Norges miljø- og biovitenskapelige universitet

Materialteori og -informatikk

Digitalisering på Ås

Moving from FAIR data principles to XAIR

Martin Thomas Horsch

Norwegian University of Life Sciences

CAPE-OPEN Annual Meeting

8th October 2024, Berlin

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i.e. "explainable-AI-ready"

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The well-known FAIR principles

Findability

F1. Globally unique **persistent identifiers (PID)**
F2. **Enriched with metadata**
F3. Data identifier included in metadata
F4. Registered in **searchable platform**

Accessibility

A1. **Retrievable from PID** via a standard protocol
A1.1. Open and freely implementable protocol
A1.2. … **authentication/authorization** if necessary
A2. Metadata remain accessible (beyond data)

Interoperability

I1. **Formal language** used for **knowledge representation**
I2. Metadata use **vocabularies** that are themselves FAIR
I3. Semantic web principles, **data can refer to other data**

Reusability

R1. Metadata include a plurality of accurate and relevant attributes
R1.1. Release data and metadata with an accessible **data usage license**
R1.2. Data are annotated with a detailed **provenance description**
R1.3. Relevant disciplinary and **community standards** are fulfilled

[1]M. D. Wilkinson *et al.*, "The FAIR Guiding Principles …," doi:10.1038/sdata.2016.18, **2016**.

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**.

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 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**.

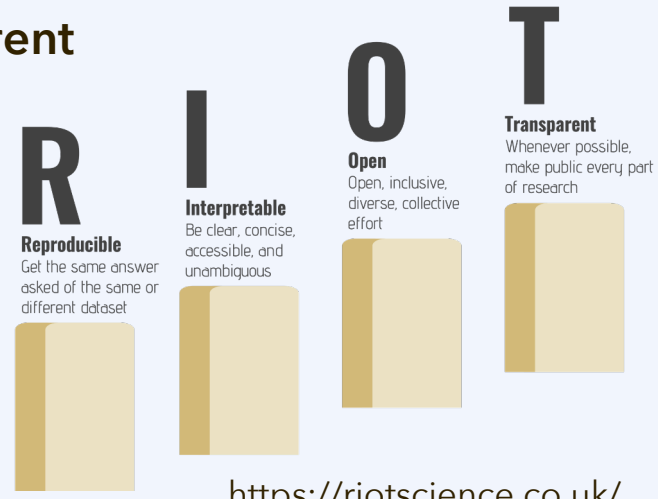
[2]P. Humphreys, in M. Carrier, A. Nordmann, *Science in the Context of Application*, *pp.* 131–142, Springer, **2011**.

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

Good practices beyond FAIR

RIOT:[1] Reproducible, interpretable, open, transparent

- Origin: UK Reproducibility Network (UKRN)
- UKRN encouraged foundation of the other reproducibility networks, such as NORRN, the Norwegian Reproducibility Network
- Local "RIOT science clubs" were founded



https://riotscience.co.uk/

CARE:[2] Collective benefit, authority to control, responsibility, ethics

- Origin: Global Indigenous Data Alliance
- Uptake supported by the Research Data Alliance
- Orientation: Sovereignty and epistemic justice

https://www.gida-global.org/care/

[1]E. Ganley *et al.*, *BMC Res. Notes* **15**: 51, doi:10.1186/s13104-022-05932-5, **2022**.

[2]S. Russo Carroll *et al.*, *Sci. Data* **8**: 108, doi:10.1038/s41597-021-00892-0, **2021**.

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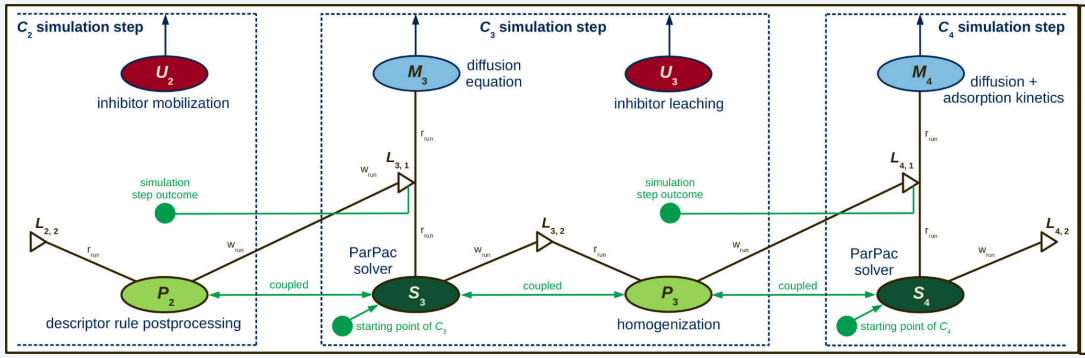
Digitalisering på Ås

