



Session: Towards Implementations of Materials and Manufacturing Commons: Digital Marketplaces

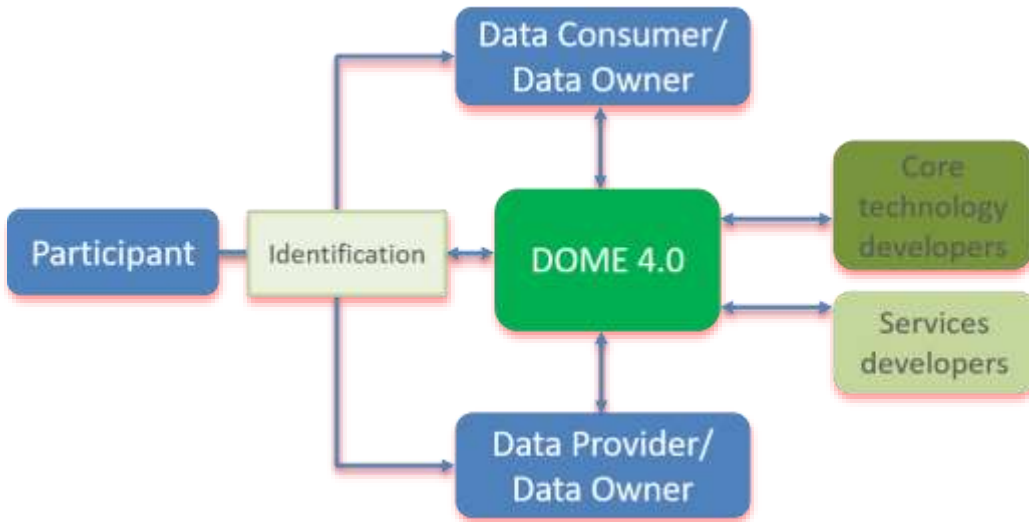
DOME 4.0 / From dataset to data documentation using ontologies

CMCL / Dr Amit Bhave

OntoCommons Workshop, April 4th-6th 2023, Fraunhofer Forum Berlin

Towards Materials and Manufacturing Commons - the enablers Digital Marketplaces, FAIR Principles and Ontologies

An overview



Digital Open Marketplace Ecosystem 4.0

- An ecosystem for transactions between **data prosumers** and **data services** providers
- **Connects** with other marketplaces, OSPs, OTEs, databases and knowledge bases
- **Semantically-enriched** core and 9 industrial/B2B showcases
- **FAIR** principles of data – Findable, Accessible, Interoperable, Reusable

