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Using Ontologies to Create Machine-Actionable Datasets: Two Case Studies

Jean-Laurent Hippolyte ^{1,*}, Marina Romanchikova ¹, Maurizio Bevilacqua ¹, Paul Duncan ¹, Samuel E. Hunt ¹, Federico Grasso Toro ², Anne-Sophie Piette ³ and Julia Neumann ⁴

¹ National Physical Laboratory, Hampton Road, Teddington TW11 0LW, UK

² Federal Institute of Metrology METAS, Lindenweg 50, CH-3003 Berne-Wabern, Switzerland

³ National Standards, FPS Economy, Koning Albert II laan 16, 1000 Brussels, Belgium

⁴ Physikalisch-Technische Bundesanstalt, Abbestraße 2, 10587 Berlin, Germany

* Correspondence: jean-laurent.hippolyte@npl.co.uk

Abstract: Achieving the highest levels of compliance with the FAIR (findable, accessible, interoperable, reusable) principles for scientific data management and stewardship requires machine-actionable semantic representations of data and metadata. Human and machine interpretation and reuse of measurement datasets rely on metrological information that is often specified inconsistently or cannot be inferred automatically, while several ontologies to capture the metrological information are available, practical implementation examples are few. This work aims to close this gap by discussing how standardised measurement data and metadata could be presented using semantic web technologies. The examples provided in this paper are machine-actionable descriptions of Earth observation and bathymetry measurement datasets, based on two ontologies of quantities and units of measurement selected for their prominence in the semantic web. The selected ontologies demonstrated a good coverage of the concepts related to quantities, dimensions, and individual units as well as systems of units, but showed variations and gaps in the coverage, completeness and traceability of other metrology concept representations such as standard uncertainty, expanded uncertainty, combined uncertainty, coverage factor, probability distribution, etc. These results highlight the need for both (I) user-friendly tools for semantic representations of measurement datasets and (II) the establishment of good practices within each scientific community. Further work will consequently investigate how to support ontology modelling for measurement uncertainty and associated concepts.

Keywords: metrology; machine actionability; ontologies; OM 2.0; QUDT; FAIR principles



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1. Introduction

In metrology, as in other sciences, the importance of well-documented and re-usable data has long been realised. However, the practical mechanisms for capturing and managing scientific data differ vastly between domains, organisations, and individual researchers. Unsurprisingly, a 2016 survey by Nature [1] revealed that more than 70% of researchers could not reproduce another scientist's experiments, and over half have failed to reproduce their own experiments. Ensuring that all data processing steps from the collection of raw data to the generation of final human-interpretable visualisations are traceable requires additional time and effort. An approach to leverage data-sharing infrastructures and systematise the replicability of research data has been proposed in the FAIR (findable, accessible, interoperable, reusable) guiding principles for scientific data management and stewardship [2].

The GO FAIR Initiative [3] expands the FAIR principles with machine-actionability; that is, the capacity of computational systems to find, access, interoperate, and reuse data with no or minimal human intervention. Specifically, for the metrology community, GO FAIR suggests the following FAIRification process: (a) considering the metrology-relevant metadata requirements and research data management (RDM) policies of national

metrology institutes (NMIs); (b) formalising these metrologically relevant considerations as machine-actionable metadata components as metadata for machines (M4M); (c) establishing good semantic representation practices for FAIR metrological information (data and metadata), which in combination with the M4M would result in a FAIR implementation profile (FIP); and, (d) leveraging the FIP to set up FAIR data infrastructures within NMIs, for example, through the use of FAIR data points or FAIR digital objects, contributing to a global internet of FAIR data and services [4].

Complete machine-actionability can be defined as the ability of machines to “make a useful decision regarding data that it has not encountered before” [2] and can only be achieved by specifying the nature and meaning of data using open standards. The availability of mature and standardised formal languages for expressing and inferring knowledge [5] has allowed the development of machine-interpretable specifications of units of measurement (known as ontologies) that build on the seminal research efforts to:

- automate the processing of numerical quantities while ensuring correct dimensional analysis in programming languages [6],
- unify the understanding of “physical dimensions, units of measure, functions of quantities, and dimensionless quantities” across engineering systems [7],
- optimise the conversion of equivalent symbolic combinations of units [8], and
- more generally provide formal specifications of coherent systems of units and dimensions [9].

However, metrology practitioners and researchers face numerous hurdles when trying to use ontologies and formal methods to describe the measurement process and data. These hurdles include a lack of familiarity with semantic technologies, the choice of competing ontologies, terminologies, or standards, differing opinions on how to represent metrological aspects of the datasets, such as units of measurement or measurement uncertainty, and an absence of practical implementation examples. A recent comparison and evaluation of the “broadness and completeness” of nine ontologies for units of measurement revealed syntactic and design issues [10].

To support the ambition of FAIRification [11] in metrology and to provide users with a practical example of using semantic technologies to structure measurement data, we set out to explore how well metrological aspects of datasets can be represented by several existing ontologies. In this study, we adopt a pragmatic approach and focus on two ontologies of units of measurement: the quantities, units, dimensions and data types ontologies (QUDT) [12] and the ontology of units of measure (OM 2.0) [13]. Beyond the two units of measurement ontologies, we take advantage of three ontologies for the contextual specification of measurements and measurement methods: (1) the semantic sensor network (SSN) ontology [14], (2) the sensor, observation, sample, and actuator (SOSA) ontology [15], and (3) the PROV ontology (PROV-O) [16,17]. A more detailed description of the five reused ontologies is given in Section 2.

Using the aforementioned ontologies, we have developed semantic models for two case studies using real-world measurement datasets. The ontologies, case study datasets, evaluation criteria and implementation workflow are summarised in Section 2. The resulting data models and evaluation results are presented in Section 3. The interpretation of the results and their implication for metrologists, researchers and ontology developers are discussed in Sections 4 and 5.