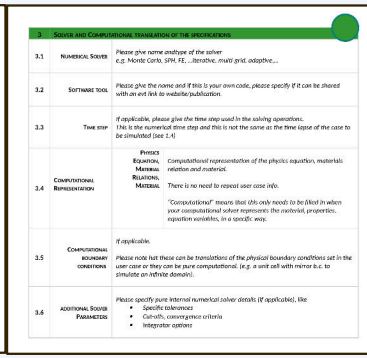
The road from FAIR to XAIR (explainable) models, simulations, and data

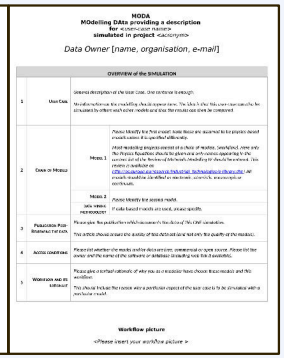
CAPE-OPEN Annual Meeting 8. oktober 2024 Materialteori og -informatikk

Standardization processes: MODA

CWA 17284:2018 MODA: Model Data



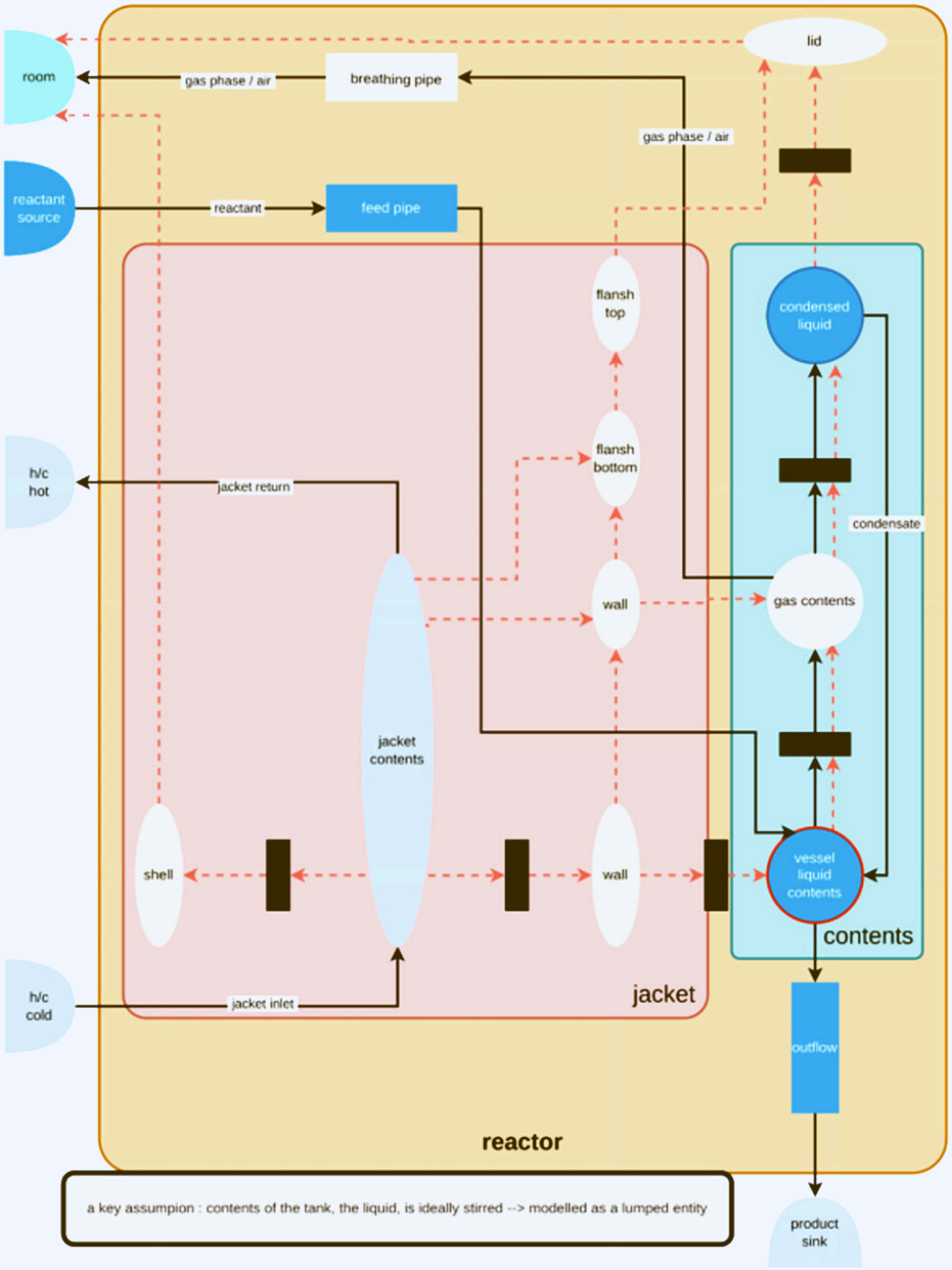




- MODA is a **closed semantic and epistemic space**: Modelling methods have to be chosen from a small list.
- MODA imposes a **given level of detail** in workflow documentation; namely, **unrealistically detailed**.[1]
- MODA documentations are **complicated** and **of limited use** to all, including to humans.[2]

