

# Battery manufacturing knowledge infrastructure requirements for multicriteria optimization based decision support in design of simulation

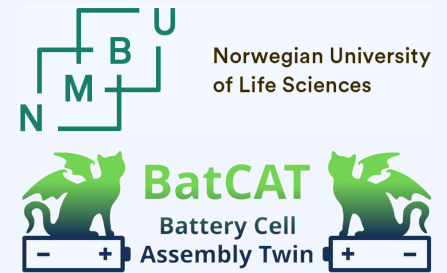
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# BatCAT project summary



- BatCAT (Battery Cell Assembly Twin) is one of the two projects, alongside BATTwin, that will realize the BATTERY 2030+ manufacturability programme from 2024 to 2027 by developing a digital twin platform and data space for battery manufacturing.
- BatCAT primarily considers vanadium-based redox-flow batteries (pilot line at VANEVO) as well as Li-ion and Na-ion coin cells (pilot line at CPI).
- MCO and logical programming will be used for a decision support system.
- Simulation methods include MD/MC with classical pair potentials, DPD with nDPD potentials, and continuum simulations, including Poisson-Nernst-Planck solvers and equivalent-circuit as well as population balance models.
- Time-series predictors will include cellular neural networks with the potential for exploitation by on-chip deployment.

# Basic requirements: Key objectives for the project

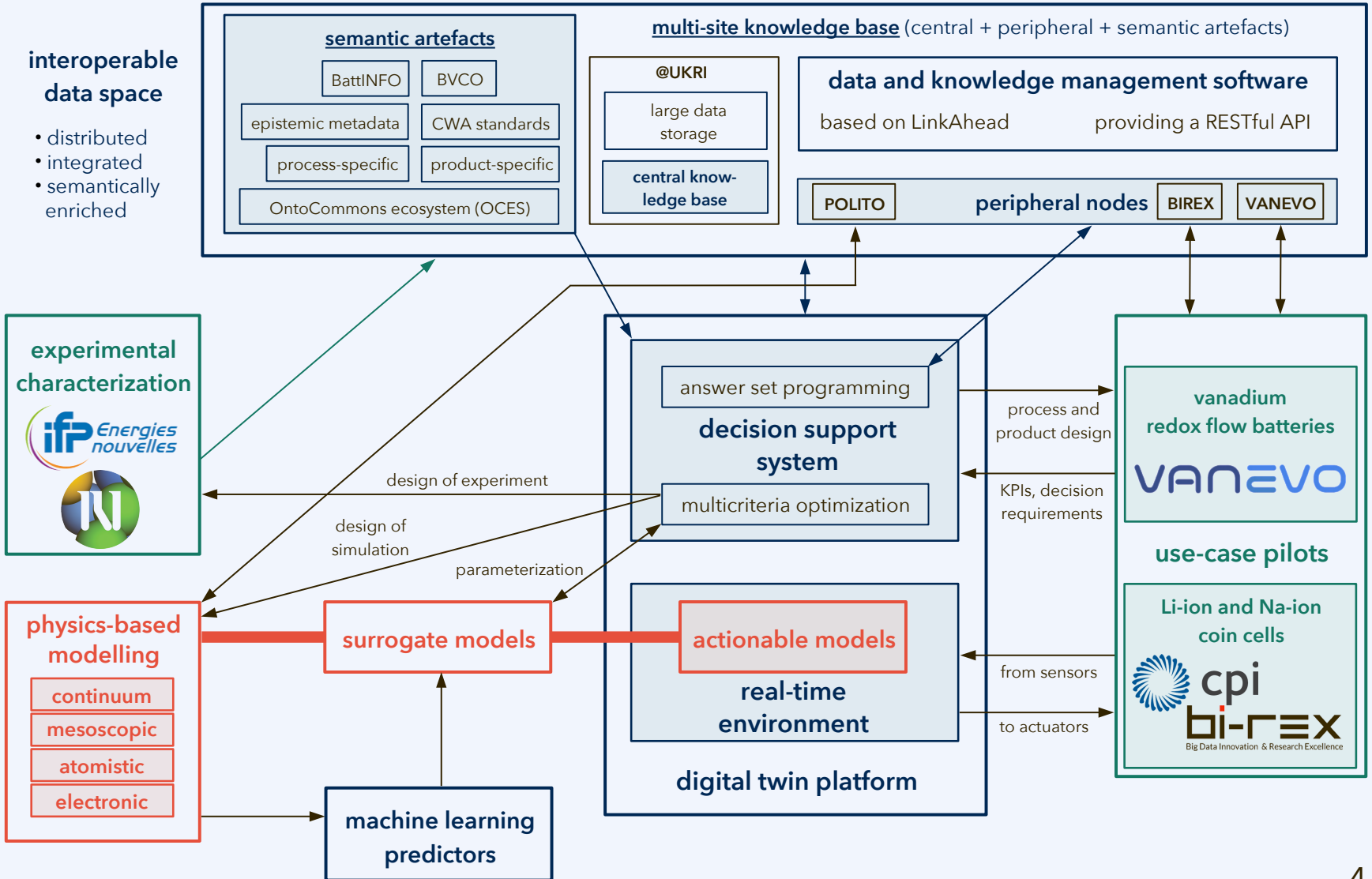
WP lead		IFPEN	POLITO	RPTU	UKRI	ITWM	CPI	GCL	NMBU
		WP1 characterization	WP2 simulation	WP3 interoperability	WP4 knowledge	WP5 digital twin	WP6 demonstration	WP7 exploitation	WP8 management
KO1	experiments and sensorics	main responsible work package	minor contribution	some contribution	some contribution	substantial contribution	minor contribution	minor contribution	minor contribution
KO2	multiphysics modelling	some contribution	main responsible work package	substantial contribution	some contribution	substantial contribution	minor contribution	minor contribution	minor contribution
KO3	technical interoperability	minor contribution	substantial contribution	main responsible work package	some contribution	substantial contribution	minor contribution	substantial contribution	minor contribution
KO4	integrated data space	substantial contribution	substantial contribution	some contribution	main responsible work package	some contribution	minor contribution	minor contribution	minor contribution
KO5	digital twin platform	some contribution	some contribution	substantial contribution	substantial contribution	main responsible work package	substantial contribution	substantial contribution	minor contribution
KO6	pilot and transferability	substantial contribution	minor contribution	some contribution	substantial contribution	substantial contribution	main responsible work package	substantial contribution	minor contribution
KO7	long-term exploitation	minor contribution	minor contribution	substantial contribution	some contribution	substantial contribution	substantial contribution	main responsible work package	substantial contribution

