Multiphysics simulation based data space and digital twin platform design for vanadium redox-flow batteries

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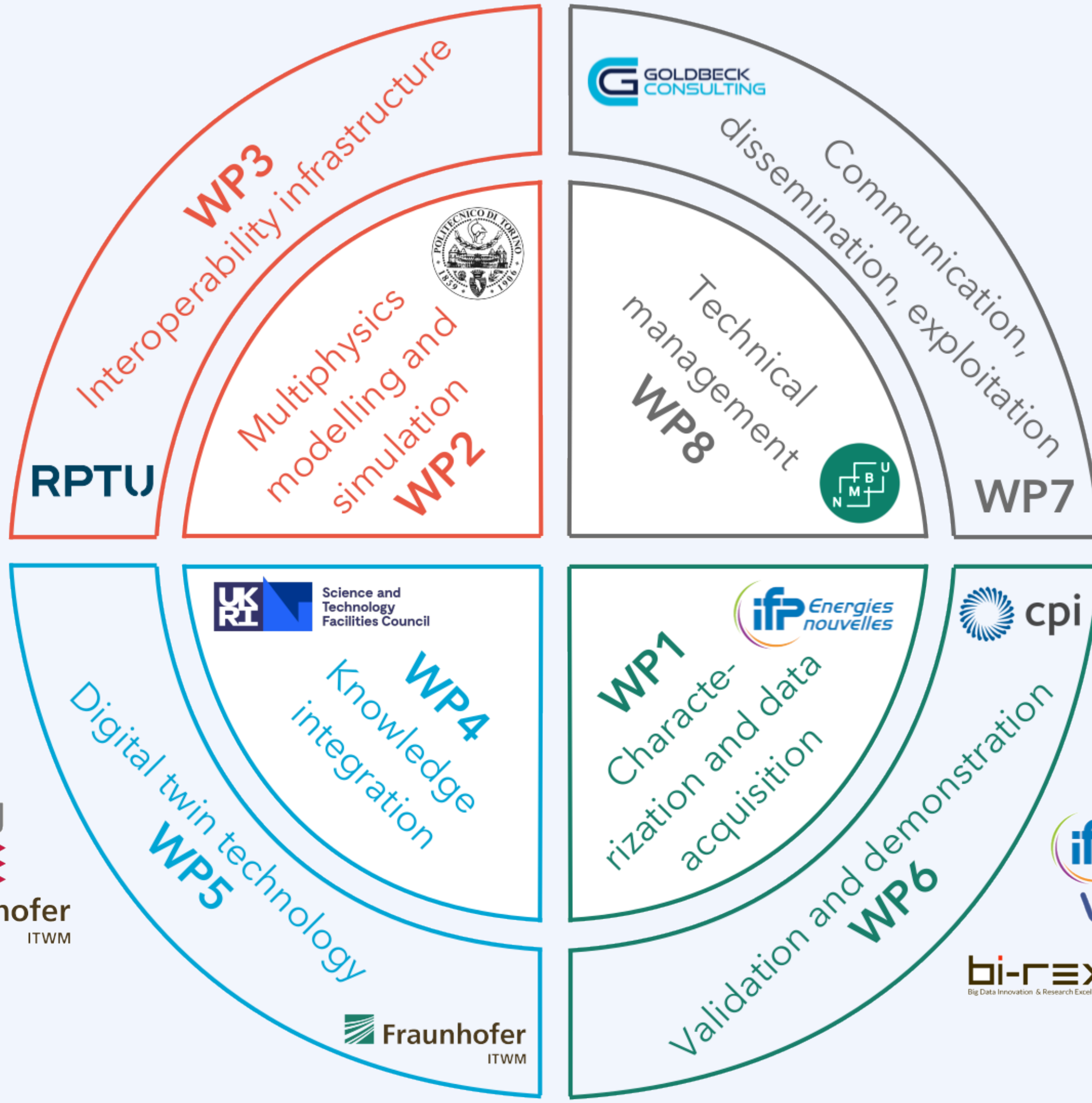
BatCAT project summary

- 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.