[1] *J. Chem. Eng Data* **65**(3): 1313–1329, doi:10.1021/acs.jced.9b00739, **2020**.

[2] ReaxPro project deliverable D2.1, «ReaxPro MODA diagrams», **2020**.



CWA 17960 ModGra

The **process model topology** is a generalized Petri net. Tokens represent **extensive physical quantities** or, alternatively, data items that can be exchanged.

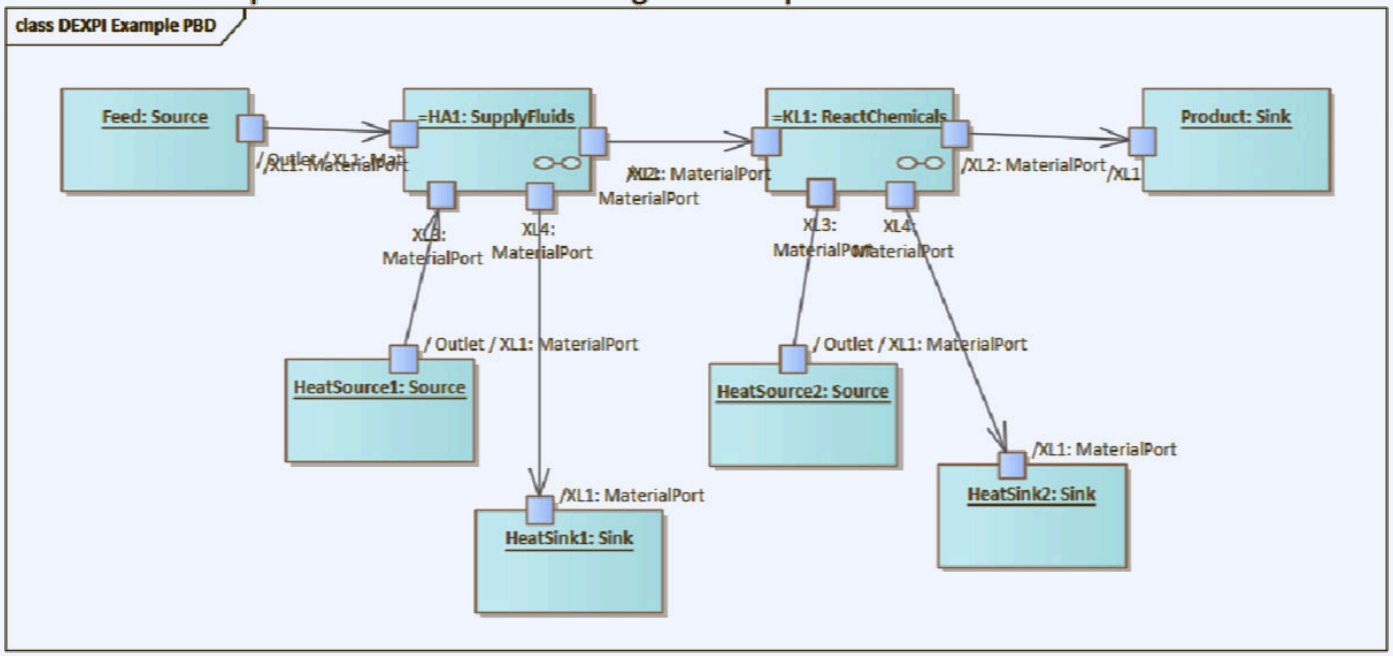
The process model's system of equations is represented by the Petri net's **transitions** and the **places** (capacities) which store the balanced quantities, or alternatively the data items.