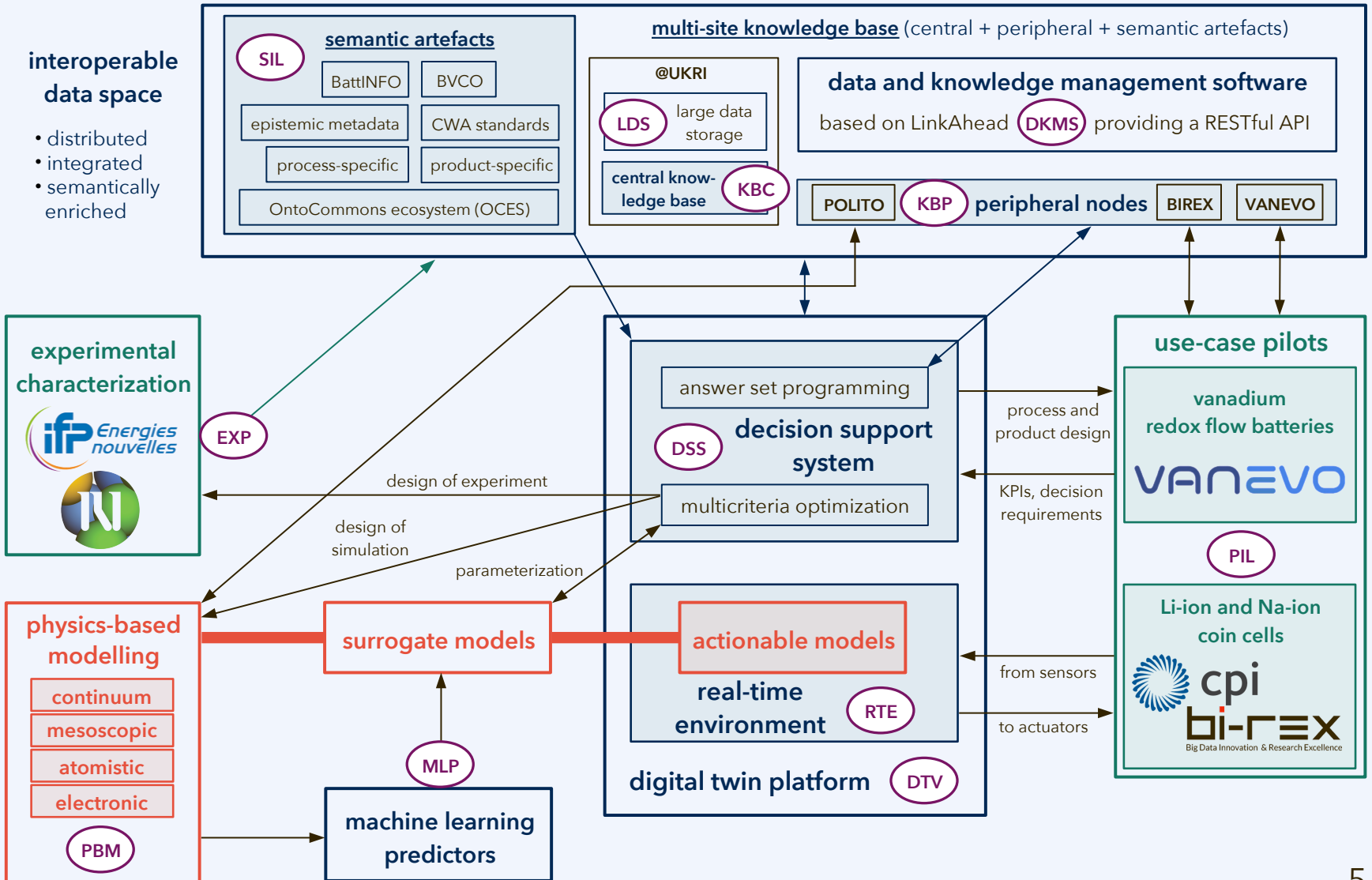
main responsible work package	substantial contribution	some contribution	minor contribution

