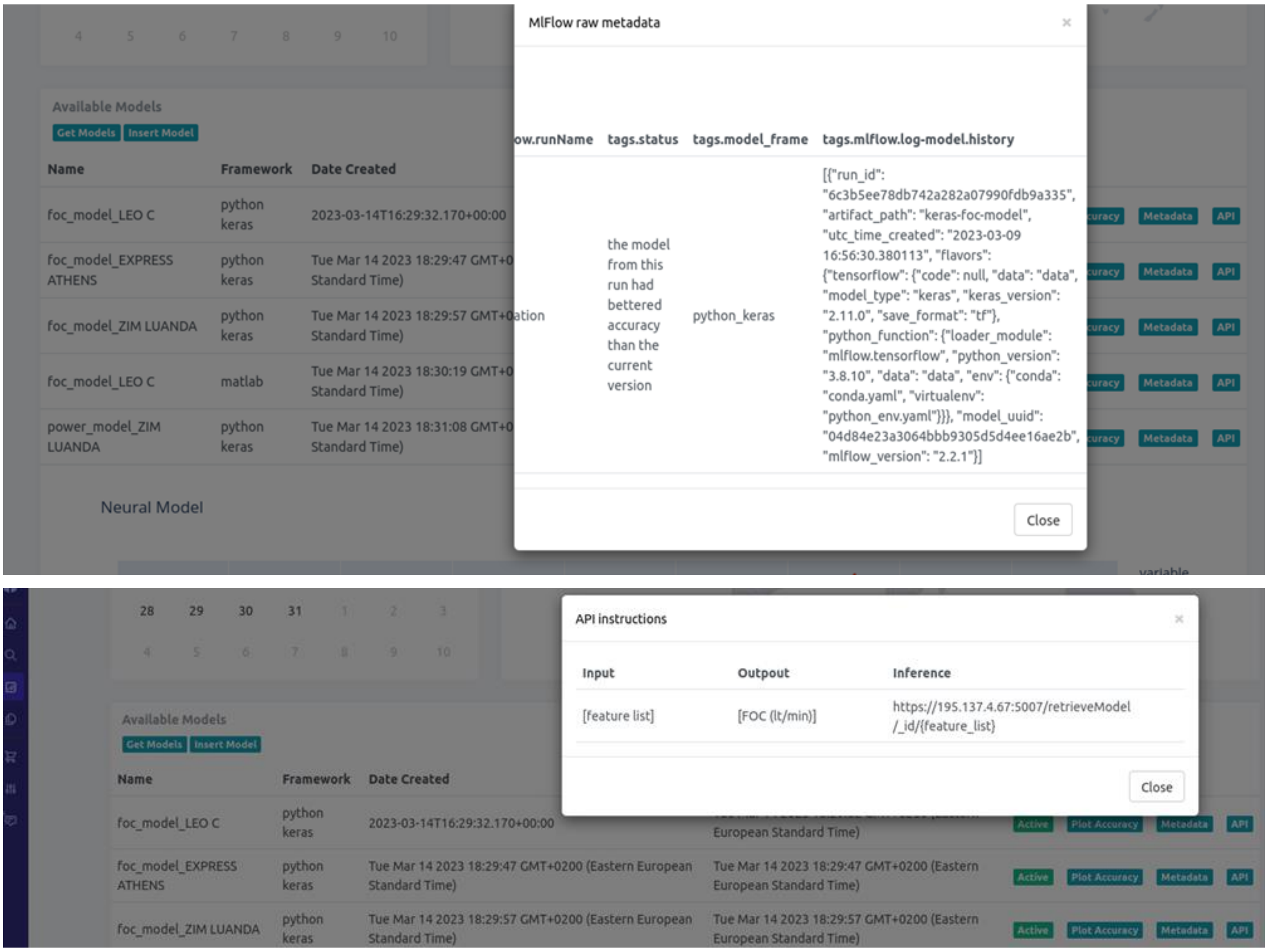

Figure 11: OML GUI. Dedicated Modals for metadata acquisition (top) & model inference instruction via KH gateway for all types of models (data driven, analytical solutions) (bottom).