An **EMMO export**, using **TriG format**, has been developed.

DEXPI and ModGra

- DEXPI and ModGra serve similar purposes. Both are developments from the CAPE community. Both can represent exchange of quantities graphically.
- ModGra is a CEN workshop agreement, while DEXPI is based on existing standards,[1] *e.g.*, DIN 6779-13, ISO 10303, and ISO 10628.

With these assumptions we build the following BFD or top-level model.

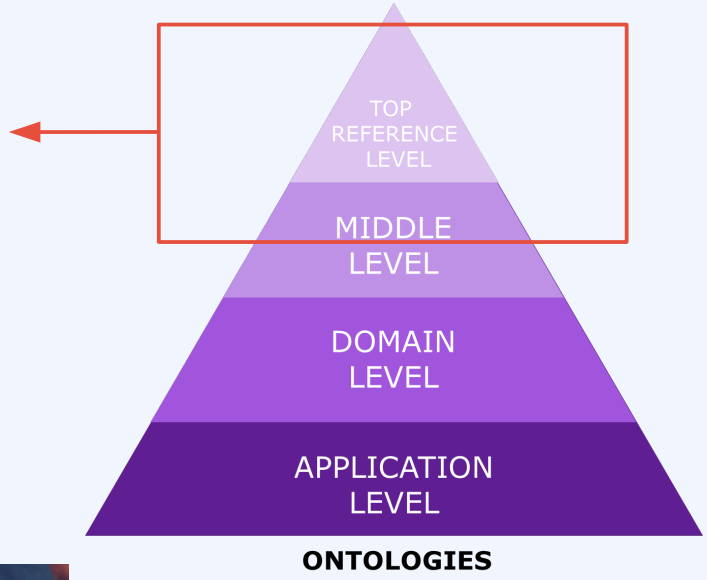


Source for diagram to the left:

[1]DEXPI Process Modelling of Process Systems and their Documentation, version 1.0, official release, **2023**.

OntoCommons CSA (2020 – 2023)

- **Community development** that brought together applied ontology, industrial digitalization, and computational science and engineering.
- OntoCommons ecosystem[1] (OCES) including the three **foundational ontologies** BFO, DOLCE, and EMMO. Development of **bridge concepts**[2] as a technique for ontology alignment.



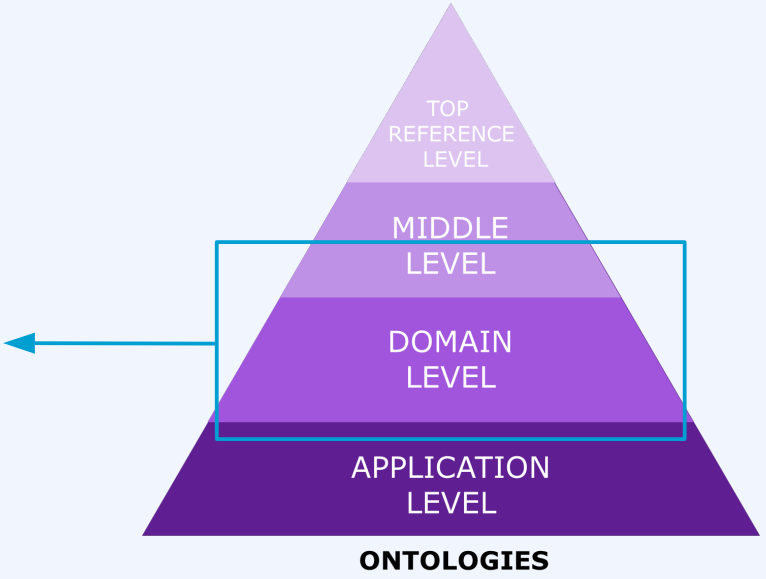
[1]M. Magas, D. Kiritsis, *Int. J. Production Res.* **60**(2): 479–492, doi:10.1080/00207543.2021.1989514, **2022**.

[2]A. de Baas *et al.*, *IEEE Access* **11**: 120372–120401, doi:10.1109/access.2023.3327725, **2023**.