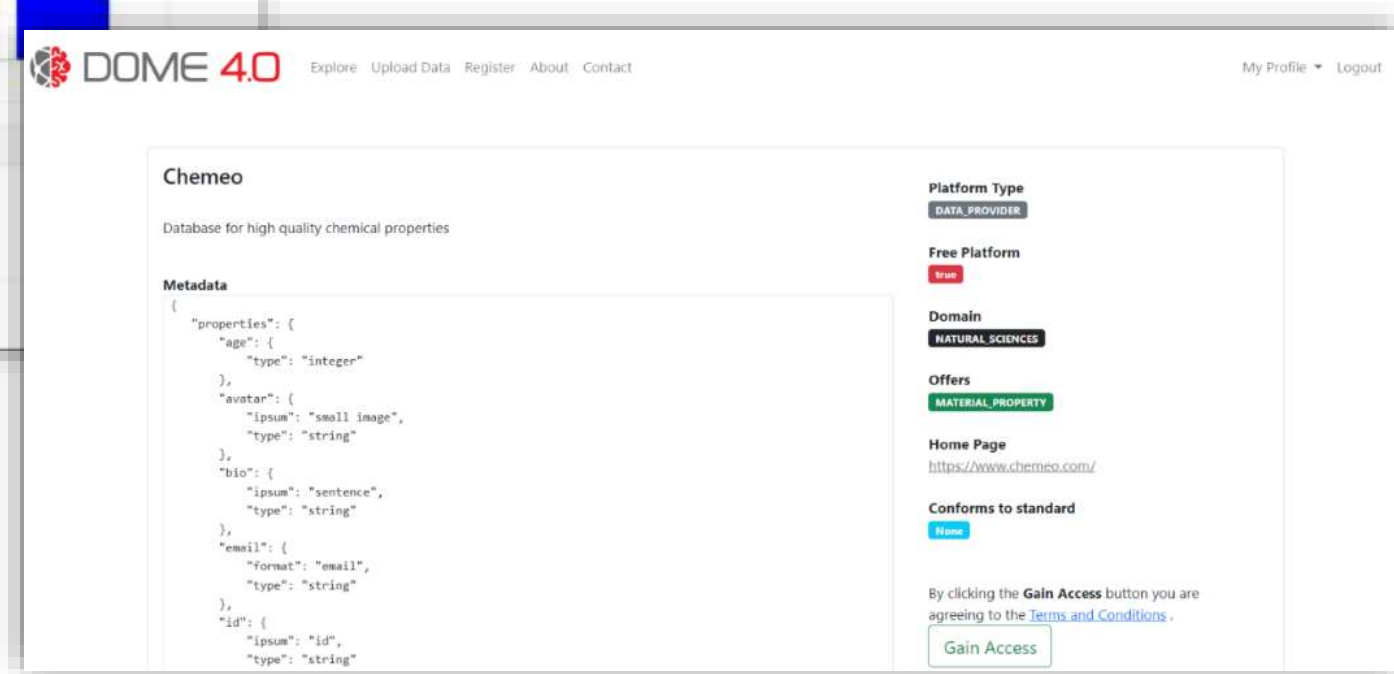
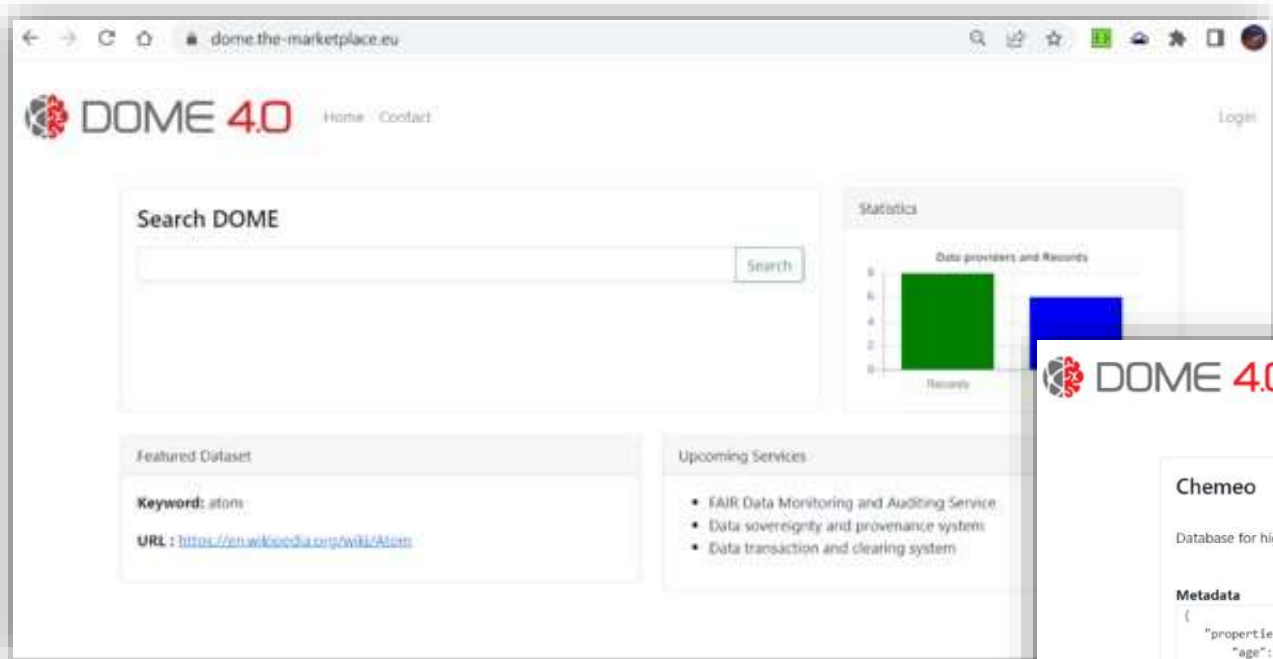


B2B Showcases

NO.	B2B SHOWCASES	DATA SOURCES	INDUSTRIAL SECTORS
1	Chemistry Knowledge Graph (KG) – marine, air quality	Ontokin KB: species, thermodynamics, chemical kinetics, sensors and geo-location data	MARINE, ENVIRONMENTAL, NANOPARTICLES
2	Light weight construction – fibre reinforced plastics	Laboratory experiments, multiscale models	PLASTICS
3	Polymeric additives for coatings: anti-corrosion	Thermodynamic, Laboratory Regulatory, Modelling	POLYMERS
4	Structural adhesives: Fatigue behaviour	Experimental data, MatWeb: Materials property data	ADHESIVES
5	Production equipment tools and service catalogues (metals, plastics, high-tech)	Semantic data repositories of MARKET4.0	MANUFACTURING
6	Turnkey services & custom workflows integrating simulations and data	Materials Cloud (Open Science, FAIR data principles)	MATERIALS
7	Formulated consumer products	gPROMS (PSE), molecular simulation (UKRI), Cheméo (Céondo), and REFPROP (NIST)	CHEMICAL PROCESSES AND MATERIALS
8	Semantic Analytics of Manufacturing Assets	Bosch I4.0 Knowledge Graph, manufacturing production data	SMART MANUFACTURING
9	Virtual development of composite materials	Experimental data, material data sheets	COMPOSITE MATERIALS