2. Materials and Methods

In this paper, semantic technologies are applied to two real-world scientific datasets, with a focus on metrological aspects, to integrate data and structural knowledge using standardised formalisms. A foundation of semantic technology are ontologies—sets of concepts and categories alongside their properties in relationships. As a tool to represent knowledge, ontologies can be generic (upper-level ontologies) or domain specific, for example representing sensor networks [18], or coordinating measurement [19] or genes [20]. The knowledge expressed in ontologies can be inferred and queried programmatically, thus

fulfilling the GO FAIR machine-actionability requirement. At the same time, it is unclear whether any given domain ontology can adequately represent metrological information to satisfy the GO FAIR requirement (c) listed in Section 1.

Good metrological practice is essential to reproducible scientific results [21]. Reproducibility requires measurement data to be systematically accompanied by consistent information on how the measurements are traceable to an international standard and how the associated measurement uncertainty is quantified. The interoperability of measurement data and their associated metadata, a prerequisite of reproducibility, relies on the proper use of machine-readable metrological concepts such as quantities and units of measurement [22]. It has been further recognised [23] that to truly represent measurement information digitally, metrological concepts such as standard, expanded and combined uncertainty must accompany measurement records and be machine actionable. From a metrological perspective, the expressivity and flexibility of ontologies can help with the curation of complex scientific data and metadata [24], the organisation of measurement device information [25] and the integration of measurement data and their quality information [26].

The applicability of ontologies to support machine readability of metrological concepts is further recognised by the International Committee for Weights and Measures (CIPM) task force set up to develop an overarching digital framework for the International System of Units (SI) [27], intended to provide tools to support the adoption of the FAIR principles and digital tools to aid in the representation of the SI units. With this in mind, a digital metrological (M) layer has been proposed [28], the goal of which is to provide a central register, holding information about quantities, scales and numerical formats relevant to measurement. The “M-layer” would provide the additional information required for digital systems to access a complete picture of metrological information. For example, the M-layer provides a triplet of information when expressing a quantity. For length, this is expressed as $l [L] < l >$ (where $< l >$ specifies the semantics of the quantity and $l[L]$ retains its value (l) and units [L]). However, there currently exists no common ontological representation of underlying metrological concepts that can be generally applied to make full use of the “M-layer” [28], even though such a representation is necessary for consistent the comparability and reproducibility of measurement information.

2.1. Selected Semantic Representations

The most expressive formalisation tool among the semantic web technologies is the OWL 2 Web Ontology Language (referred as OWL in this paper) [29]. In OWL ontologies, knowledge is formalised based on set theory, allowing us to group and recombine real-world or virtual entities of an area of interest. Ontologies are also grounded in logic, allowing us to infer knowledge about entities through automated reasoning. OWL ontologies facilitate the sharing and reuse of knowledge on the web by leveraging uniform resource identifier (URI) mechanisms and a machine-interpretable formalism. Some ontologies are included, among other kinds of digital resources, in an inventory of digital systems for the representation of units [30] published by the Digital Representation of Units of Measurement (DRUM) of the Committee on Data of the International Science Council [31]. Two of these OWL ontologies, listed in the inventory as of August 2022, are actively maintained and were used to implement the case studies:

1. The Ontology of units of Measure (OM) 2.0, version 2.0.38 released on 4 April 2022;
2. Quantities, Units, Dimensions and Data Types (QUDT) ontologies, version 2.1.19 released on 2 August 2022.

OM 2.0 is an improved version of the original ontology of units of measure and related concepts, developed to support quantitative research in the broader Ontology of Quantitative Research [32]. OM 2.0 has been applied in a large spectrum of scientific areas, including food engineering, physics, and economics [33]. The initial development of the ontology was derived from official publications such as the 1987 Symbols, Units, Nomenclature and Fundamental Constants [34], the 1976 CRC Handbook of Chemistry

and Physics [35], the 1995 Guide for the use of the International System of Units [36] and the NIST Reference on Constants, Units, and Uncertainty [37]. OM 2.0 has been actively maintained and improved according to user requests, resulting not only in the inclusion of additional physical dimensions and units, but also in structural changes, such as the capacity to define compound units [38].

QUDT was originally developed to support knowledge integration and information exchange across disciplines within NASA, as part of the NASA Exploration Initiative Ontology Models project [39]. QUDT is actively maintained and published by the eponymous non-profit organisation. QUDT has been applied in many engineering and scientific areas: for example, climate analysis [40], materials design [41], pre-clinical studies [42], and urban data management [43]. QUDT's initial development was based on the 2006 8th edition of the SI Brochure [44], the NIST Reference on Constants, Units, and Uncertainty [37], the 2006 CODATA recommended values of the fundamental physical constants [45], the ISO 80000 Standards for Units and Quantities [46] and the UNECE code list for Units of Measure Used in International Trade [47].

Both OM 2.0 and QUDT have a focus on supporting interoperability between machines, interfacing between humans and machines, and sharing knowledge between humans by preventing ambiguities in the specification of units that could lead to misinterpretation [12].

A crucial requirement of machine-actionability is that no data element should be characterised in isolation. Semantic connections between datasets and information about who/what/how/why they have been generated help humans as well as machines browse, query and interpret data.

Figure 1 is a class diagram that shows how observations can be linked to physical entities and activities reusing upper-level concepts from the SSN and PROV-O ontologies. Each box in the diagram represents a concept. The concept names are prefixed by the ontology that defines them. For example, the concept of *Sensor* in the SOSA ontology is denoted as *sosa:Sensor*. The arrows express how concepts relate to each other. Regular arrows denote a directed association. The direction of the arrow and the label on top of it give an idea of the meaning of the association. For example, *Observations* are made by *Sensors*. Triangle-headed arrows denote a generalisation/specialisation kind of relationship. For example, *Sensors*, *Platforms* and *Collections* are specialised types of *Entities*. Diamond-headed arrows denote an aggregation, where the concept next to the diamond is a kind of container for the concept at the other end of the arrow. For example, *Platform* is a generic concept for any system that contains (hosts) *Sensors*.