Review of Domain Interoperability[1]

OntoCommons CSA collected and supported the design and alignment of **domain-level interoperability standards**. There, CAPE-OPEN and OntoCape were discussed a few times.[1]

The overall analysis of modes of interoperability, relevant tools and components, and recommendations was delivered in the form of **RoDI: The Review of Domain Interoperability**.[2]



	data	**human**	**organization**	**software**
data (d)	$d \leftrightarrow d$	$d \leftrightarrow h$	$d \leftrightarrow o$	$d \leftrightarrow s$
human (h)	—	$h \leftrightarrow h$	$h \leftrightarrow o$	$h \leftrightarrow s$
organization (o)	—	—	$o \leftrightarrow o$	$o \leftrightarrow s$
software (s)	—	—	—	$s \leftrightarrow s$

Matrix structure for interoperability requirements: Who interoperates with whom?

[1] S. Chiacchiera *et al.*, OntoCommons deliverable 3.9, "First focus workshop on domain ontologies," **2021**.

[2] S. Chiacchiera *et al.*, OntoCommons deliverable 3.8, "Finalized Review of Domain Interoperability," **2023**.

“XAIR principles” working group

XAI: Explainable artificial intelligence

AIR: Artificial-intelligence ready

XAIR: Explainable AI-ready

Data are **XAIR** to the degree that they are semantically enriched so that **best use** can be made of **interpretable learning** techniques. These include XAI in the narrow sense (learning by induction) and logical reasoning (deduction).

Tendency: **Making data trustworthy through explanations** will increasingly become a requirement. Data must become explainable-AI-ready (XAIR).

Slogan: “FAIR and XAIR data.” (Sounds similar to the idiom “fair and square.”)

“XAIR principles” working group

Months 1 to 10: **Synopsis of literature work on core concepts**

- Identify the core concepts, analyse and summarize the literature characterizing these concepts.
- M10, report, public, "**Synopsis of XAIR core concepts**."

Months 11 to 16: **Work on actionable core concepts**

- Discussion of use cases; annotation of examples; draft of mid-level and domain ontologies.
- M16, report, public, "Request for comments on actionable XAIR core concepts."

Months 17 to 22: **Work and consultation on XAIR principles**

- Community discussion toward “XAIR principles.”
- M22, report, public, "Request for comments on XAIR data and metadata […] principles […]".

Months 23 to 34: **Stable release of mid and domain ontologies**

- Ontologies for XAIR are finalized to the extent that no major changes will occur in the future.
- M34, ontologies, public, "[…] Ontologies covering the XAIR key concepts […]".

Months 35 to 40: **XAIR forward plan and ontology governance**

- Critical analysis of accomplishments and forward-looking discussion.
- M40, report, public, "XAIR forward plan and ontology governance."

DCLXVI 2024 International Workshop

Designing the Conceptual Landscape for a XAIR Validation Infrastructure

RPTU Kaiserslautern, Germany, 11th December 2024

What information needs to be conveyed to users so that data and models can become **explainable-AI-ready** (XAIR)?

The core concepts for explainable-AI-readiness will be discussed at the **DCLXVI 2024 Workshop** in Kaiserslautern, organized by the Horizon Europe projects AI4Work and BatCAT.

Submit your manuscript by 22nd October 2024. The proceedings will be published in the Springer series Lecture Notes in Networks and Systems.

AI4Work: HEur GA 101135990. BatCAT: HEur GA 101137725.

https://batcat.info/dclxvi/

ai4work

BatCAT
Battery Cell Assembly Twin

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Documentation of epistemic metadata

Semantic architecture: 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.

Imperial College London

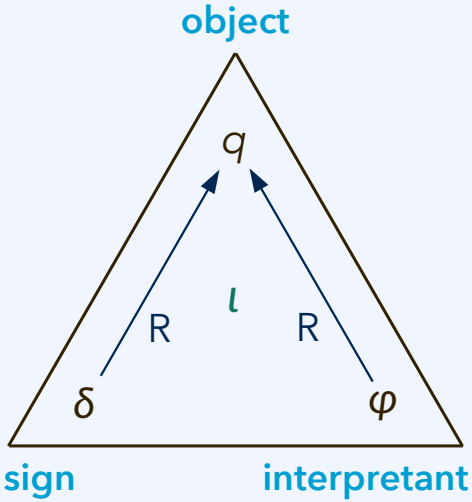
RPTU Rheinland-Pfälzische Technische Universität

Science and Technology Facilities Council

Ontology of epistemic metadata: Knowledge claims

Peircean semiotics is applied to the description of cognitive processes, *e.g.*, consider a process in which dataset δ is analysed, yielding knowledge claim φ:

- The data δ are about some research question q.
  So δ is a representamen for q; it has the role of the **sign**.
- The research question q is the **object** of the semiosis.
- As an outcome of the semiosis, claim φ is obtained, which is a new representamen for q, the **interpretant**.