- KO1:** In situ measurements and **characterization**, targeting cell manufacturing and behaviour.
- KO2:** Multiscale and **multiphysics modelling**, targeting scalability and computational efficiency.
- KO3:** Technical interoperability and **linking of models, data, and processes**.
- KO4:** **Knowledge base** for a federated, integrated, and semantically enriched data space.
- KO5:** Interpretable industrial **decision support system** and Industry 5.0 **real-time environment**.
- KO6:** Demonstrate the developments in a **pilot production line** and verify transferability.
- KO7:** Create the preconditions for a **long-term exploitation** of the project outcomes.

# BatCAT architecture



# BatCAT architecture: Design targets



# Requirements analysis

The following tasks conduct internal & external **stakeholder interviews** as part of an **agile requirements analysis** jointly, with task T4.1 taking the lead:

T4.1: "Knowledge infrastructure requirements analysis" (lead: NMBU, contrib.: AAU, DTU, IS)

T4.3: "Data and metadata landscape" (lead: UKRI, contrib.: CPI, IFPEN, NIC, SIMULA)

- T4.1&3 deliver **D4.1**, "Data landscape & infrastructure related requirements," by **M9**.

T6.1: "Industrial & use-case requirements analysis" (lead: VANEVO, contrib.: BIREX, CPI, DTU)

- T6.1 delivers **D6.1**, "Use-case requirements for validation," by **M9**.