Activities such as measurement campaigns produce datasets. Those datasets are considered *Collections* of virtual entities whose primary source is a physical *Sensor*, for example, a radiometer. *Sensors* are mounted on hosting physical systems called *Platforms*, for example, an Earth orbiting satellite. Information about how *Sensors* are hosted by a given *Platform* (for example, the operational time period) can be specified via the SSN concept of *Deployment*. Individual readings from a *Sensor* are contained in an *Observation*, that links the measurement *Result* with the specifications of the *Observable property*. Section 3 gives more details about the semantic representation of *Observations*, *Results* and *Observable properties* with respect to two case studies and two different ontologies of quantities and units of measurement.

2.2. Evaluation Criteria

In the present work, the OM 2.0 and QUDT ontologies were evaluated using the following four criteria:

1. The coverage of the metrology concepts by each ontology, assessing how the two ontologies fulfil the requirements of both case studies in terms of semantic representation of metrological data;

2. Machine-actionability and compliance with the FAIR principles, assessing how the two ontologies facilitate automated processing, interoperability, and reusability of the datasets;
3. Alignment with the “M-layer”, assessing how the two ontologies comply with the semantically consistent triplet of information $q [Q] < q >$ (where q is the value, $[Q]$ is the unit and $< q >$ specifies the semantics of the quantity) [28]; and
4. Traceability to standards, understanding how they link with official/authoritative/normative resources.

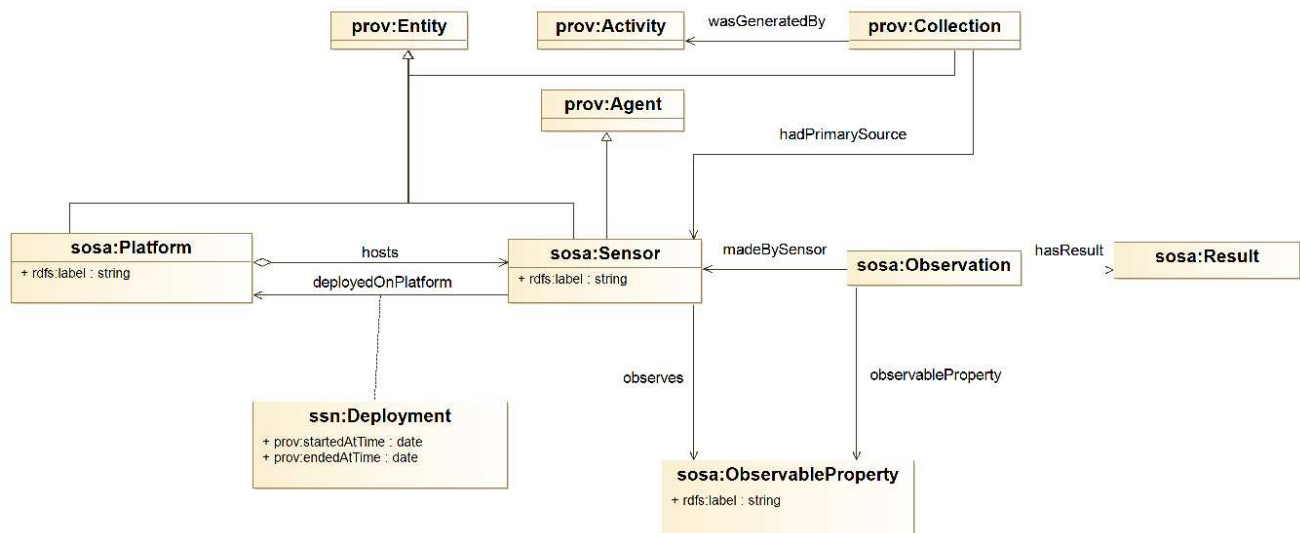


Figure 1. Contextualising measurements using PROV-O and SSN.

2.3. Dataset 1: Earth Observation

Timestamped and geolocated radiance, measured from Earth observation satellites, is one of the basic physical quantities that can form fundamental climate data records (FCDRs). High-level climate analysis relies on the combination and transformation of FCDRs. In this case study, we look at FCDRs formed from the advanced very high-resolution radiometers (AVHRR) or advanced along track scanning radiometers (AATSR) sensors, mounted on Earth observation satellites, that can be used to measure Earth radiance in the thermal infrared region. As this dataset was intended for historical climate analysis, it aimed at harmonising (inter-calibrating) the Earth radiance data captured by multiple satellites (Envisat using an AATSR, MetOp-A and eight NOAA satellites using AVHRRs) with different operating lifetimes between 1992 and 2018 [48]. The satellites and their operational lifetimes are visualised in Figure 2.

The key measurand, the incoming Earth radiance at a specific location and time and wavelength, is derived from (1) direct telemetry observables, such as the digital count number from space, (2) sensor calibration parameters, such as the internal calibration target (ICT) for count numbers, and (3) information about the state of the sensor, such as the instrument temperature.

2.4. Dataset 2: Bathymetry

Bathymetry describes a process of measuring seafloor topography by scanning the seabed with a fan-shaped acoustic beam emitted by a multibeam echosounder (MBES) instrument. The key measurand is the seafloor topography, that is, the result of combining measurements of the seafloor depth and the coordinates relative to the horizontal datum. A horizontal datum is the specific coordinate system on the surface of the Earth that is used to locate points measured in a survey.

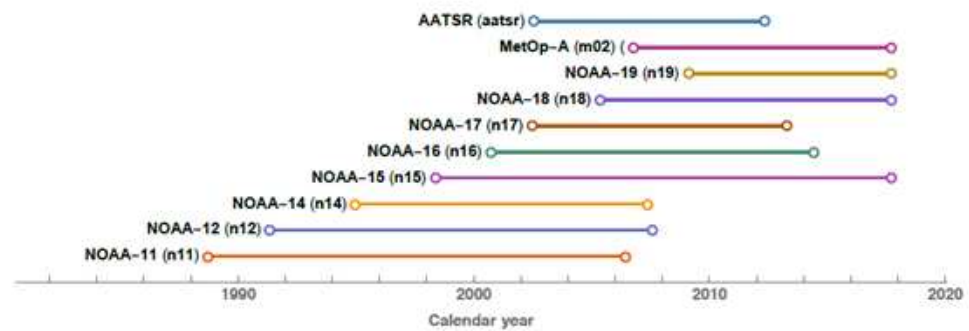


Figure 2. Timeline of NOAA and MetOp satellites acquisition overlapping in time for harmonization purposes [48].