DOME 4.0 Platform

Minimum Viable Prototype (MVP) on DigitalOcean



Digital Marketplaces Status and Experience

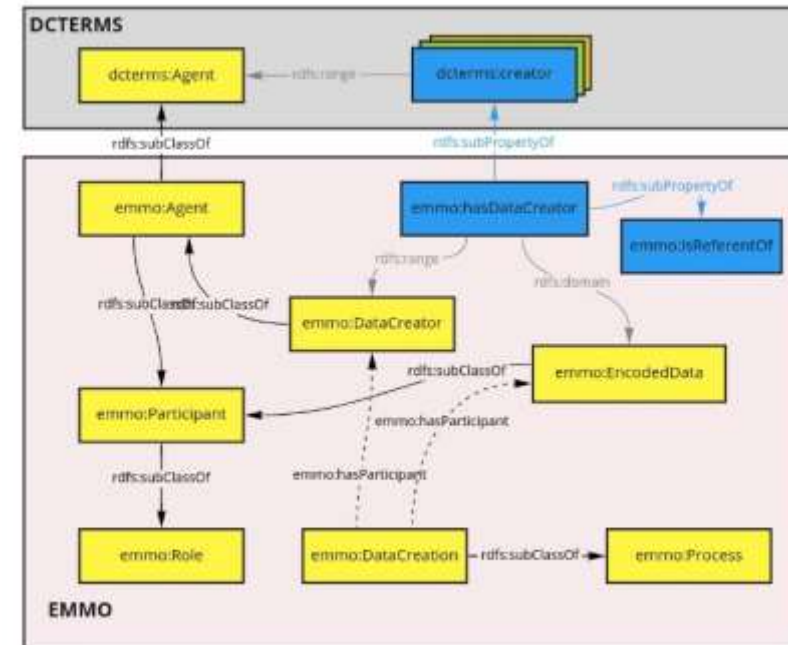
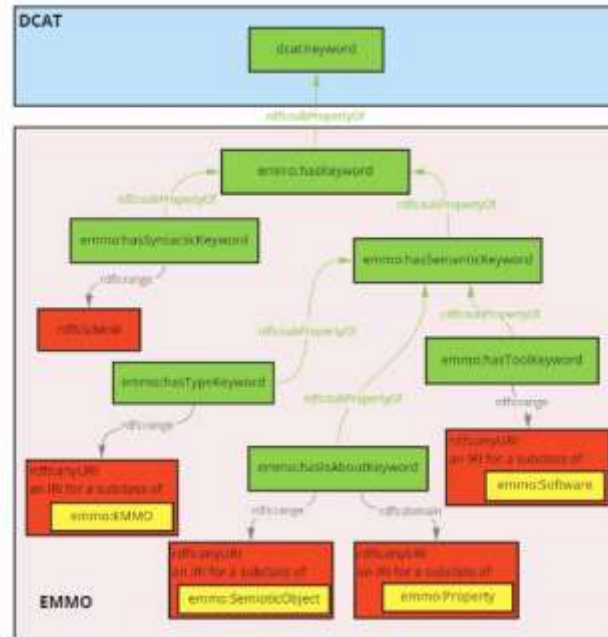
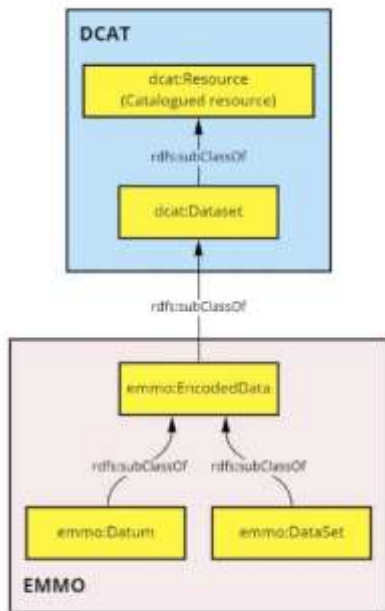
- * What were/are the main **challenges** in the **ontology development pipeline**?
 - * Practitioner's approach and agile software methodology chosen within DOME 4.0
 - * DOME 4.0 ecosystem ontology concepts based on DCAT, MSM, EuroSciVoc, EMMO, EVMPO, etc.
 - * Ontologies reuse demonstrated in certain showcases
 - * Communication between domain experts and ontology developers – expertise within the consortium
- * How did you overcome these challenges?
 - * Release, break, learn and improve in cycles
- * If you used a published Ontology development strategy please state it
(e.g.: LOT, Ontology 101, SAMOD, NeOn, ...)
 - * DCAT semantic enrichment and mapping with EMMO in close cooperation with OntoCommons
 - * No specific ontology development strategy adopted for DOME 4.0 ecosystem and the selected initial B2B showcases

Digital Marketplaces Status and Experience

- * How much value do the ontologies currently bring to your system?
 - * How much value could they potentially bring to your system?
 - * Linking decentralised data sources, software and enabling interoperability
 - * Critical for scalability for smart infrastructure, smart cities and energy applications considered in DOME 4.0.
- * Can your system cope well with ontology updates?
 - * Incomplete: This is an important aspect and while we have performed some investigations on the individual showcases, a comprehensive testing and development will be required.
- * How does your system handle missing ontology terms?
 - * Currently developed via user-intervention/manually
- * Please address the questions above if relevant for your case