BatCAT focus areas and partners

Focus area
simulation

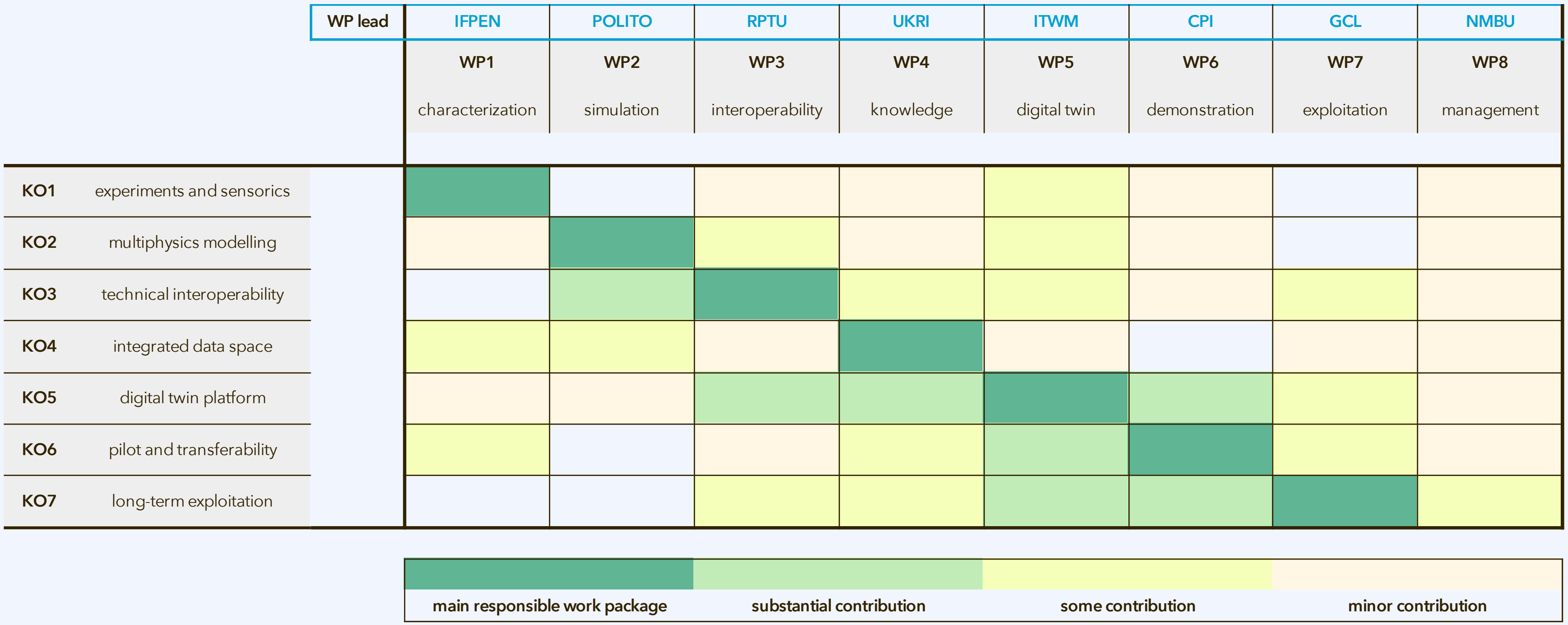


Focus area
management

Focus area
data

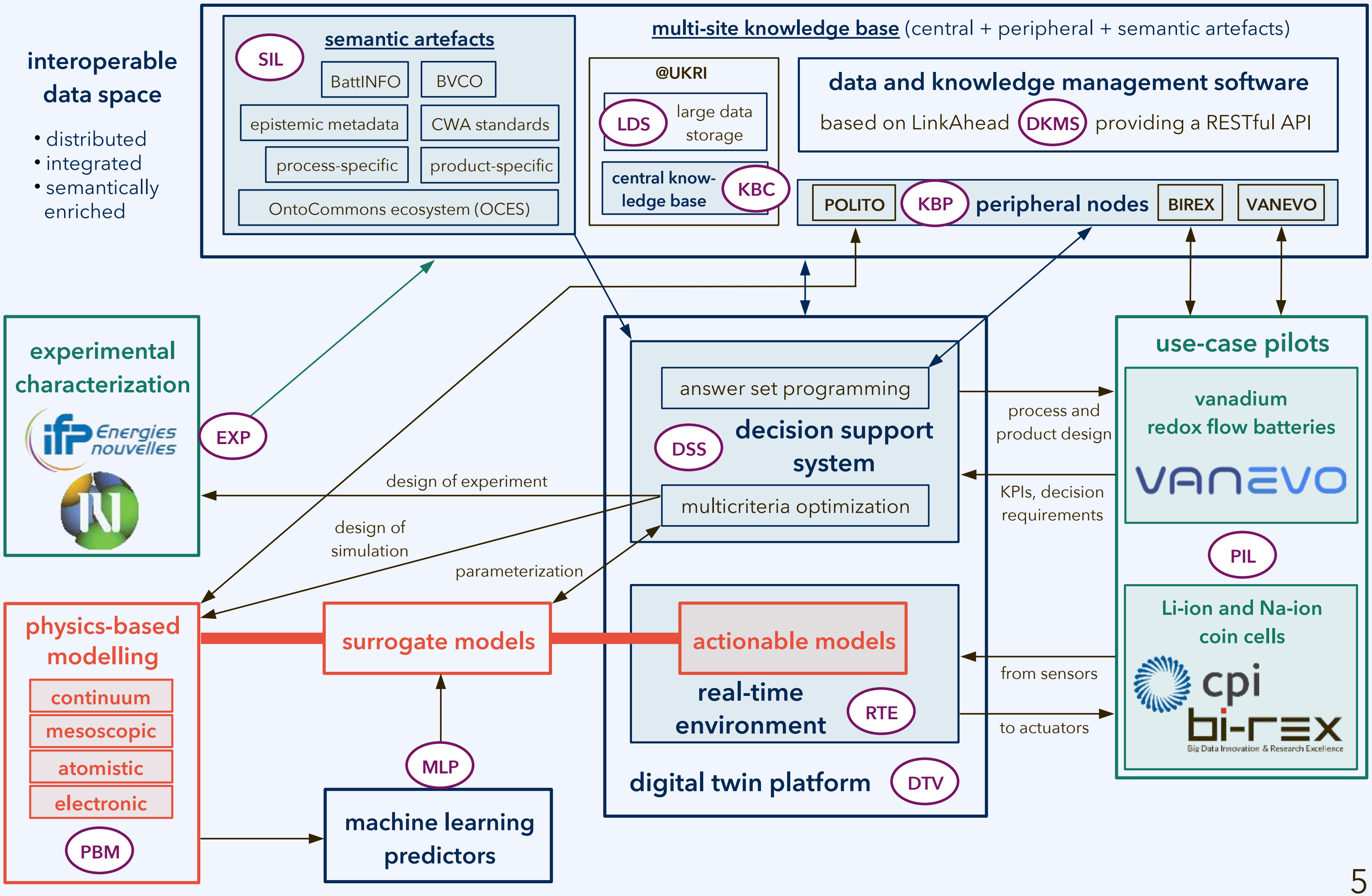
Focus area
process

Requirements: Key objectives of BatCAT



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.

Requirements analysis: Design targets



Requirements analysis: Methodology

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 proceeded 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** for revision and extension of deduced requirements.
4) Analysis and catalogue of requirements (**deliverables** D4.1 and D6.1).

Requirements documentation

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" priorization:** "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".)

Multiphysics simulation in BatCAT

For both use cases:

MikTherm coupling/ linking — RPTU

MolMod DB model repository — RPTU

proprietary **MCO tool** — Fraunhofer ITWM

We are also exploring free MCO tools.