The dataset used in this study was acquired during the July 2019 survey of the Oosthinder sandbanks in the Belgian part of the North Sea [49]. The seafloor depth data illustrated in Figure 3 are stored in ASCII format, while the metadata are partially captured by MBES instrument proprietary software and manually entered by scientists. More details about Dataset 2 can be found in Supplement 2.

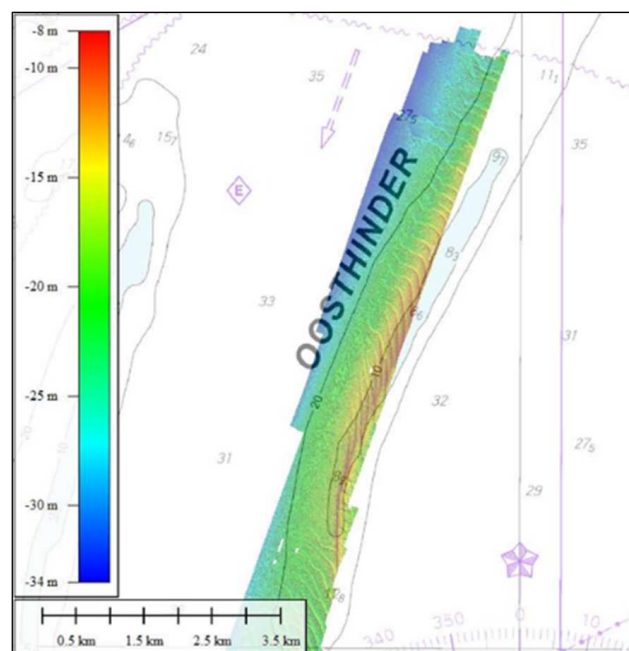


Figure 3. Graphic visualisation of the bathymetric model of the Oosthinder sandbanks, as measured in July 2019 [49].

2.5. Implementation Workflow

The overall goal of the implementation is to demonstrate how the use of ontologies for research dataset descriptions, including metrological features, can be made machine-actionable. The implementation consisted of the steps shown in Figure 4. First, we collected information about the targeted datasets: metadata, documentation and associated scientific publications. The information was then used to implement three kinds of OWL assertions (constructs that allow to state facts about the datasets) that describe:

1. the context in which the dataset was created (provenance);
2. the devices that were used to make the measurements; and
3. the measurement results.

For each case study dataset, two distinct assertion ontologies were then produced, depending on which of the two ontologies of quantities and units of measurement presented

in Section 2.1 was used. The four resulting ontologies were generated using the ontology processing library Apache Jena <https://jena.apache.org/> (accessed on 18 January 2023) [50] and, to facilitate human checking, they are written with the Turtle <https://www.w3.org/TR/turtle/> (accessed on 18 January 2023) notation. The ontologies were then stored into ontology repositories hosted in the Ontotext GraphDB <https://www.ontotext.com/products/graphdb/> (accessed on 18 January 2023) triple store, so that they can be browsed and queried using the SPARQL query language <https://www.w3.org/TR/sparql11-query/> (accessed on 18 January 2023). SPARQL is a standardised protocol and query language for semantic web resources [51], including OWL ontologies. SPARQL underpins ontology-driven machine-actionability by acting as an interface between the formal knowledge representation of OWL ontologies and programs that aim to exploit that knowledge. We created three sets of SPARQL queries:

1. queries that are independent from the ontologies of units of measurement;
2. queries specific to OM 2.0; and
3. queries specific to QUDT.

The generic queries allow us to retrieve contextual information, for example, about when or where the measurements were performed. The specific queries not only demonstrate the retrieval of information about the quantity kind or the unit, but they also show how the semantics captured by QUDT and OM 2.0 combined with the arithmetic capabilities of SPARQL can be used to perform unit conversions.

The four OWL ontologies, the example SPARQL queries and the expected query results as well as additional information about the case study datasets are available online [52].

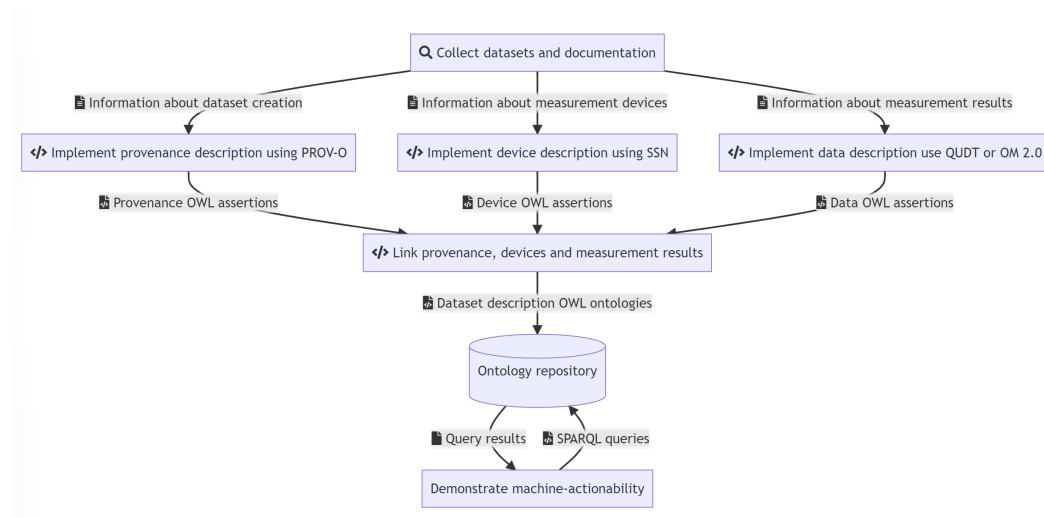


Figure 4. Implementation workflow.