Enabling semantic data exchange

*EMMO compliant semantic data exchange ontology created in alignment with the OntoCommons project



DOME 4.0 ecosystem ontology

Aim: An ontology to support the **integration of multiple web-based sources of data and services**, in the areas of **materials modelling and manufacturing**. Support core components of DOME 4.0 platform (e.g., UI filters, broker, connectors to external sources)

Key points: Reuse of assets (see below an extract of RDF-like ones), alignment to EMMO (1.0.0-beta4 version)

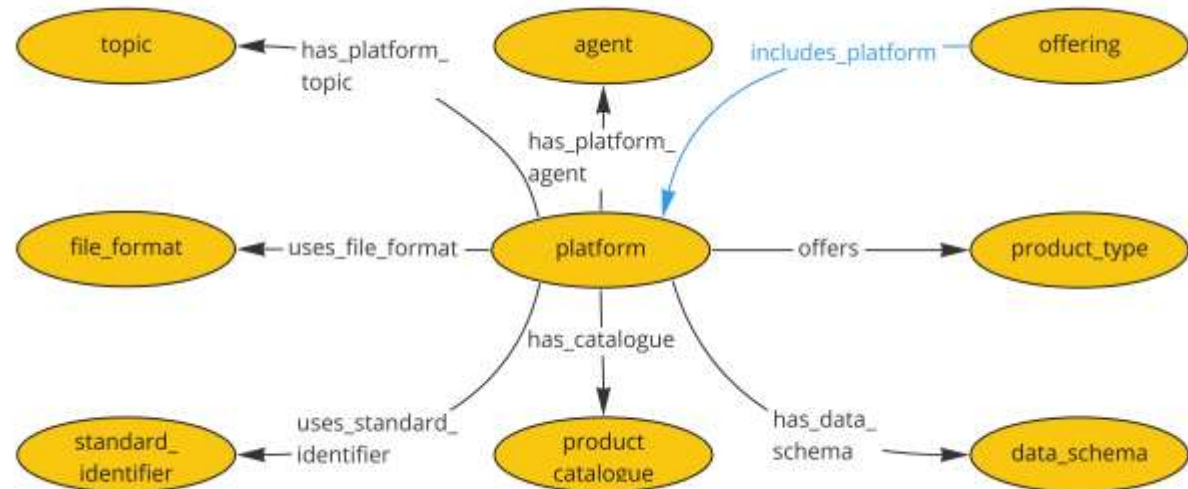
EMMO: Elementary Multiperspective Ontology (TLO)

EVMPPO: European Virtual MarketPlace Ontology (MLO) (cf. VIMMP and EMMC projects)

EuroSciVoc: European Science Vocabulary

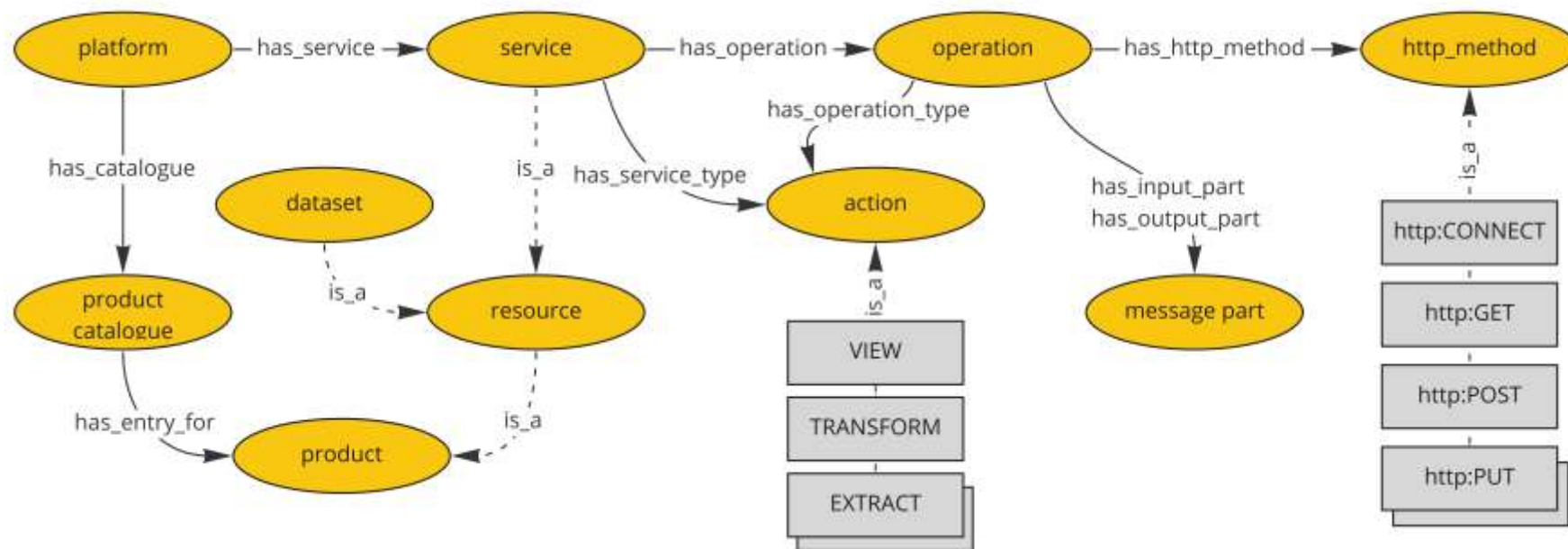
DCAT: Data Catalog Vocabulary

MSM: Minimal Service Model (cf. SOA4All project)