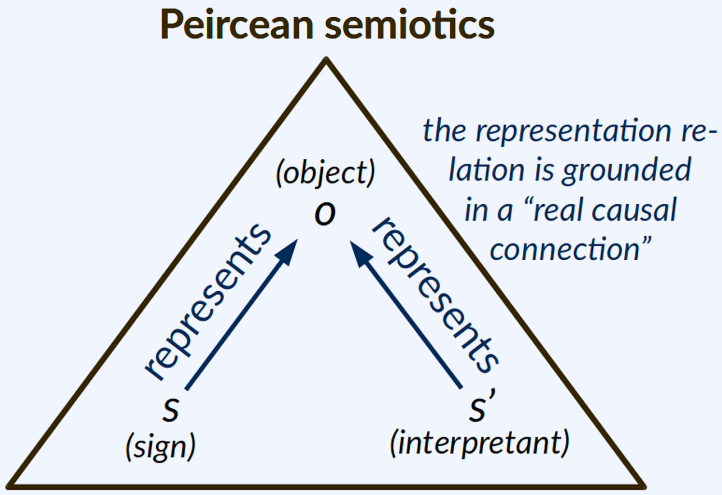
InformationProcessing
(*i.e.*, a Peircean semiosis)

The part of the PIMS-II ontology that deals with Peircean semiotics is also axiomatized in first-order logic,[1] in addition to the OWL implementation.[2]

C. S. Peirce

[1] «Mereosemiotics: Parts and signs», in *Proc. JOWO 2021 (FOUST)*, **2021**.
[2] OWL implementation under http://www.molmod.info/semantics/pims-ii.ttl

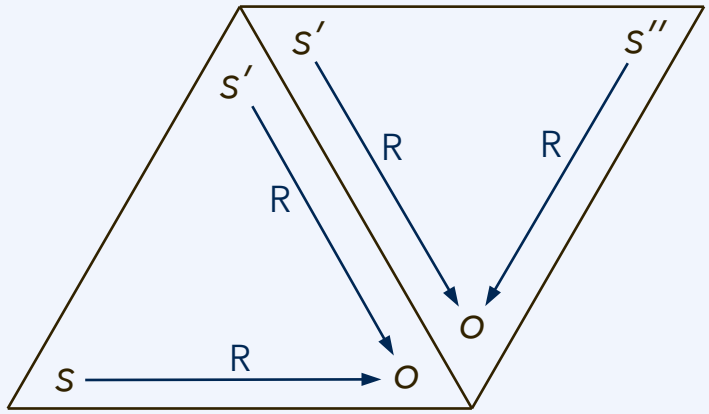
Provenance: Documentation with flexible resolution



Cognitive process (example):

- First, experimental data *s* for material *o* are used to parameterize a model, obtaining model *s′*.
- Then, a simulation is done using model *s′*, yielding the simulation result *s″* (which also represents *o*).

Research workflows as cognitive processes:[1]



Each cognitive step starts from one representation relation, *e.g.*, *Rso*, and creates a new one, *Rs′o*.

The successor step reuses *Rs′o* and creates the next relation, *Rs″o*.

[1] In *Proc. JOWO 2021*, CEUR *vol.* **2969**: *p.* 3 (FOUST), **2021**.

Validation and falsification

Common formulation and schema for reproducibility claims (RCs):

«Whenever research process κ'' is carried out, it must lead to the outcome φ''.»

we argue that there is a mechanism from pragmatics at work here

1) Reseacher *a* did κ and found φ.

   Here, *a* also made the **positive reproducibility claim $\psi = \Box(\varphi'' \mid \kappa'')$.**

2) Reseacher *b* did γ, **consistent with κ''**, and found ζ, **inconsistent with φ''**.

   Here, *b* made the **negative reproducibility claim $\Diamond(\neg\varphi'' \mid \kappa'') \equiv \neg\Box(\varphi'' \mid \kappa'') \equiv \neg\psi$.**

3) What is relevant there is the **contradiction between ψ and $\neg\psi$**.

provenance metadata κ
provenance paradata κ'

provenance orthodata $\kappa'' = \kappa - \kappa'$

«repeat κ, but no need to retain κ'»

knowledge claim metadata φ
knowledge claim paradata φ'

knowledge claim orthodata $\varphi'' = \varphi - \varphi'$

«obtain φ again, except for φ' maybe»

Epistemic grounding

See also the reference ontology of trust **ONTrust** by Baratella *et al.*[1, 2]