For the redox-flow use case:

MD using ms2

surrogate

DPD using DL_MESO

surrogate

surrogate

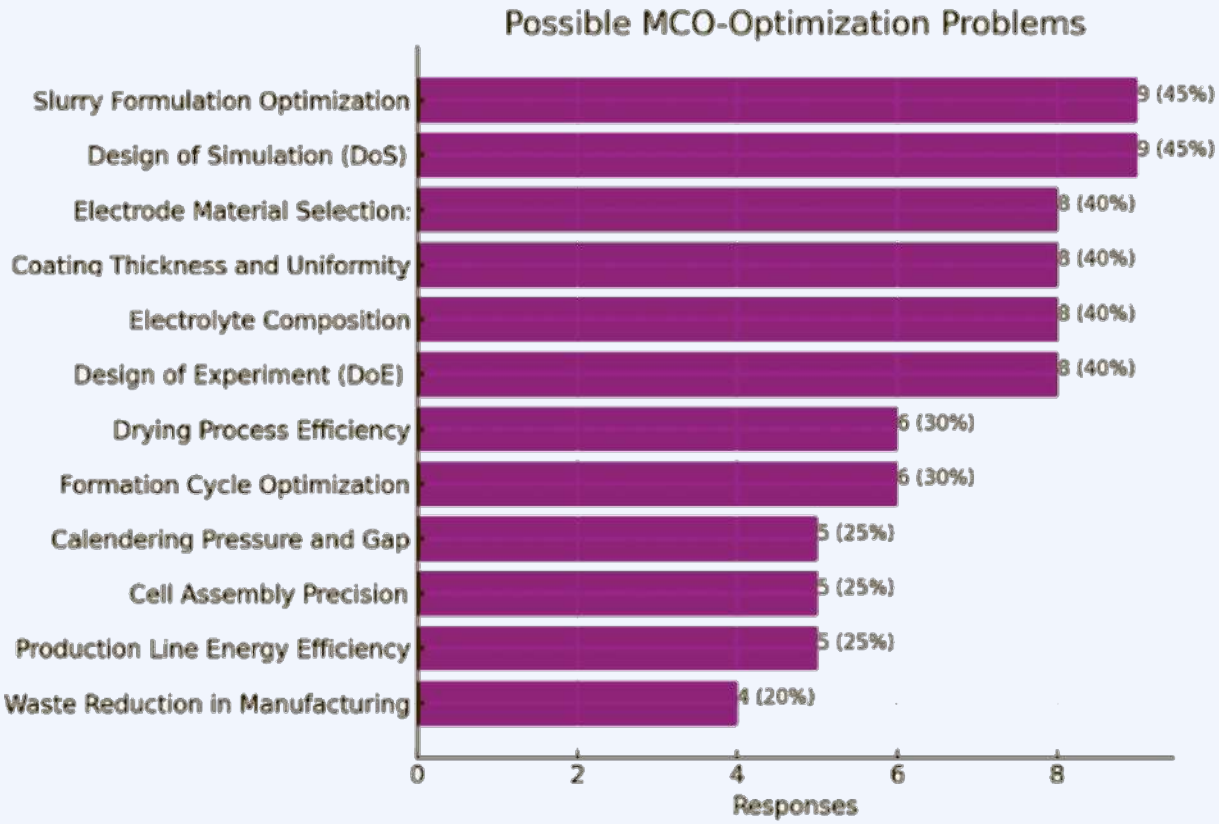
continuum models using FEniCS

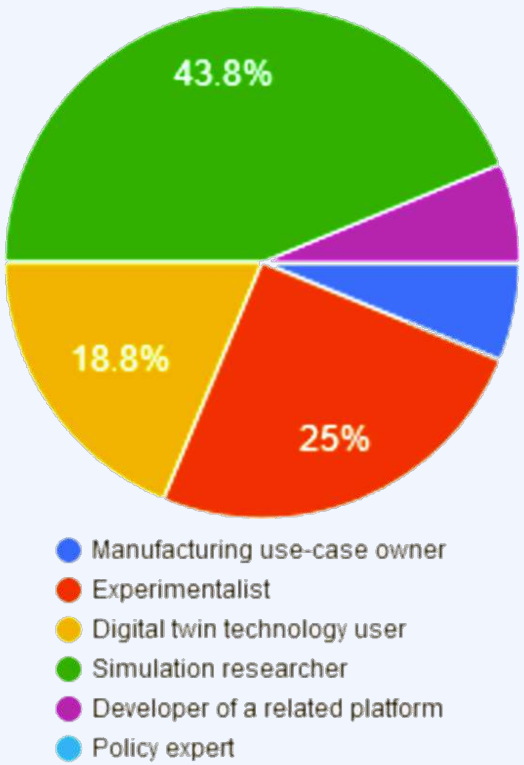
surrogate

MCO, **ASP**, and **actionable modelling**

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.