3. Results

Both case studies originally contained limited non-standardised metadata and extensive human-readable documentation. The concepts and relationships formally expressed in the two selected ontologies, OM 2.0 and QUDT, were leveraged to implement machine-actionable representations of the measurements and their respective contexts. The implementation principles are based on the formal alignments and example code snippets provided in W3C's SSN recommendation [53]. The four resulting ontologies (Earth observation using QUDT, Earth observation using OM 2.0, bathymetry using QUDT and bathymetry using OM 2.0) are exclusively composed of assertion axioms, facts about specific real-world entities or specific data elements. Non-specific terminology related to context specification is reused from PROV-O and SSN (following the structure illustrated in Figure 1), while non-specific terminology related to physical quantities and units are reused from either OM 2.0 or QUDT.

3.1. Earth Observation Semantic Representation

The original dataset [54] is a set of independent files that mostly contain time-series data in NetCDF <https://www.unidata.ucar.edu/software/netcdf/> (accessed on 18 January 2023) format, an open file format for array-oriented scientific data that is commonly used in climatology. As illustrated by the QUDT-based example in Figure 5, we modelled each element of a time series as an observation made by a specific sensor and characterised by a specific observed property linked to a QUDT quantity kind, a result quantity value composed of a numerical value (not depicted) and a unit, and a result date and time (not depicted).

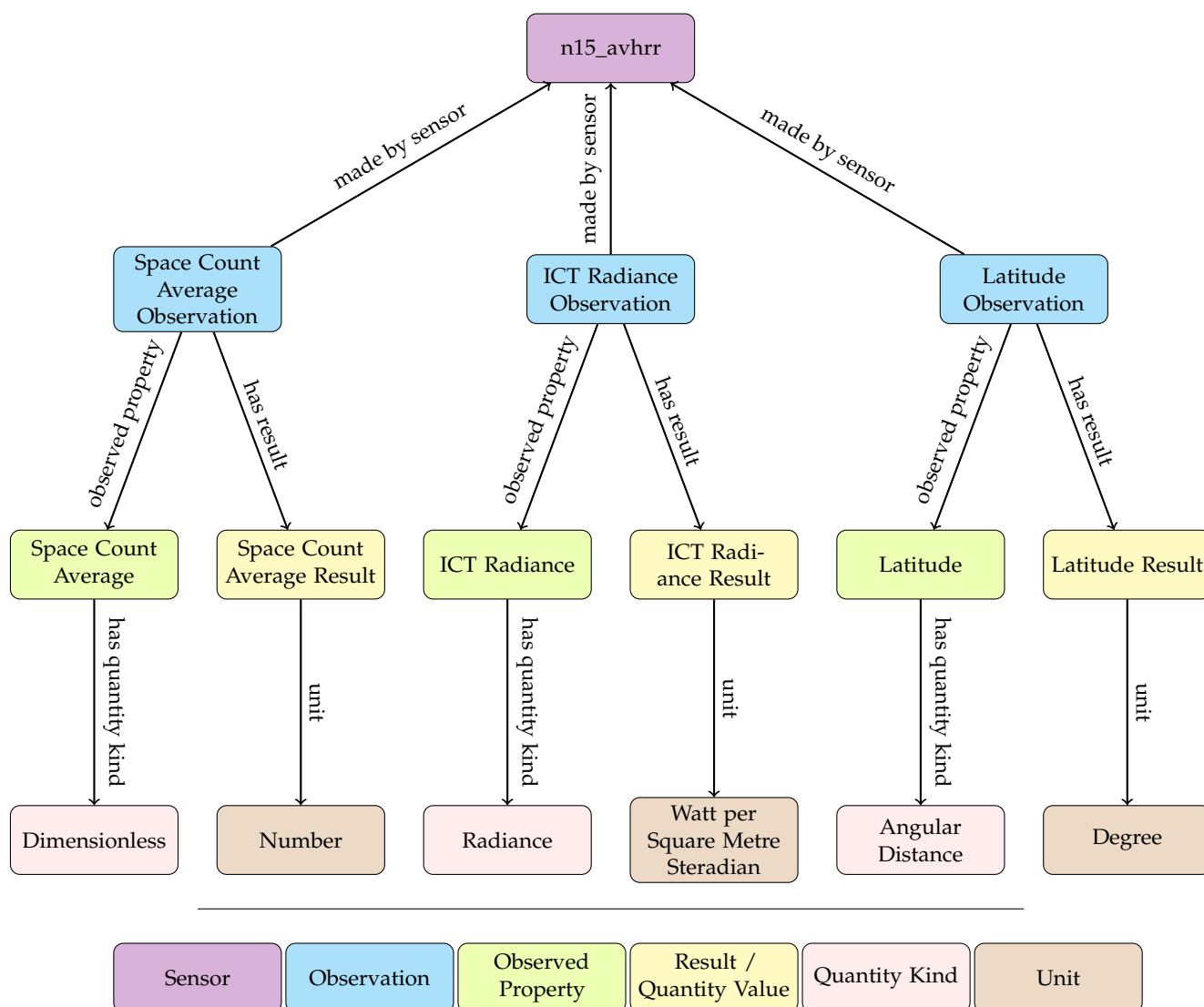


Figure 5. Example semantic representation of satellite observations (using QUDT).

The ontology concepts used in OM 2.0 and the QUDT implementations of the Earth observation case study are summarised in Table 1, where we have given a qualitative but subjective assessment of each concept using red/amber/green background colours. Green indicates that the concept/relationship is defined in the measurement ontology and seems appropriate for the case study. Amber indicates that we made some compromise by using the concept/relationships, either because the semantics do not exactly match (for example, using a generic dimensionless quantity for a count), or the semantics expressed in the measurement ontology are incomplete (for example, standard uncertainty in QUDT is a single numerical value, without any semantic mechanism to associate the influence

factors or parameters such as probability distributions). Finally, red denotes that a relevant concept/relationship is missing from the measurement ontology.