DOME 4.0 Ecosystem ontology

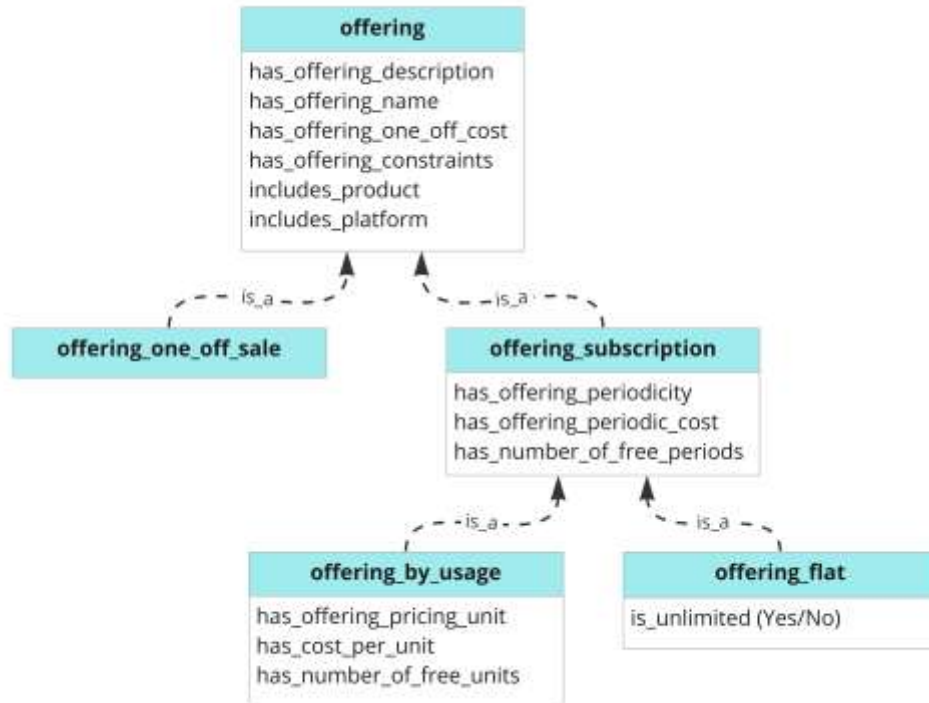
Another view: extract of major concepts and relations between them, focusing on **product catalogue** and **services**. Concepts from MSM, DCAT and HTTP and RoMM (in the action class) are reused.



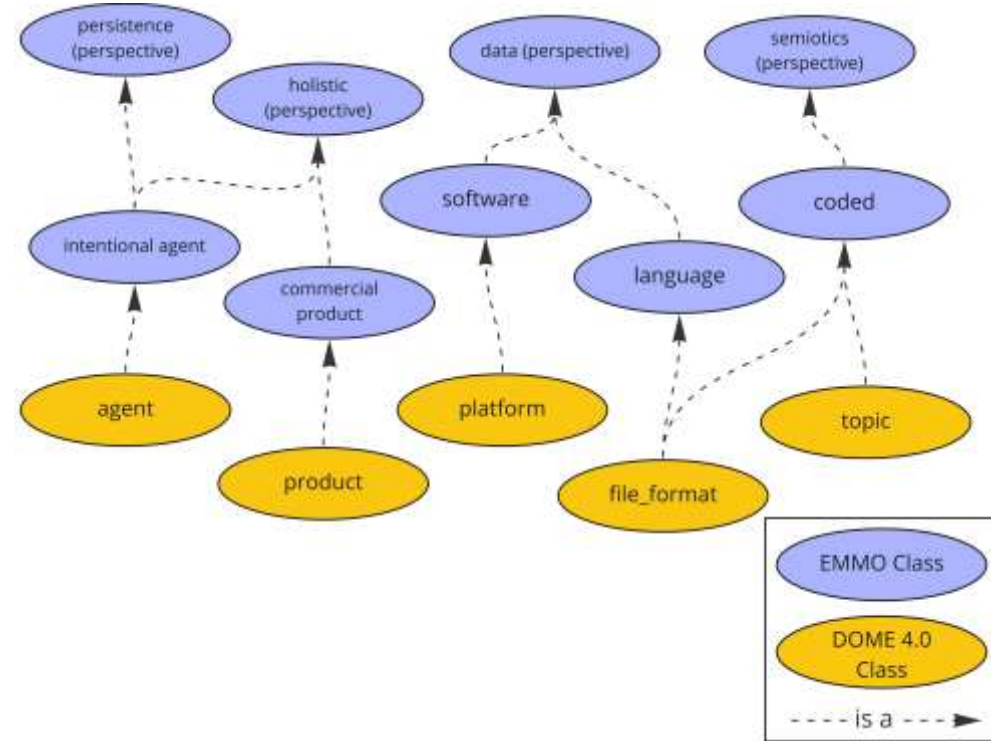
RoMM: A.F. De Baas (ed.), *What makes a material function?*, known as "Review of Materials Modelling". A book, part of a wider effort toward a common vocabulary for the field.