The aforementioned architecture as a whole, is supported by a set of No-Sql DBs (non-relational databases) that aim to create an adaptive support layer of additional repositories of models with their associated parameters. MongoDB was selected in particular in order to store a variety of parameters describing non-data driven solutions (MATLAB, SIMULINK, etc) (Figure 12), alongside their executables in binary format. A dedicated API with instructions on how to query and consume the executables corresponding to analytical models was developed and hosted for experimentation in the OML GUI where the user can either directly infer the selected model or be informed via appropriately placed widgets and placeholders (Figure 12, 13) on how to insert, query and consume models via the dedicated endpoint specified (API). Mongo-DB will act complimentary with the KG module in order to support and accelerate the implementations of the broader OML frame. In a later stage, databases will be replaced by the fully functional and operable KG.

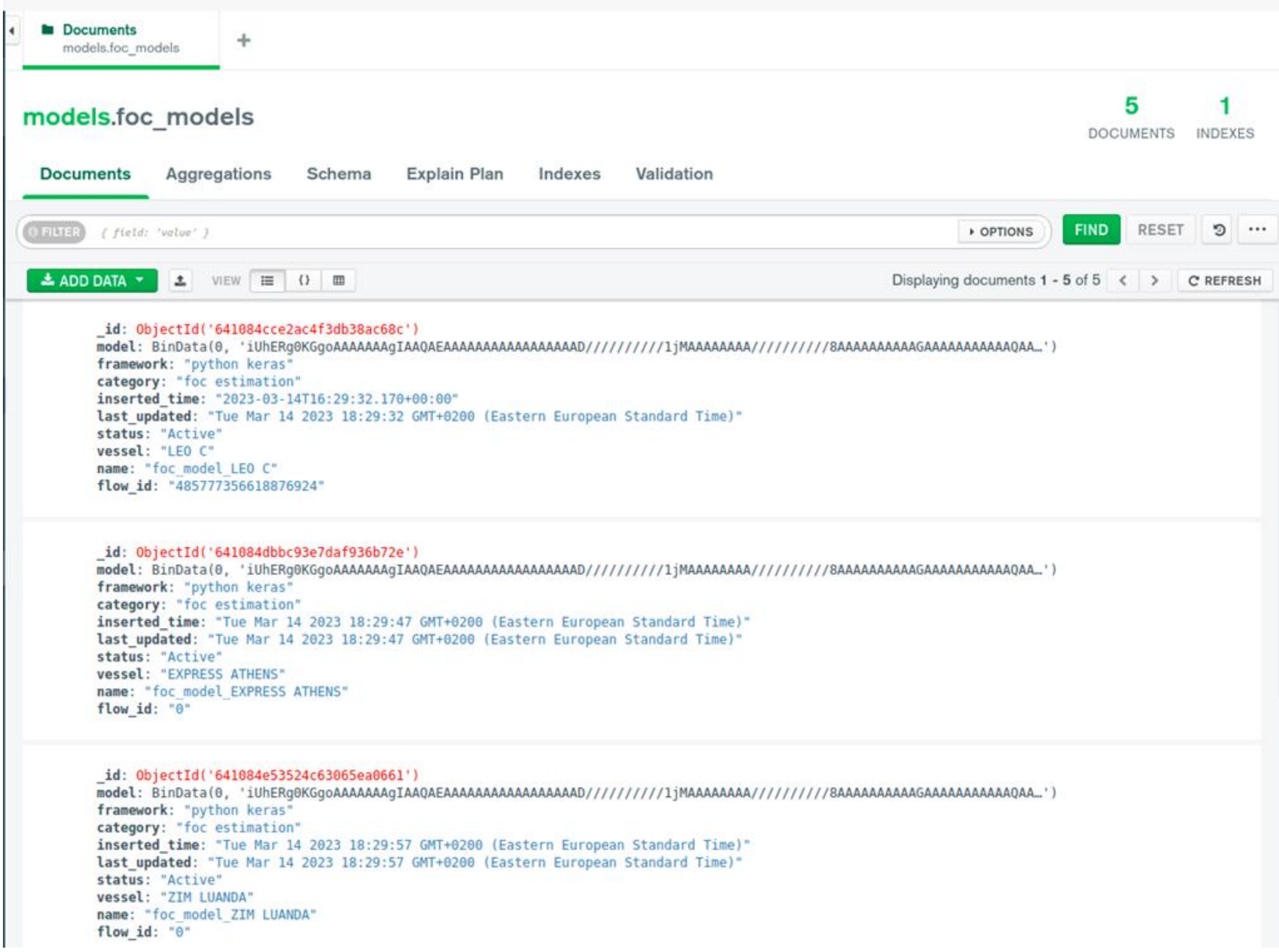

Figure 12: MongoDB snapshot repository.