Table 1. Summary of metrology-relevant features implemented for the satellite case study using OM 2.0 and QUDT. Colour denotes how well a concept is defined in the ontology (green: fully, amber: partially, red: missing).

		OM 2.0 entity	QUDT entity
Physical quantities	Space count average	Number class	Dimensionless, instance of QuantityKind class
	ICT count average		
	Earth count	Radiance class	Radiance, instance of QuantityKind class
	ICT radiance		
	Instrument temperature	ThermodynamicTemperature class	ThermodynamicTemperature, instance of QuantityKind class
	Latitude	EclipticLatitude class	AngularDistance, instance of QuantityKind class
	Longitude	EclipticLongitude class	
Units of measurement	Sun-Zenith angle	Angle class	Angle, instance of QuantityKind class
	Satellite-Zenith angle		
	counts	one, instance of PrefixedUnit class	NUM, instance of CountingUnit class, applicable unit of the Dimensionless quantity kind
	°	degree, instance of Unit class	DEG, instance of Unit class, applicable unit of the AngularDistance quantity kind
	K	kelvin, instance of TemperatureUnit class	K, instance of Unit class, applicable unit of the ThermodynamicTemperature quantity kind
Metrology	Wm ² sr ^{−1}	wattPerSquareMetreSteradian, instance of RadianceUnit class	W_PER_M2_SR, instance of Unit class, applicable unit of the Radiance quantity kind
	Systematic uncertainty	n/a	standardUncertainty property
	Random uncertainty	n/a	standardUncertainty property
	Class of observed quantity error correlation	n/a	n/a
	Error correlation matrix	n/a	n/a

3.2. Bathymetric Data Semantic Representation

The original data are a text file that contains the measurements discretised as a matrix of 4351 columns and 10367 rows, where each element is the measured value for a 1 m² area. The origin of the matrix is the datum located at 51°29′24.8″ N, 2°36′08.9″ E. The original tabular format enforced a rectangular shape that does not reflect the actual shape of the surveyed area, with the replacement value −99,999 recorded for locations where no depth measurement was performed. As a result, we decided to only represent cells with actual measurement data in the ontology. The meaningful cells are represented following the structure illustrated with Figure 6. Unlike the Earth observation case study, the timestamp information of each data element is not retained. Consequently, observations cannot be grouped by result time. We reused the concept of “Sample” from SSN to group depth observations with their location relative to the horizontal datum. Each sample is semantically represented as being part of the larger feature of interest that is the sandbank.

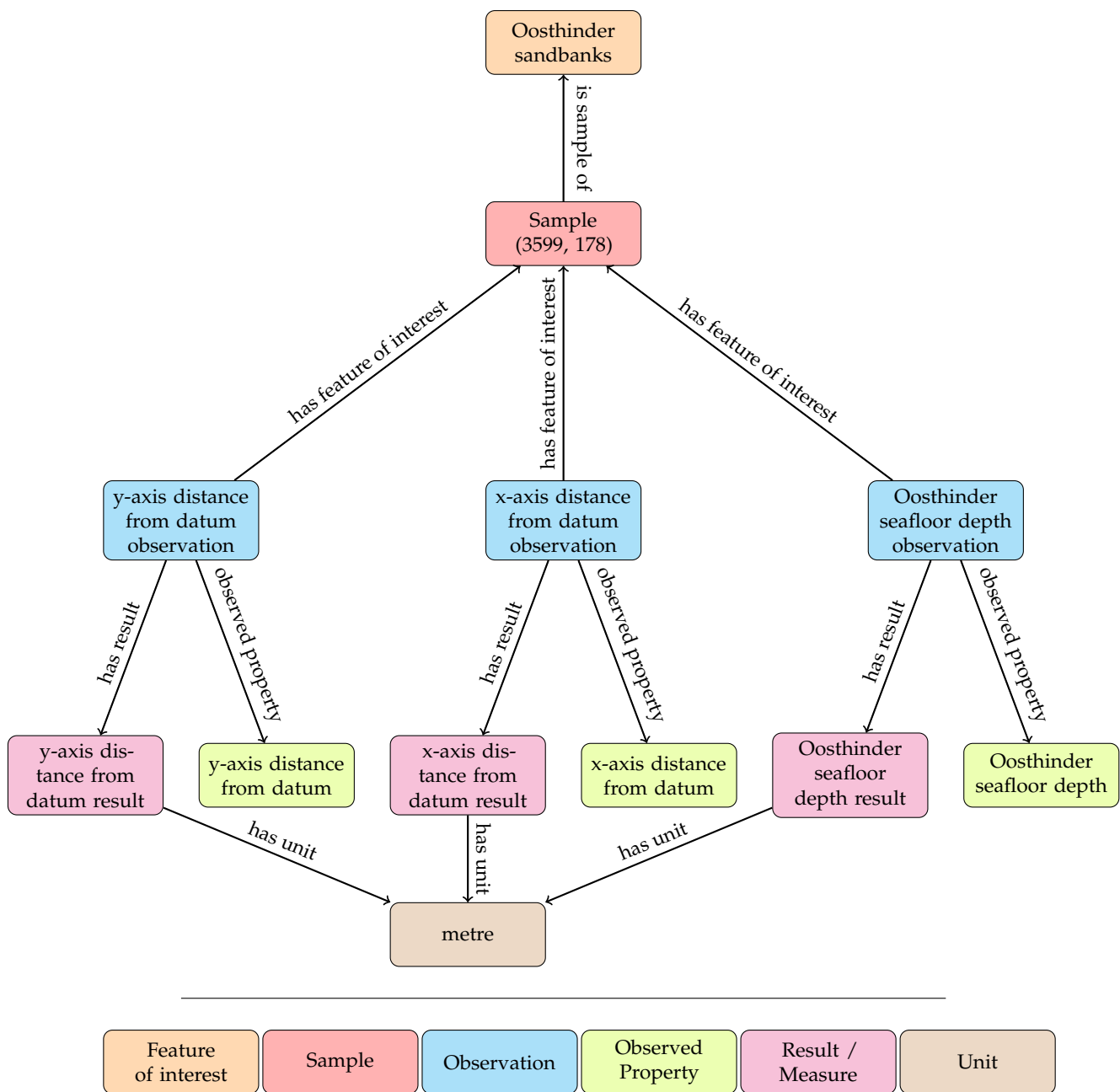


Figure 6. Example semantic representation of bathymetry observations (using OM 2.0).