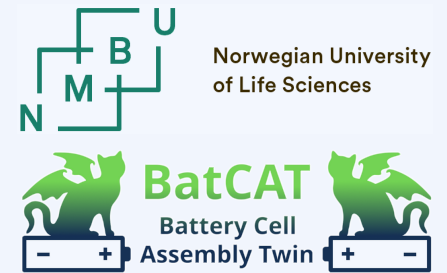
T7.2: "Citizens' role and societal & gender dimensions" (lead: NMBU, contrib.: DTU, POLITO)

- "positive and potentially adverse aspects of the societal (incl. citizens', gender) dimensions of the impact, conducting an agile requirements analysis from early on"

We proceed in the following stages:

- 1) Preparatory **first-stage interviews** (30 minutes), exchange of ideas.
- 2) **Second-stage interviews** (30 minutes), developing concrete user stories.
- 3) **Half-day workshop** (24.6.) for revision and extension of deduced requirements.
- 4) Analysis and catalogue of requirements (**deliverables** D4.1 and D6.1).

# Requirements analysis



**Agile reqs analysis** based on **user stories** and **epics**.

We collected & accepted 56 user stories, which are categorized according to:

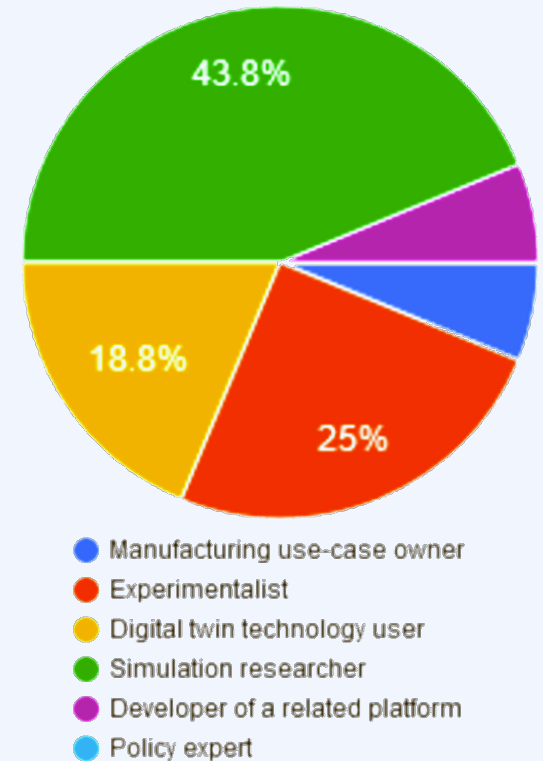
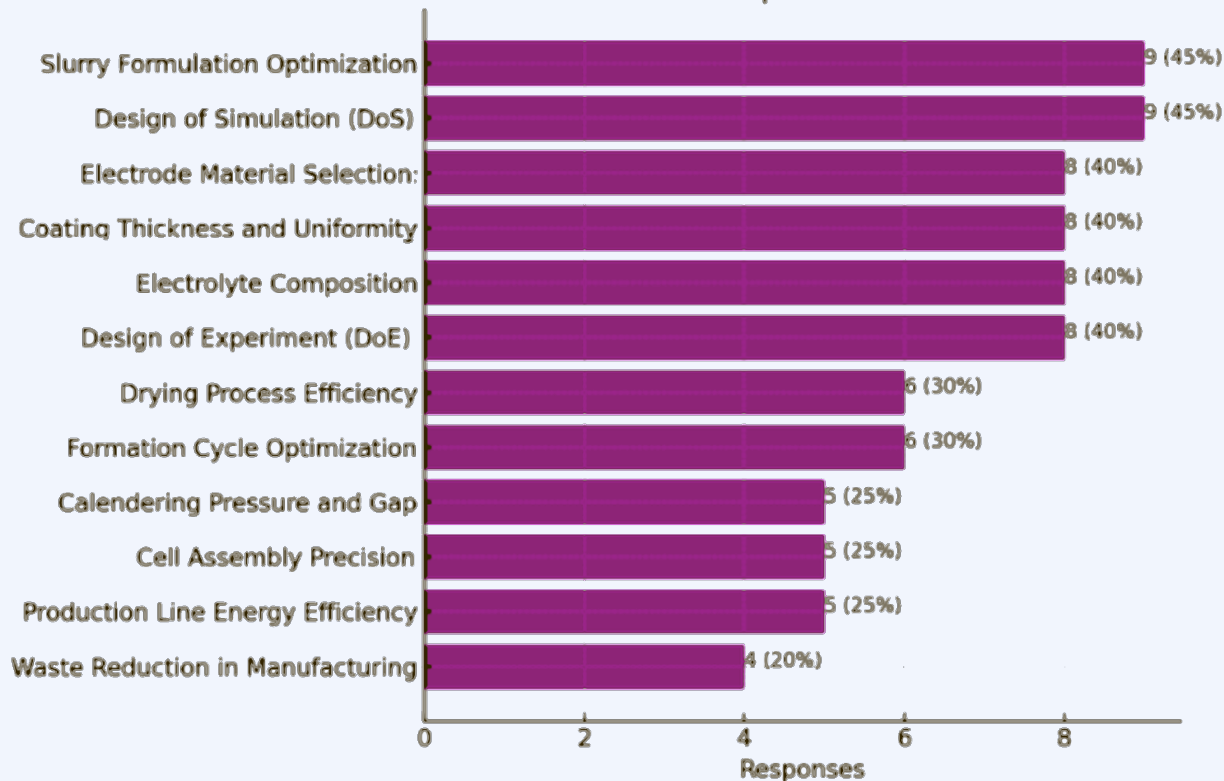
- **Persona:** What kind of user/developer has such a requirement?
  - Personas: (1) AI: Administrator - internal, (2) DI: Digital twin technology user - internal, ..., (8) EE: Experimentalist - external, (9) PE: Policy expert - external
- **Epic:** What is being pursued as an overarching aim?
  - The 56 user stories are grouped into 23 epics.
- **Design target:** What is it for?
  - There are 12 design targets (see architecture figure), plus a separate category for non-functional requirements (without specific design target).
- **“MoSCoW” prioritization:** “Must”, “should”, “could”, or “will not”?