3.5 Repository of Simulation Models for New Building Design / 3D Modeling

There are various repositories of simulation models and 3D modelling tools available for the maritime sector. One such repository is the Maritime Simulation and Resource Centre (MSRC) in Canada, which offers a wide range of simulation tools and services for the maritime industry. They provide simulation models for ship manoeuvring, port operations, offshore drilling, and more. Another example is the Ship Design, Operation, and Simulation (SDOS) Center at the University of Strathclyde in the UK, which focuses on developing ship design and operation models using advanced simulation and optimization techniques. Additionally, there are several 3D modelling software tools available in the market that can be used for ship design and marine engineering, such as AutoCAD, Rhino, and ShipConstructor. These tools help ship designers and engineers to create and visualise 3D models of ships, marine structures, and offshore platforms, which can aid in design optimization, visualisation, and communication.

- ShipSim: is a software suite that provides modeling and simulation tools for the maritime industry. It includes modules for ship design, hydrodynamic analysis, and maneuvering simulations, among others.

- MARIN: is a research institute that specializes in hydrodynamic research and simulation for the maritime industry. They offer a range of simulation software tools and services, including ship design software, hydrodynamic analysis, and seakeeping simulations.
- DNV GL: is a classification society that provides services to the maritime industry, including ship classification, certification, and verification. They offer a range of simulation software tools and services, including 3D modeling software, hydrodynamic analysis, and structural analysis.
- ShipConstructor: s a software suite that provides 3D modeling tools for ship design and construction. It includes modules for hull modeling, outfitting design, and production planning.

Navisworks: is a 3D modeling software that is commonly used in the maritime sector for ship design and construction. It allows for the creation of detailed 3D models that can be used for visualization, design reviews, and construction planning.

These are just a few examples of the many resources available for simulation models and 3D modeling in the maritime sector.

4 Quantum Analogues Derivation

The recent utilization of quantum advantage and quantum acceleration has demonstrated the viability of quantum approaches in a variety of use-cases, such as decryption, quantum internet, and quantum machine learning (QML). Of these, QML, which is based on variational quantum circuits (VQC), has shown great promise in surpassing the performance of classical neural networks (CNNs). However, the current limitations of quantum technology have necessitated the development of novel quantum neural network architectures, such as Dissipative Quantum Neural Networks (DQNN), to address energy efficiency issues in wireless communication systems.

Axon has conducted a study using DQNN to test its practicality in addressing these energy efficiency issues, which is aligned with the decarbonization objective of the DT4GS project. The results of the simulation demonstrate the following key findings:

- DQNN is highly robust to noisy training datasets, as evidenced by its ability to produce accurate results using real-world problem datasets, such as RSSI in wireless communications.
- When compared to CNNs, QNNs produce comparable results with only a quarter of the available training datasets. This finding is significant as it implies that we can reduce the amount of electric power used in the training phase of machine learning, leading to green computation and decarbonization.

In light of these findings, Axon is considering applying QNNs or Quantum LSTM neural networks to compare against a classical model trained by VLTN. However, since Axon lacks full information about the classical model, such as the purpose of the prediction model, the size of the dataset, the number of inputs and outputs, it remains undecided on which types of quantum neural networks to use. Axon is therefore preparing to work closely with VLTN and other partners to explore the power of QLSTM for time series data prediction. A manuscript on this work will be prepared soon.

5 OML Management Plan

In this section we demonstrate the backbone of a management plan for OML that aims to outline the basic steps in order to continue the employment and further expand the framework proposed in the context of D2.6 in the right direction. It also aims to define OML lifecycle through the project time, as well as to establish a clear pathway to reach the projected goals and KPIs.

5.1 Validation Scenarios

A series of user acceptance tests and validation scenarios will be defined during the next months in order to set the benchmarking criteria and KPIs to validate the core functionality of OML and T2.4 in general. Validation scenarios will include the participation of other DT4GS modules related, directly or indirectly to OML to derive the ideal set of streamlined scenarios that will evaluate and validate the first version of the platform. In the Figure 13 below, we demonstrate a UML that aims to depict the workflow adopted to manage requirements elicitation (technical, high level), validation scenarios and release plans for T2.4.