Digital product passport (DPP)

For optimal use by manufacturers, the digital twin needs to track the information required for the battery DPP as specified by the **Batteries Regulation**.

In addition to the **DPP for batteries**, there are **advanced materials** included in the batteries (*e.g.*, VFRB electrolyte, membrane, and electrodes).

The **DigiPass CSA** project is responsible for developing specifications and interoperable systems and tools the **digital materials and product passport**, *i.e.*, the DPP for advanced materials.

DigiPass CSA is forming an expert group on advanced materials in batteries.

Norwegian University of Life Sciences

BatCAT Battery Cell Assembly Twin

VANEVO

FLOW BATTERIES EUROPE
A united voice for flow batteries

DigiPass
Know your products!

Digital materials & product passport: DigiPass CSA

WP7: Semantic interoperability and data spaces

WP2: Digital materials and product passport

WP10: Sustainability and business plan

WP6: Metadata standardization

WP3: Data acquisition and knowledge generation

DigiPass
Know your products!

Helmholtz-Zentrum hereon
WP11 & WP12

WP4: Best practices

WP8: DigiPass ecosystem
WP9: Collaboration, dissemination, training

Demonstration case: Pre-painted metals supply cain

WP1: Materials data and information systems

WP5: Innovation process

Demonstration case: Advanced materials for renewable energy sources

Digital materials & product passport

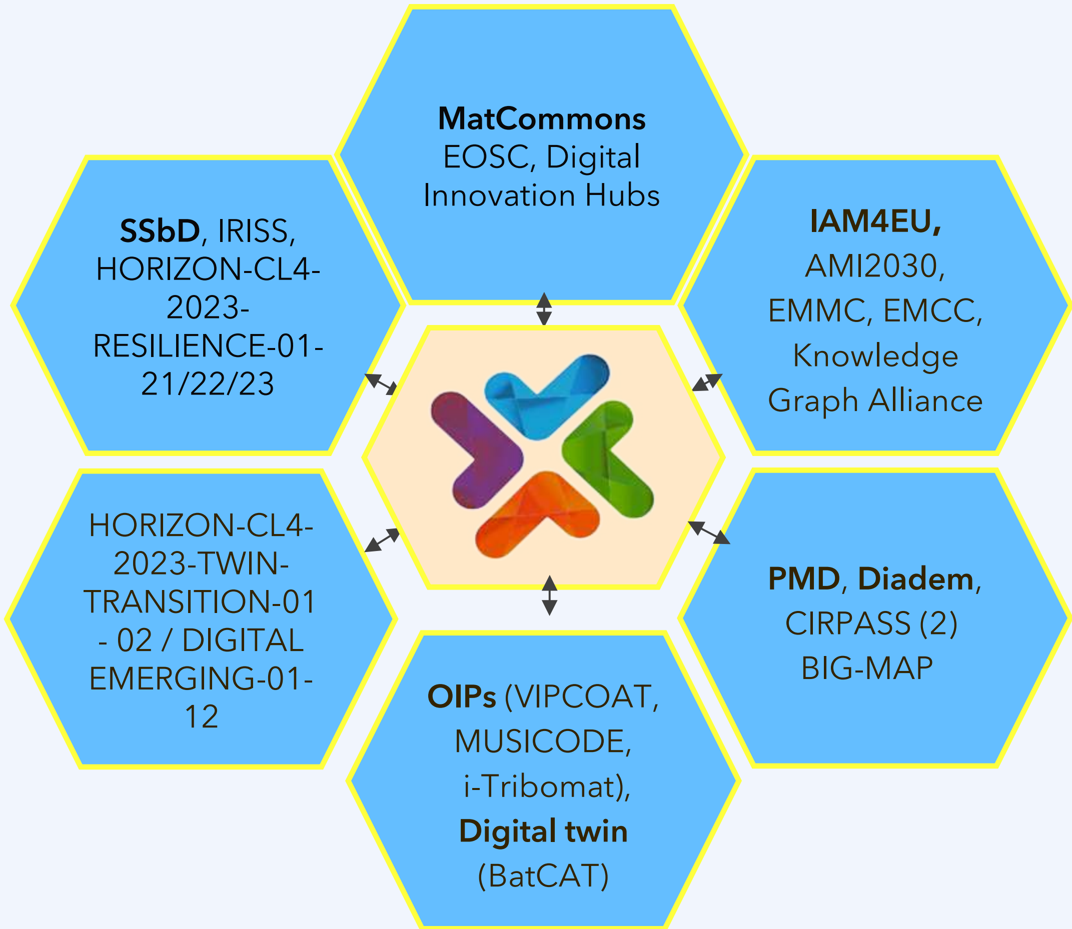
DMPP **demonstrators**:

Case 1:
Advanced composites

Case 2:
Advanced materials for renewable energy sources

Case 3:
Safety of nanomaterials

Case 4:
Pre-painted metals

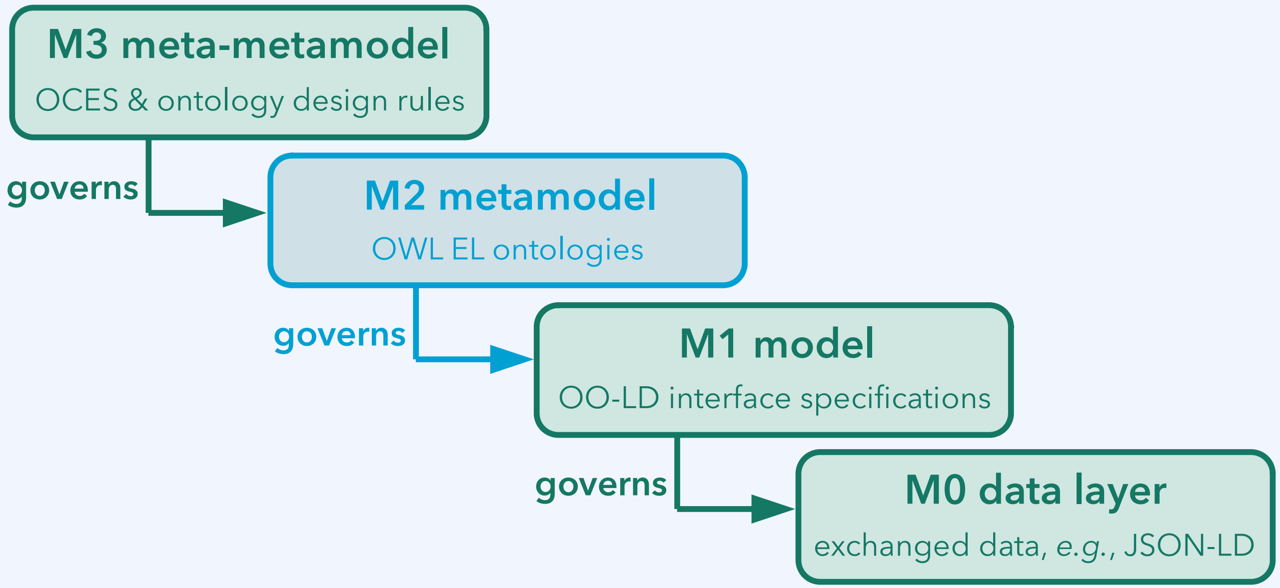


Expert groups to be formed within 2024:

(1) Trust and immutability **(2)** Material digital passport **(3)** Battery materials