The ontology concepts used in OM 2.0 and QUDT implementations of the bathymetry case study are summarised in Table 2, with a colour-based qualitative assessment similar to Table 1. It can be noted that we used a workaround solution to specify the uncertainty from the sensor, applying the concept of system property from SSN's system capabilities module to the uncertainty value of the sensor provided by the experimenters.

Table 2. Summary of metrology-relevant features implemented for the bathymetry case study using OM 2.0 and QUDT. Colour denotes how well a concept is defined in the ontology (green: fully, amber: partially, red: missing).

		OM 2.0 entity	QUDT entity
Physical quantities	Depth	Depth class	Depth, instance of QuantityKind class
	x distance to datum	Distance class	Distance, instance of QuantityKind class
	y distance to datum	Radiance class	
Units of measurement	metre	metre, instance of LengthUnit class	M, instance of Unit class, applicable unit of the Length quantity kind
Metrology	Measurement uncertainty	n/a	standardUncertainty property

4. Discussion

Using OM 2.0 and QUDT ontologies we were able to realise the metrological layer [28]. Both allow one to enrich the SSN concept of an observation result with properties to associate a value and a structured unit definition. Despite employing distinct approaches and having varying levels of detail for different kinds of quantity, both models offer semantically rich descriptions of the kind of quantity and dimension.

4.1. Context Information Retrieval

By writing and running SPARQL queries, we were able to retrieve enough information from the dataset descriptions to demonstrate machine-actionability. Due to the reuse of SSN and PROV-O to describe the context of the measurements, some queries are independent from OM 2.0 and QUDT. For example, a query to reproduce the timeline in Figure 2, would simply list all instances of the SSN class for deployment present in the ontology for Dataset 1, enabling access to the name of the deployed satellite, and the start date and end date of its lifecycle. More generally, linking observations to a semantic representation of their sensor makes any information about the sensing infrastructure accessible, and linking the observation with a semantic representation of the dataset makes any provenance information accessible. We showed it was possible to query sufficient information from both ontologies developed for Dataset 2 to reproduce the map shown in Figure 3; these pieces of information are the global coordinates of horizontal data in the World Geodetic System WGS84 and the coordinates of the measurement samples relative to the horizontal data and their measured depth values. OM 2.0 and QUDT provide short readable labels and textual descriptions in English alongside the commonly used symbols. Taking advantage of the arithmetic and assignment functionalities of the SPARQL language [51], we also ran two example queries that performed unit conversions. The first query displayed the measurement values from Dataset 2 in feet, while the original implementation in the ontologies was in metres. The second query displayed the instrument temperature measurement values in degrees Celsius, whereby the original implementation was in kelvin.

4.2. Machine-Actionability of Metrology Concepts

Both ontologies showed variations in the coverage and completeness of metrology concept representations. From a metrological point of view, OM 2.0 and QUDT allow users to query semantically rich information about the measurand associated with an observation or the unit associated with a measured value. For example, the Distance measurand is defined in OM 2.0 and QUDT. In OM 2.0, it is formally defined as a specialisation of Length using OWL language constructs, thus inheriting the semantic links with all units applicable to the Length dimension. QUDT takes a less stringent approach by defining Length as the broader concept of Distance, both modelled as specific quantity kinds. In addition, QUDT potentially enables dimensional analysis by further characterising quantity kinds with dimension vectors. Dimension vectors combine the exponents of eight dimensions: length L , mass M , time T , electric current I , thermodynamic temperature θ , amount of substance N , luminous intensity J and a term for dimensionless quantities D . For example, the dimension

vector of the Distance quantity kind is represented as $\dim \text{Distance} = L^1 M^0 T^0 I^0 \theta^0 N^0 J^0 D^0$ (the dimension vector of the Length quantity) and the dimension vector of the Radiance quantity kind is $\dim \text{Radiance} = L^0 M^1 T^{-3} I^0 \theta^0 N^0 J^0 D^0$ (the dimension vector of the Power per Area Angle quantity). OM 2.0 and QUDT provide formal definitions for systems of units, derived units, and unit prefixes, thus allowing inference against base units and automated conversions. In terms of traceability of units of measurement, QUDT additionally allows us to retrieve standardised unit codes from the International Electrotechnical Commission's Common Data Dictionary (IEC 61360) [55], the United Nations Economic Commission for Europe's Codes for Units of Measure Used in International Trade [47], and the Unified Code for Units of Measure (UCUM) [56].

In terms of core metrological concepts, QUDT defines a measurand under the umbrella term "Quantity Kind" with the definition "any observable property that can be measured and quantified numerically" and requires information such as units and dimensions. Comparing this to the description of measurand in the International Vocabulary of Metrology (VIM) [57], a "quantity intended to be measured" which requires "knowledge on the kind of quantity, description of the state of the phenomenon, body, or substance carrying the quantity, including any relevant component, and the chemical entities involved", suggests that the QUDT description alone cannot express the accepted definition of measurand to provide traceability [23]. The OM 2.0 design, on the other hand, does not give an explicit definition of an overarching concept of quantity kind. Instead, it defines a concept of quantity as "a representation of a quantifiable (standardised) aspect of a phenomenon" and provides a multiplicity of sub-concepts (for example, an Angle class is defined as a subclass of the Quantity class). In other terms, in OM 2.0, concrete realisations of quantities (a value associated with a unit) must be instances of a specific sub-concept of quantity; in QUDT, concrete quantities must be associated with a realisation of a kind of quantity. Although OM 2.0 adopts a different viewpoint, it still fails to provide full traceability to the VIM in that matter.