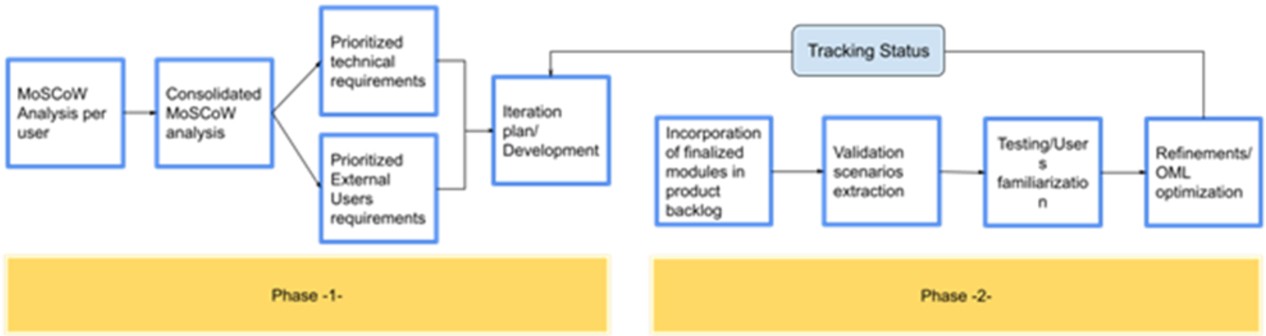

Figure 13: OML user requirements / validation scenarios / management flow.

OML control operation is defined in two phases. During the trial period the system requirements will be specified via a MoSCow analysis, and the first release of the platform will be evaluated internally. The results of the evaluation will define the optimization and further development criteria of the system. In the second phase after the final version of the system (OML V2), the concluding evaluation by external users will define possible improvements and necessary adjustments for the initiation of a market-ready exploitable service. The control and evaluation of systems and services will be based on a set of evaluation criteria derived by continuous training and user familiarisation programs with the system and its functionalities (Training Workshops, Computer Based Training-CBT) with the ultimate goal of collecting as many specifications and improvement criteria as possible.

5.2 Stakeholders Engagement

In order to ensure the success of OML and its integration into the DT4GS ecosystem, it is essential to engage with relevant stakeholders. This includes engaging with potential end-users of the platform, such as operators and service providers, as well as engaging with relevant regulatory bodies and standardization organizations.

To achieve this, OML will conduct stakeholder engagement activities throughout the project lifecycle, including workshops, consultations, and regular communication channels such as newsletters and social media. The aim of these activities will be to gather feedback, build relationships, and ensure that the development of OML remains aligned with the needs and expectations of its stakeholders. To facilitate the process, we will establish a clear segregation of potential stakeholders based on a set individual and indicative attributes (power, legitimacy, urgency), utilising the stakeholders salience model. Furthermore, through a stakeholders engagement matrix we will be able to continuously monitor the needs, expectations, interests and potential impact in order to infer their desired engagement level. AN example of a stakeholders engagement matrix is depicted below.

Stakeholder	Power / Interest	Unaware	Resistant	Neutral	Supportive	Leading
Stakeholder 1	high / low	C			D	
Stakeholder 2	high / medium			C	D	
Stakeholder 3	medium / high				D C	
...						
Stakeholder n	high / high				C	D

Figure 14: Stakeholder engagement matrix with a power / interest classification column.

In addition, OML will also work closely with other DT4GS modules and partners to ensure that the platform is integrated seamlessly into the wider ecosystem. This will include regular communication and collaboration with partners involved in related modules, such as T2.3 (Modelling, Analysis, Simulation, and Optimisation Tools) and T3.1, T3.2 (KH, Ship and company specific DT configuration and Deployment support services.).

Overall, stakeholder engagement will be a key element of the OML management plan, ensuring that the platform is developed in a way that meets the needs and expectations of its users, partners, and regulatory bodies.

6 Conclusions

In this deliverable we presented a prototype version of a novel Open Model Library for the maritime sector that aims to provide a versatile ecosystem for model storage, versioning and deployment with the introduction and utilisation of SOTA automated administrative workflows and support mechanisms. Through this various set of tools and services, OML will be able to create an adaptive multi-tenant platform engaging all users attached to the waterborne sector to partake either actively to the envisaged framework by defining their own set of models or consuming, as end - users, tailor - made services adapted to their own set of long- or short-term goals.

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