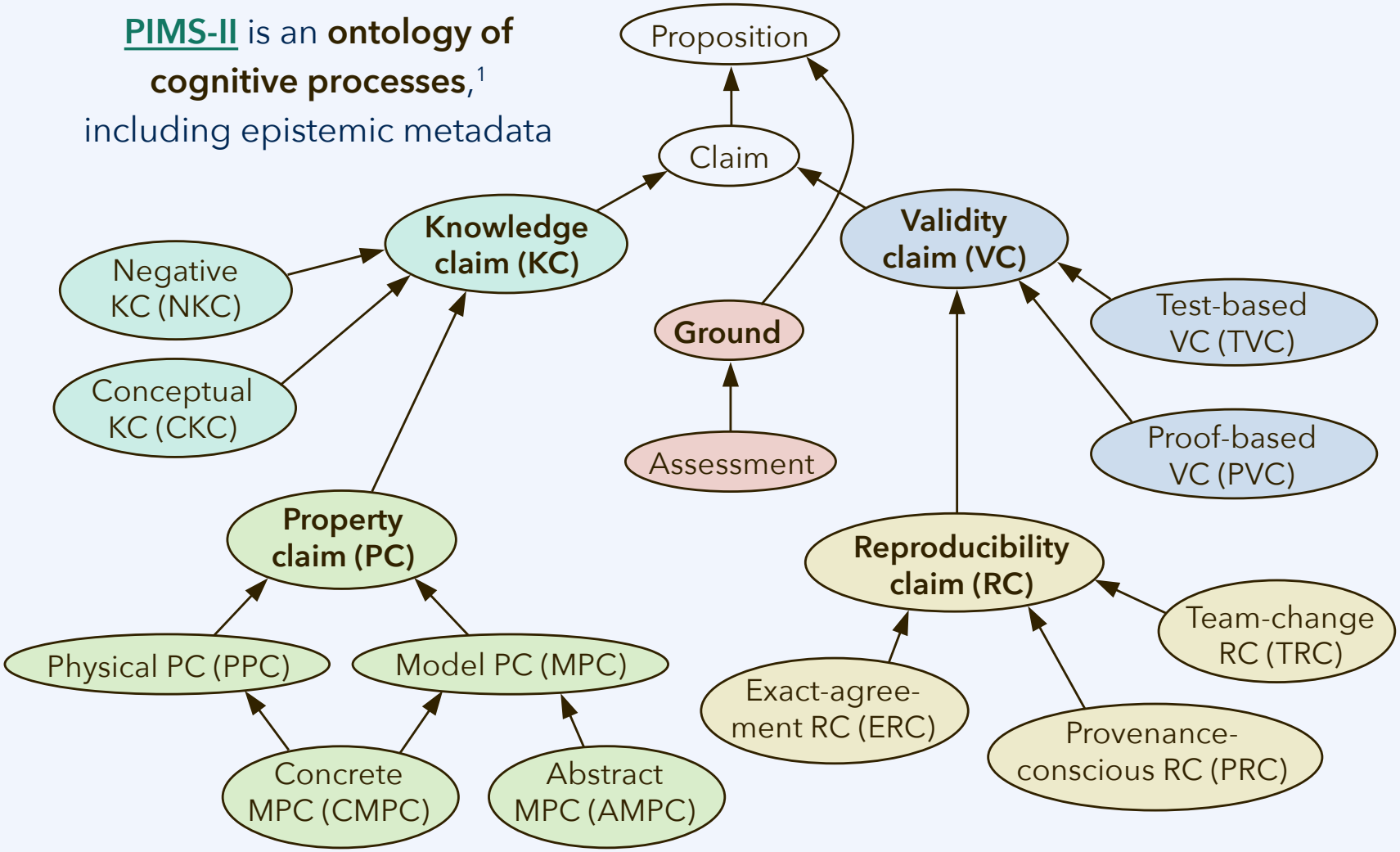
	trust	reliance
Type-1 The **results** establish their own validity.	*Typical:* Mathematical argument (proof) over of a conceptual framework designed around widely accepted definitions and axioms.	*Schema:* A new theory is more reliable because it is simpler, covers more phenomena, or represents underlying physics. (**theoretical virtues**)
Type-2 The **provenance** of the results tells that they are valid.	*Case study example:* Chatwell and Vrabec argue: It is OK to use a cutoff radius of 5.5σ for the LJ potential, since this was done in three cited works from the literature.	*Typical:* We used a model, method, and simulation code validated in the past and – usually – very accurate. (**process reliabilism**)

[1]Baratella *et al.*, «The many facets of trust», in *Proc. FOIS 2023*, doi:10.3233/faia231115, **2024**.