Example: As a **policy expert**, in order to **enable RFB manufacturers** to calculate entries for the **digital product passport**, I want (myself/manufacturers) to use the **decision support system** to predict the carbon footprint at process/product design stage. (“S”: “Should”.)

# Decision support by multicriteria optimization

Multicriteria optimization (MCO) will be used for a variety of purposes. Right now we are prioritizing design of simulation (DoS) for surrogate model creation.

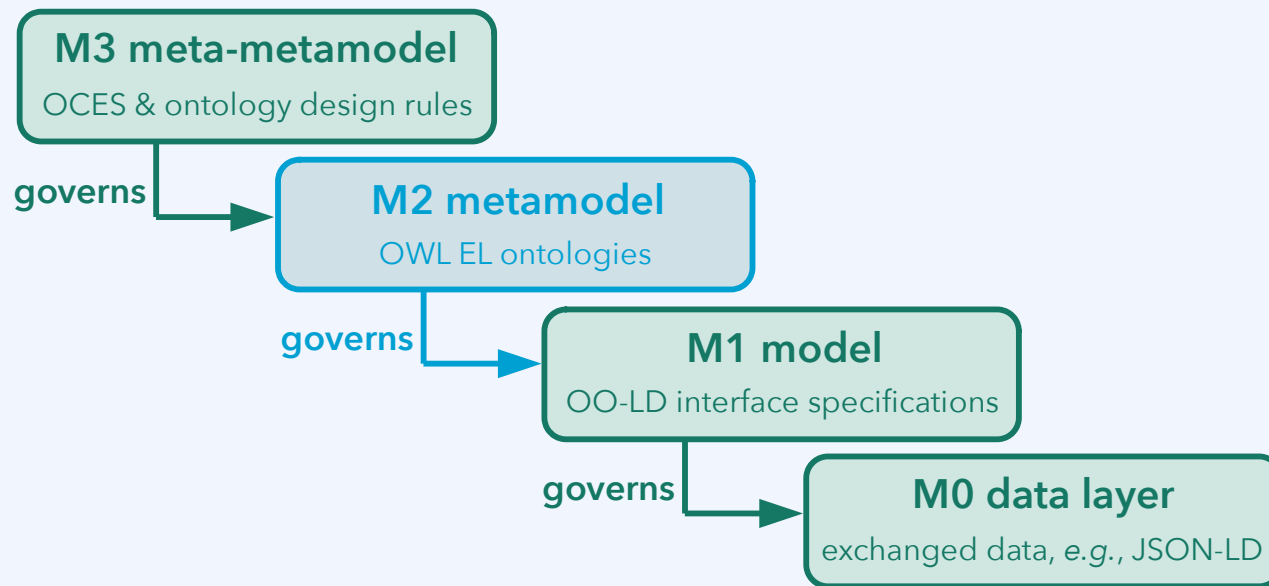
Possible MCO-Optimization Problems





# Semantic interoperability layer

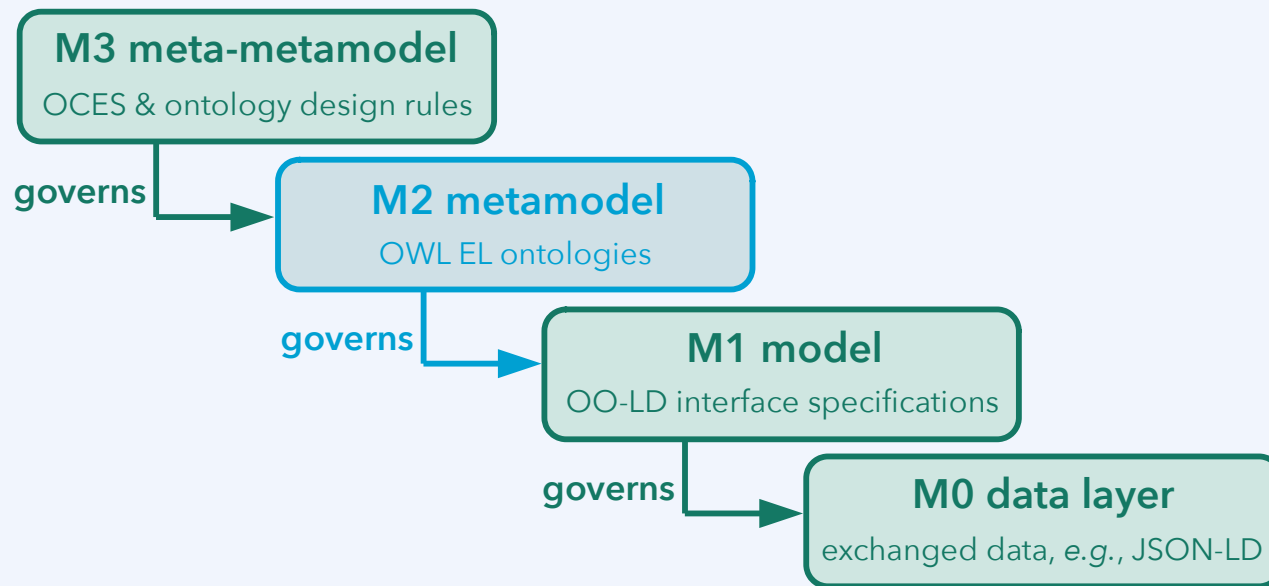
Four layers of metamodelling according to the Meta Object Facility (MOF):



Some of the reused ontologies (e.g. BattINFO and BVCO) are EMMO-related, others are aligned with DOLCE; bridge concepts/OCES can be used at the meta-ontological level. For interfaces, we agreed with KlproBatt (which has the same kind of problem and data) on using the same technology (OO-LD).

# Semantic interoperability layer requirements

Four layers of metamodelling according to the Meta Object Facility (MOF):



Requirements for the design target “semantic interoperability layer (SIL)” are collected in the form of user stories and, in addition, competency questions.