DOME 4.0 Ecosystem ontology

Business/sustainability: The **offering** class, its subclasses and their properties.



An extract of the **alignment** of DOME concepts to the EMMO ones.



Digital Marketplaces Status and Experience

- * Did you consider **FAIR principles** in the **developed ontologies** in your marketplace?
 - * In DOME 4.0 - FAIR monitoring applied to data
 - * Ontologies across the ecosystem and the B2B showcases not yet fully documented.
- * If you use a particular tool please state it if possible (e.g.: MatPortal, widoco, github ...)
 - * Needs to be documented across the B2B showcases
- * In what way your ontologies promote FAIR principles?
 - * Note yet done uniformly across the DOME 4.0 platform and the showcases
 - * For Showcase 1 for example: IRIs for F, Agents enable A, ontologies for I and T-Box facilitates reuse
- * Does your system promote FAIR principles with means other than ontologies?
 - * Ontologies as the prime driver for promoting all four aspects of “FAIR”

FAIR ratings on datasets

- F-UJI – web service that assess FAIRness of research data, <https://www.f-uji.net/index.php>
- Comparison between two datasets

Optimade data in JSON format (4%)

Assessment Results:
Evaluated Resource:

Save JSON New

FAIR level: initial

Resource PID/URL: https://ontolans.optimade/structures/wave_limit:10

DataCite support: enabled

Metric Version: metrics_v0.5


Metric Specification: <https://doi.org/10.3281/remote.4081211>

Software version: 2.2.0

Download assessment results: [JSON](#)

Save and share assessment results:

Summary:



	Score earned:	Fair level:
Findable:	1 of 7	initial
Accessible:	0 of 3	incomplete
Interoperable:	0 of 4	incomplete
Reusable:	0 of 10	incomplete

Ship emissions data in RDF format (18%)

Assessment Results:
Evaluated Resource:

Save JSON New

FAIR level: initial

Resource PID/URL: <https://plot.ontolans.optimade.com/multin/bc158d2e5b170c65a61887898e058627ee70fd68136d717a7de14672c2b64db9010/em10.xml>

DataCite support: enabled

Metric Version: metrics_v0.5


Metric Specification: <https://doi.org/10.3281/remote.4081211>

Software version: 2.2.0

Download assessment results: [JSON](#)

Save and share assessment results:

Summary:



	Score earned:	Fair level:
Findable:	1.5 of 7	initial
Accessible:	1 of 3	initial
Interoperable:	2 of 4	moderate
Reusable:	0 of 10	incomplete

Digital Marketplaces Status and Experience

- * Can you tell us about your experience **integrating your data sets** with the developed ontology / semantic tools ?
 - * Ecosystem level: Concepts based on DCAT, MSM, EuroSciVoc, etc.
 - * Showcase level: ontologies and agents used in Showcase 1
- * Can you demonstrate (or show a conceptual design) how the developed ontologies are used for data sharing?
 - * DOME 4.0 with MARKET 4.0 – IDS connector and OPTIMADE
 - * DOME 4.0 with AiiDALab for data and simulation
 - * DOME 4.0 – Showcase 1 for cross-sector maritime AQ – Smart Port City