Semantic interoperability layer

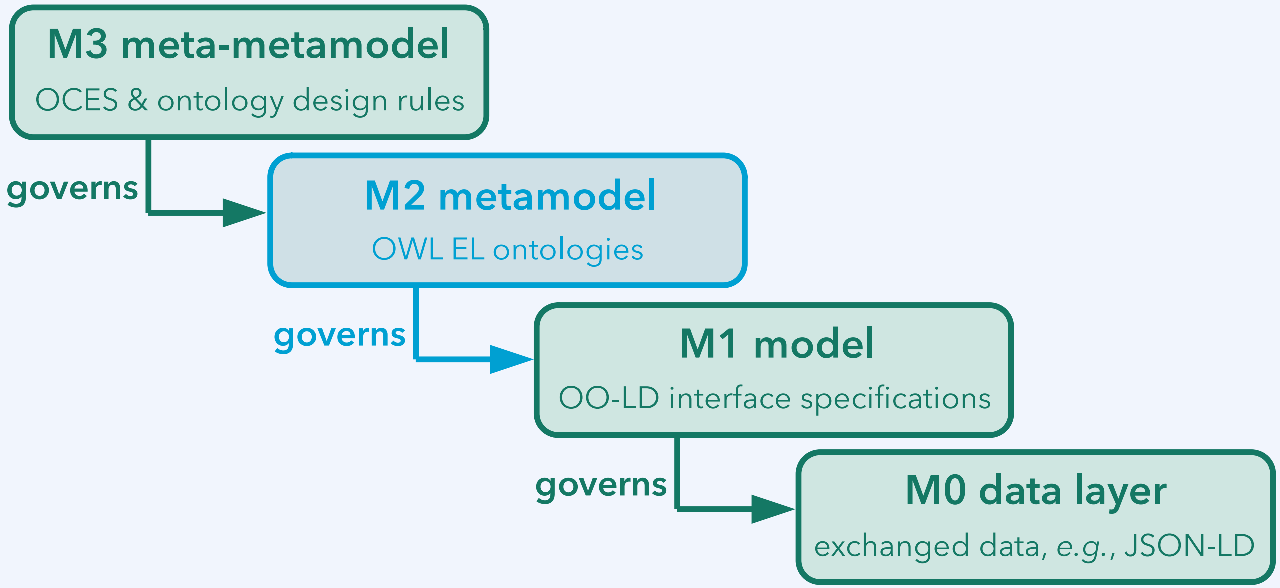
Four layers of metamodelling according to the Meta Object Facility (MOF):



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 KIproBatt (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?*

Opacity vs. transparency

European AI Act: "To address concerns related to **opacity** and [...] fulfil their obligations under this Regulation, **transparency** should be required for high-risk AI systems before they are placed on the market [...]. High-risk AI systems should [...] enable deployers to understand how the AI system works [...]. High-risk AI systems should be accompanied by **appropriate information**".

Epistemic opacity:

The concept was introduced by **Humphreys** in *Extending Ourselves*[1]

[1]P. Humphreys, *Extending Ourselves Computational Science, Empiricism, and Scientific Method*, **2004**.

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Epistemic opacity can occur when simulation-based and data-driven methods are used. The concept was introduced by **Humphreys** in *Extending Ourselves*[1] (2004), developed further in later work,[2] and has had a substantial impact.[3]

> **Epistemic opacity** (Humphreys, 2011): A «process is **epistemically opaque** relative to a cognitive agent X at time t [... if ...] X does not know at t all of the **epistemically relevant elements**»[2]

[1]P. Humphreys, *Extending Ourselves Computational Science, Empiricism, and Scientific Method*, **2004**.

[2]P. Humphreys, in M. Carrier, A. Nordmann, *Science in the Context of Application, pp.* 131–142, Springer, **2011**.

[3]J. M. Durán, N. Formanek, *Minds and Machines* **28**(4): 645–666, doi:10.1007/s11023-018-9481-6, **2018**.

Epistemic metadata

Epistemic metadata are the information that **establishes the knowledge status** of data or digital objects.[1]

Questions we must answer to establish the knowledge status:

a) "what **knowledge claim** φ has been formulated?,"
b) "where do the data and the claim come from?" (**provenance**),
c) "what **validity claim** was made about φ?,"
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**.

In *Proc. JOWO 2022*, CEUR *vol.* **3249**: *p. 2 (CAOS)*, CEUR-WS, **2022**.
In *Proc. ICAPAI 2023*, doi:10.1109/icapai58366.2023.10193944, IEEE, **2023**.
In *Proc. FOIS 2023*, *pp.* 302–319, doi:10.3233/faia231136, IOS, **2023**.