4.3. Limitations of the Results

This study has limitations with respect to the design and extent of the provenance and metrological descriptions that were implemented as OWL ontologies. Firstly, we were able to capitalise on the existing expertise in ontology design to implement the dataset description ontologies; this would be a learning curve for most scientists. Secondly, the flexibility provided by the OWL language allowed us to make design decisions that could potentially hinder interoperability and reusability, even though we limited our choices of dataset descriptors to the concepts referenced by well-established ontologies. This issue is general to any ontology reuse or re-engineering task. Discrepancies are observed even when asking ontology experts to classify arbitrary domain concepts within the structure of an upper (i.e. more abstract) ontology [58]. Users of ontologies of units of measure, such as the authors, could misunderstand the design intent of the creators of the reused ontologies. Differences in scientific background could result in subtle differences in the understanding of textual definitions. Users could also make mistakes when manually implementing their dataset descriptions. It is also possible that important metadata, provenance or traceability information, such as calibration procedures, mathematical specifications etc. were overlooked due to time constraints. Integration of this metadata would be required to achieve a full semantic description of the quality of data [26], and consequently constitutes a direction for future research. Finally, it must be considered that any ontology can only be as useful as the requirements it was developed to fulfil. The reused ontologies OM 2.0 and QUDT were designed to represent quantities, dimensions, systems of units, and units of measure, rather than support other metrological concepts, such as measurement uncertainty. Other types of semantic representations, such as the SmartCom Digital-SI XML exchange format [59], the UML knowledge model for measurement process [60], or the modelling language for measurement uncertainty evaluation [61], have been created for that purpose.

The integration of the XML schema definitions of the aforementioned models with the presented work would require additional transformation and modelling effort.

5. Conclusions

Metrology and semantic technologies are essential to reproducibility; however, existing ontologies are lacking formal representations of key metrological concepts. While overall, the freedom and flexibility of implementation provided by OM 2.0 and QUDT are useful, the very same features may result in a highly labour-intensive process of data modelling, even for experienced users. The amount of effort needed to create a useful model for a given dataset and a given use case within a given scientific domain could be greatly reduced if examples were provided. The OWL implementations of Earth observation and bathymetry measurement case studies reported in this paper aim to provide such examples to enhance the machine-actionability of the metrological information associated with scientific measurements. Even though we reused the SSN and PROV-O ontologies to contextualise the measurement results, and limited the semantic specifications to either OM 2.0 or QUDT, many arbitrary design decisions had to be made in the OWL implementations. This excessive freedom of choice highlights the need for the establishment of good practices, for example, in the framework of a community-driven FAIRification process. In the long term, more human-friendly tools to generate the ontologies would be helpful, for example, graphical user interfaces or semi-automated generation embedded in data acquisition software. From the point of view of a data (re-)user, some open science repositories streamline semantic querying of datasets by exposing SPARQL endpoints, i.e., web services that can process SPARQL queries sent by software programs. To guarantee the interoperability and enable automated reuse, the development of tools to edit metrologically sound ontologies for dataset descriptions and the deployment of infrastructures to host them will require a good degree of consensus on the specific requirements for semantic representation within scientific communities.

Future work will investigate the integration of the existing ontological and non-ontological models to represent the metrological concepts essential for correct interpretation of the measurement results [22] of the two case studies. Recently developed XML schemas and ontologies, such as the SmartCom Digital-SI XML exchange format [59], the UML knowledge model for measurement process [60], the modelling language for measurement uncertainty evaluation [61], and the ontology for measurement process and uncertainty of results [19] show promise with regard to simplicity of integration and the completeness of the metrological concepts. To further enhance the machine-actionability of the provenance description of the measurement datasets, the I-ADOPT framework ontology [62] and the SciData ontology [63] could be reused, in conjunction with the PROV-O ontology, to achieve a more fine-grained specification of the contextual information and better standardisation of the terms related to scientific experiments, calculations, and theories. We believe that a practical integration of metrological schemas with the case studies presented in this paper will also help answer the open question: is it better to extend existing ontologies of units of measure with further metrology concepts (resulting in greater integration), or to develop a separate metrology ontology that would be agnostic to units of measure ontology (resulting in better interoperability)? A flexible ontology, dedicated to metrological concepts and agnostic to ontologies for quantities and units of measurement, could offer more freedom for scientific communities to develop and implement practices for both FAIR and metrologically accurate representation of their data.

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Abbreviations

The following abbreviations are used in this manuscript:

AATSR	Advanced Along Track Scanning Radiometer
AVHRR	Advanced Very High-Resolution Radiometer
BIPM	International Bureau of Weights and Measures
CIPM	International Committee for Weights and Measures
CODATA	Committee on Data of the International Science Council
DRUM	Digital Representation of Units of Measurement
FAIR	Findable, Accessible, Interoperable, Reusable
FCDR	Fundamental Climate Data Record
FIP	FAIR Implementation Profile
IEC	International Electrotechnical Commission
ISO	International Organization for Standardization
M4M	Metadata for Machines
M-layer	Metrological Layer
MBES	MultiBeam EchoSounder
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NOAA	National Oceanic and Atmospheric Administration
NMI	National Metrology Institute
OM 2.0	Ontology of units of Measure version 2.0
OWL	the OWL 2 Web Ontology Language
PROV-O	PROVenance Ontology
QUDT	Quantities, Units, Dimensions and Data Types ontologies
RDM	Research Data Management
SI	International System of Units
SSN	Semantic Sensor Network
UML	Unified Modeling Language
WGS84	World Geodetic System
XML	Extensible Markup Language

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