Across marketplaces and databases

Manufacturing

MARKET 4.0



Data prosumers

Materials

OPTIMADE



About us

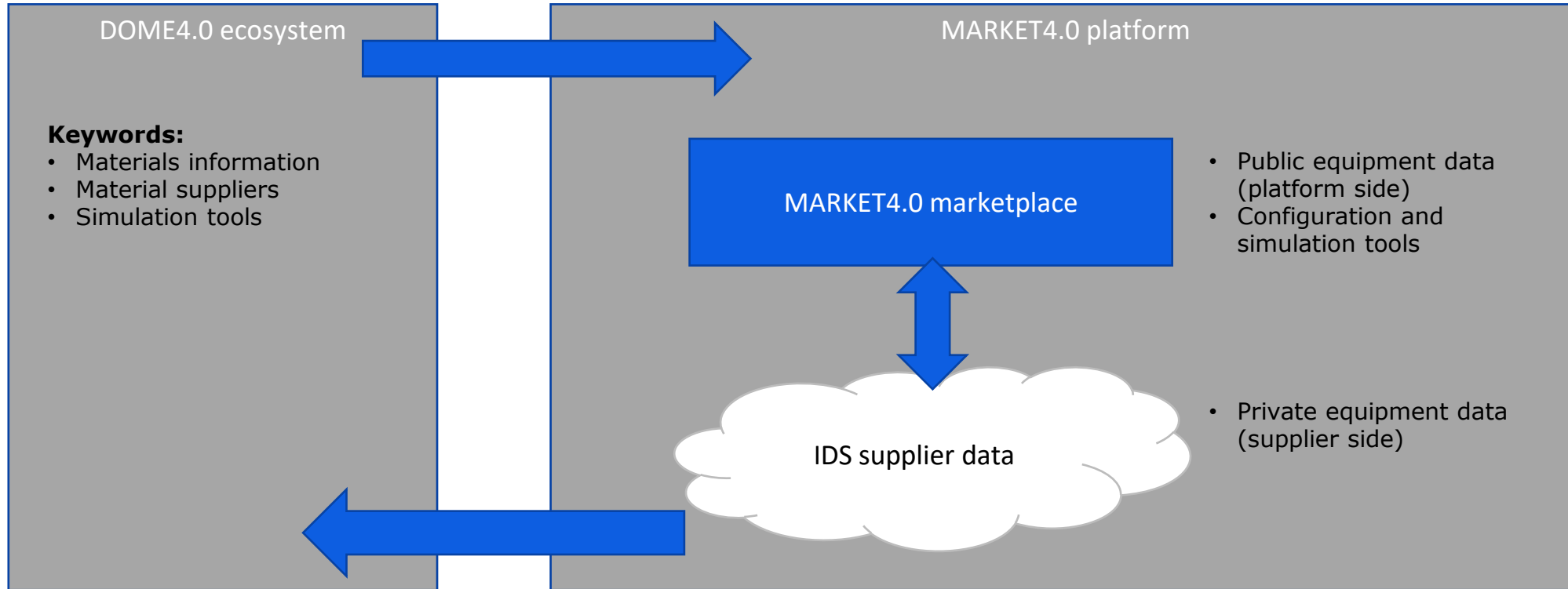
The Open Databases Integration for Materials Design (OPTIMADE) consortium aims to make materials databases interoperable by developing a specification for a common REST API.

Motivation

Designing new materials suitable for specific applications is a long, complex, and costly process. Researchers think of new ideas based on intuition and experience. Their synthesis and evaluation require a tremendous amount of trial and error. In the last few years, there has been a major game change in materials design. Thanks to the exponential growth of computer power, and the development of robust first-principles