Requirements for epistemic metadata: Case study

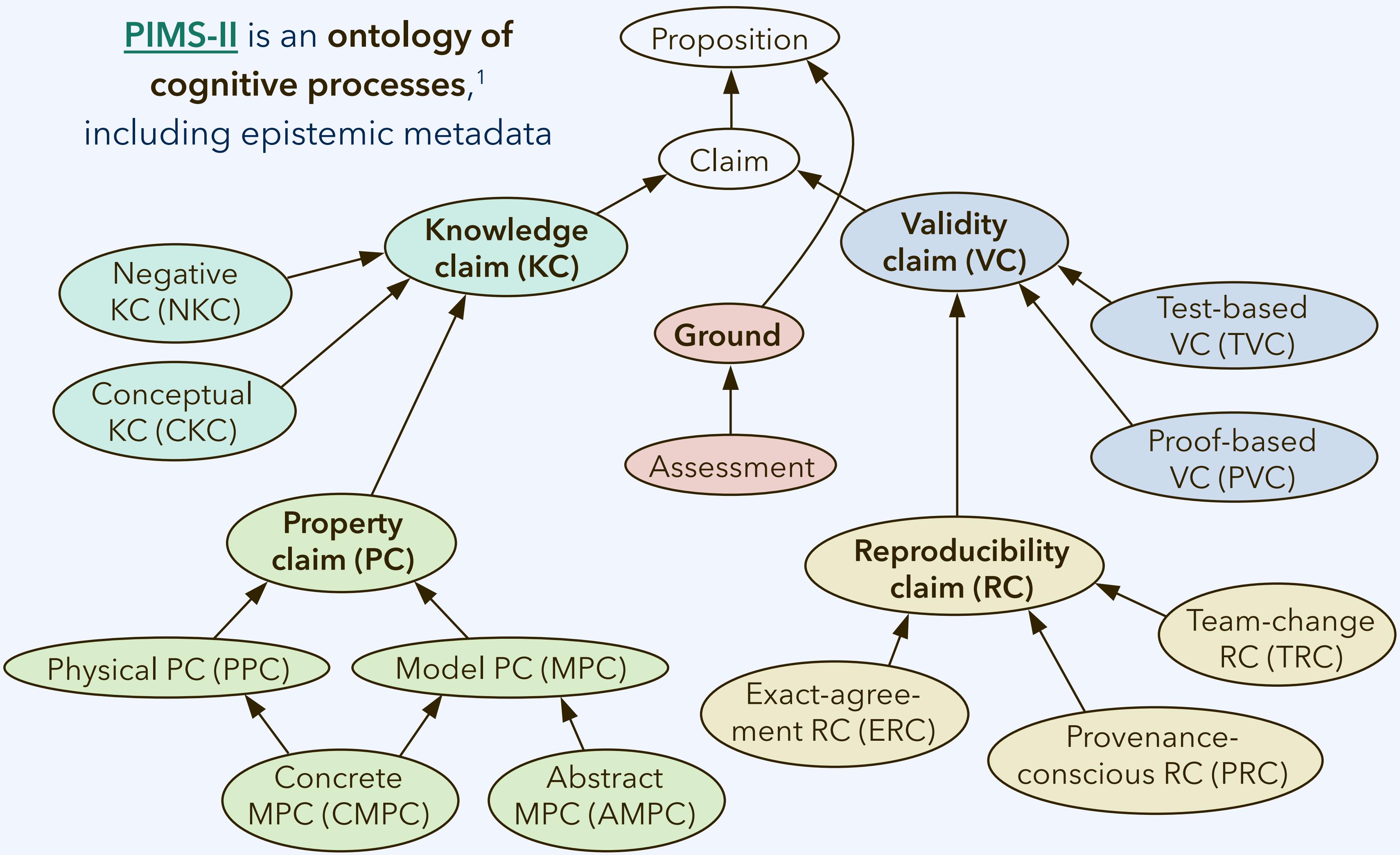
Epistemic metadata and their documentation were explored for the domain of molecular modelling and simulation within engineering thermodynamics:

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.

Mid-level ontology of epistemic metadata

PIMS-II is an **ontology of cognitive processes**,[1] including epistemic metadata



[1] OWL implementation under http://www.molmod.info/semantics/pims-ii.ttl

Refactoring of mid-level ontology

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
- All modules of the ontology are directly aligned with DOLCE

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Digitalisering på Ås

BatCAT Battery Cell Assembly Twin

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