*Example: What are the constraints of the (given) optimization problem, expressed as answer set programming rules and facts?*

# Semantic architecture: Epistemic metadata

**Epistemic metadata** are the information that **establishes the knowledge status** of data or digital objects.<sup>1</sup>

**Questions we must answer to establish the knowledge status:**

- a) “what **knowledge claim**  $\varphi$  has been formulated?,”
- b) “where do the data and the claim come from?” (**provenance**),
- c) “what **validity claim** was made about  $\varphi$ ?,”
- d) “why should we accept any of this?” (**grounding**).

Key epistemic metadata items are the **knowledge claims** made based on data, their **provenance**, **validation** and **reproducibility**, and **epistemic grounding**.

<sup>1</sup>«Documentation of epistemic metadata by a mid-level ontology of cognitive processes», in *Proc. JOWO 2022*, CEUR vol. **3249**: p. 2 (CAOS), CEUR-WS, **2022**.

# Requirements for epistemic metadata: Case study

**Epistemic metadata** and their documentation were explored for the domain of molecular modelling and simulation within engineering thermodynamics:

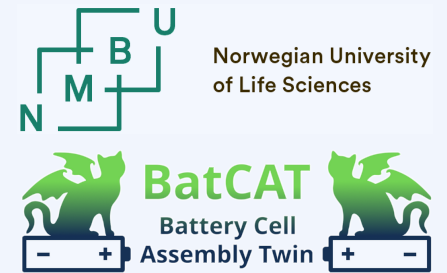
**First stage report (10 cases)**, doi:10.5281/zenodo.7516532, **2023**.

Discussion of *five papers each* from *two research groups* (London, Berlin) without involving the papers' authors. Obtained a tentative **taxonomy for epistemic metadata**, later implemented into the PIMS-II ontology.

**Second stage report (12 claims)**, doi:10.5281/zenodo.7608074, **2023**.

Discussion of *two claims each* from *six papers*, with two papers each from three research groups (London, Berlin, Kaiserslautern), involving the papers' authors. Discussed aspects such as the **grounding of knowledge claims** with authors.

# Refactoring of mid-level ontologies



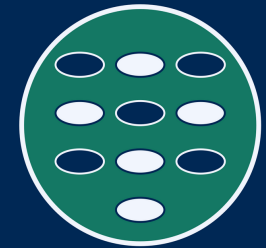
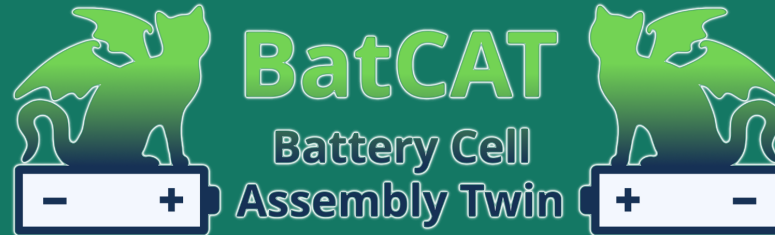
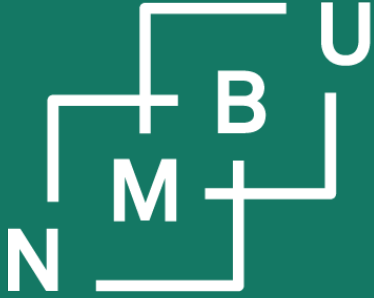
PURL for the new system, MSO-EM (ontologies for **modelling, simulation, optimization**, and **epistemic metadata**), which is under construction:

<https://www.purl.org/mso-em>

BatCAT organizational github: <https://github.com/HE-BatCAT>

Design principles:

- Strong alignment with DOLCE (through DOLCE Lite)
- OWL2 EL profile expressivity level
- Ongoing development, with easy stable access to versioned releases
- Simple modules, each with maximum three taxonomy levels and maximum three top concepts
- Backwards compatibility with equivalences to the preceding mid-level ontology development (PIMS-II) to the maximum possible extent



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