Connector, marketplace and data space


DOME4.0 user searches for equipment data or data sets

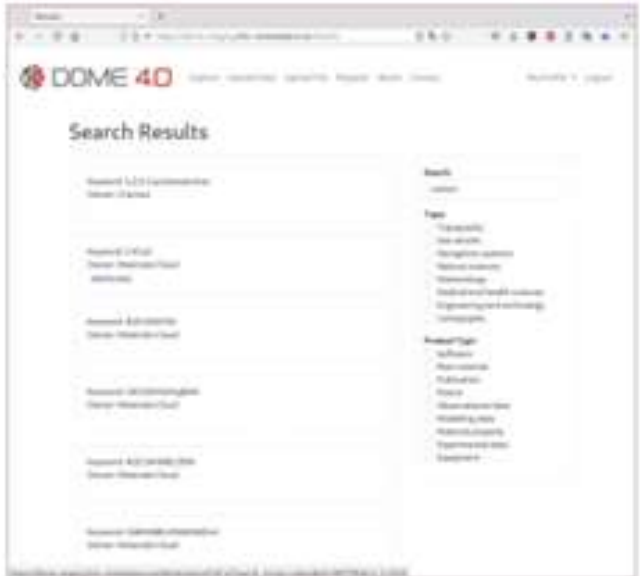


MARKET4.0 user searches for material information / simulation tools


DOME 4.0 – materials data and simulation








Step 1: Search for material



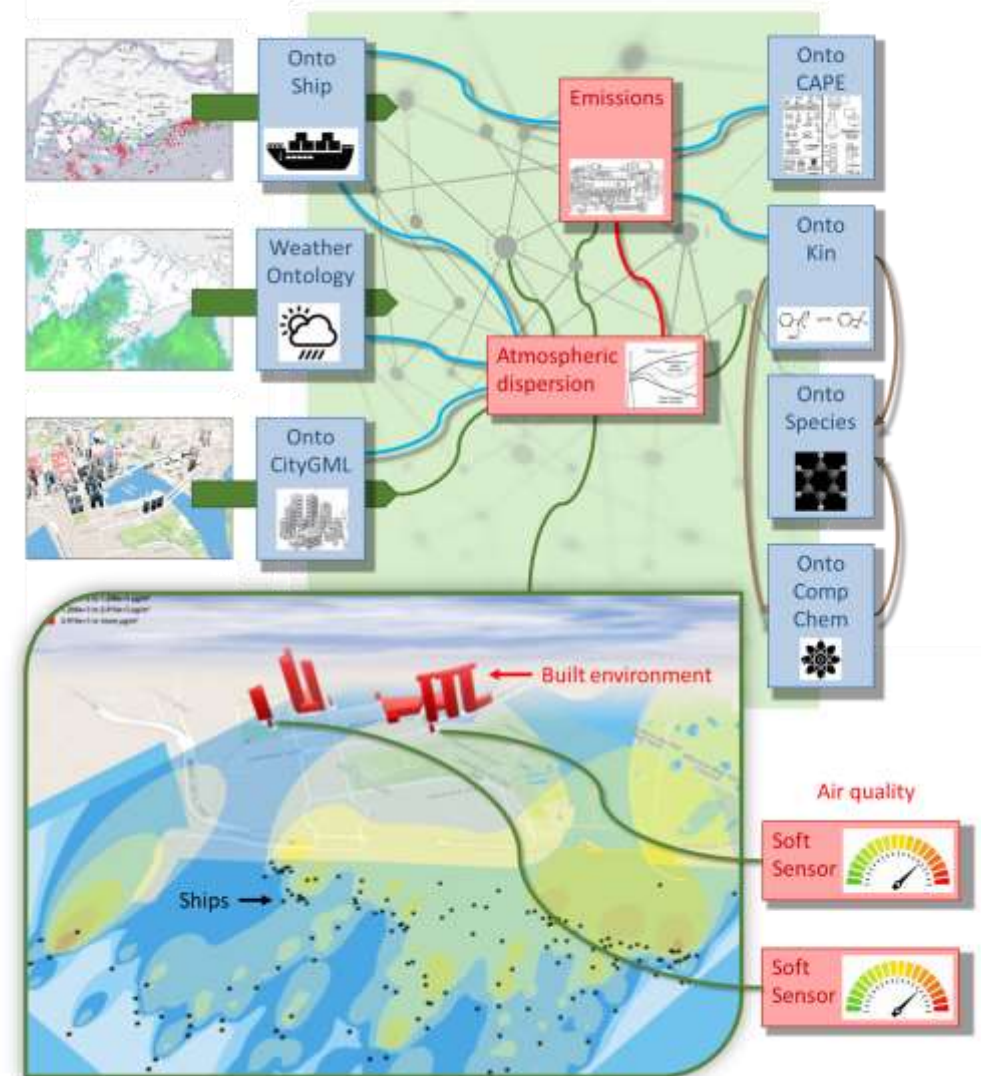
Step 2: Get info for material



Step 3: Hand data off to AiiDALab

Cross-sector data sharing showcases

- * Air Quality (AQ) virtual sensor
 - Augment physical sensors at port/harbor cities
 - Emissions source apportionment
- * Utilise real-time weather data
- * Utilise real-time ship location data from external databases
- * Account for city buildings data
- * Multiple commercial and open-source software
- * Support decision making for local authorities and industry



Digital Marketplaces Status and Experience

- * Do you use / offer / connect to any form of **data space** in your Marketplace environment?
 - * Currently access rights provided to all users once authenticated
 - * Access rights based on restricted views still under development
- * How useful is the platform **outside of the consortium** at the moment?
 - * Not useful outside the consortium yet
 - * Data prosumer onboarding plans from outside the consortium – planned via DOME 4.0 *hackathon* in 2024
- * Do you have a **sustainability concept** for your platform?
 - * Not yet for the entire ecosystem with all the showcases functional
 - * Features of the ecosystem and specific showcases or use cases can prove sustainable for reuse
 - * Support for maintenance of the ecosystem and TRL advancement (4 to 6-7) for new sectors
- * Please explain as far as possible, which were the considerations to influence your choices

DOME 4.0 Hackathon and IEOD



HOME THE PROJECT B2B SHOWCASES LIBRARY NEWS/EVENTS CONTACT

DOME 4.0 Organized An Industrial Engagement Open Day And Hackathons



Digital Marketplaces Status and Experience

- * Name one **concept that works** well in your platform and **another** that poses a **major challenge**.
 - * MVP of the platform for specific features (e.g. search, participant authentication, etc.) along with some of the offline B2B showcases
 - * Major challenge: Still working out how best to deploy resources for implementations vs improvements (e.g. Hyperledger blockchain vs a simplistic database logging solution)

- * List **five lessons learned** during the course of the platform development in the project?
 - * Waterfall method superseded by Agile – frequent releases, break, improve
 - * MVP even with minimal features became an anchor point for core development and use cases
 - * Semantic enrichment based on existing DCAT and EMMO in collaboration with OntoCommons
 - * Multiple B2B showcases of varied semantic maturity
 - * Substantial resource required for the technical development related to the B2B showcases – but worthwhile for dissemination and exploitation purposes

Summary

MVP – simple with initial features, basis for all further development

EMMO-DCAT – bridging between W3C lite ontologies with a highly expressive framework

Ecosystem ontology based on project scope and reuse

Standardisation with *OntoCommons*, EMMC, and EAB

Connected to marketplaces and other projects

The 9 B2B showcases – in progress

Project name: **DOME 4.0** **Digital Open Marketplace Ecosystem 4.0**

Call DT-NMBP-40-2020:
Creating an open marketplace for industrial data (RIA)

The European Union Horizon 2020
Grant Agreement no. 953163





Thank you!

Questions?



www.dome40.eu



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