[2]https://github.com/unibz-core/trust-ontology

Mid-level ontology of epistemic metadata

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

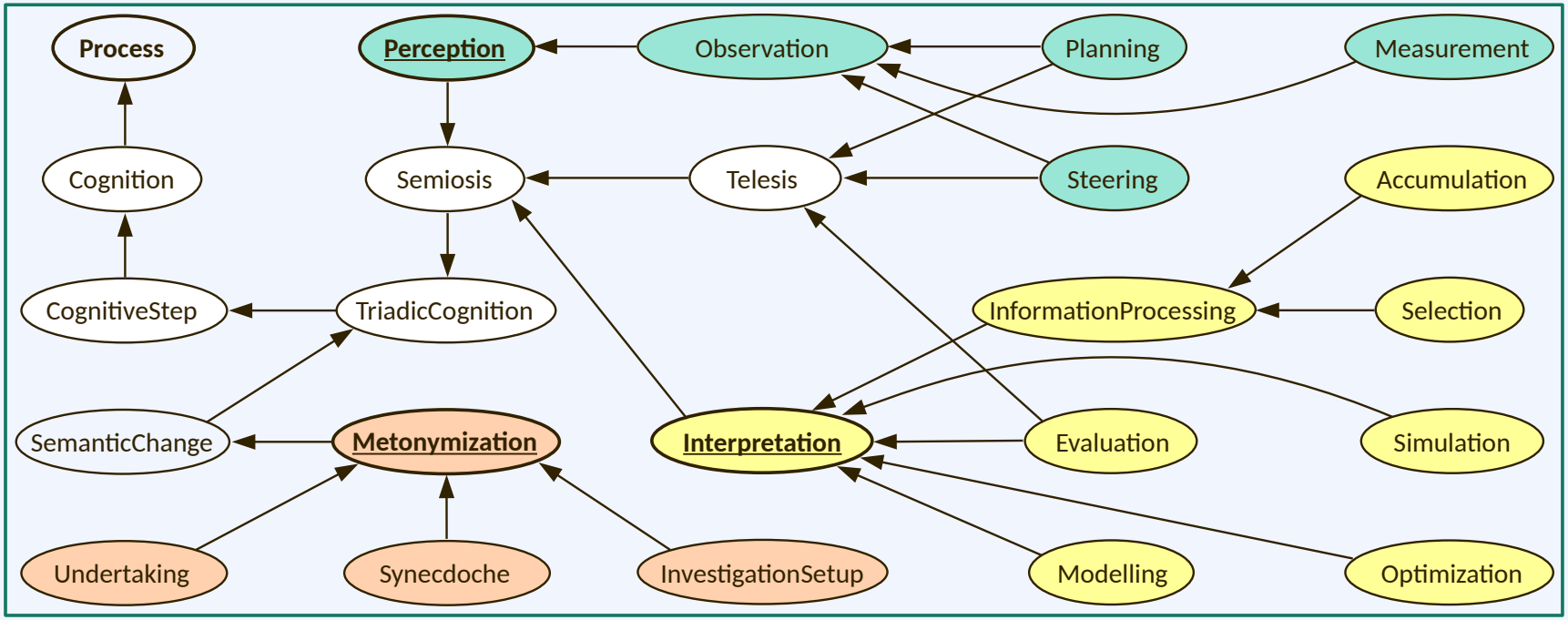


[1]OWL implementation under http://www.molmod.info/semantics/pims-ii.ttl

Mid-level ontology of epistemic metadata

In PIMS-II, scientific workflows are described in terms of cognitive processes.[1–3]

perception requires the presence of the perceived object



metonymization preserves the „real causal connection" (Peirce) between the sign and its old & new referents

interpretation and **metonymization** do not require physical presence of the referents

[1]M. T. Horsch, no. 3 in *Proc. JOWO 2021*, **2021**.

[2]P. Klein *et al.*, no. 26 in *Proc. JOWO 2021*, **2021**.

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

Mid-level ontology refactoring

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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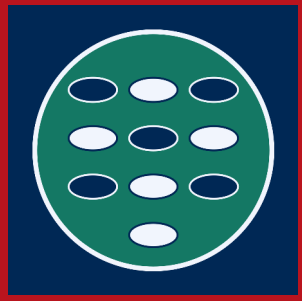
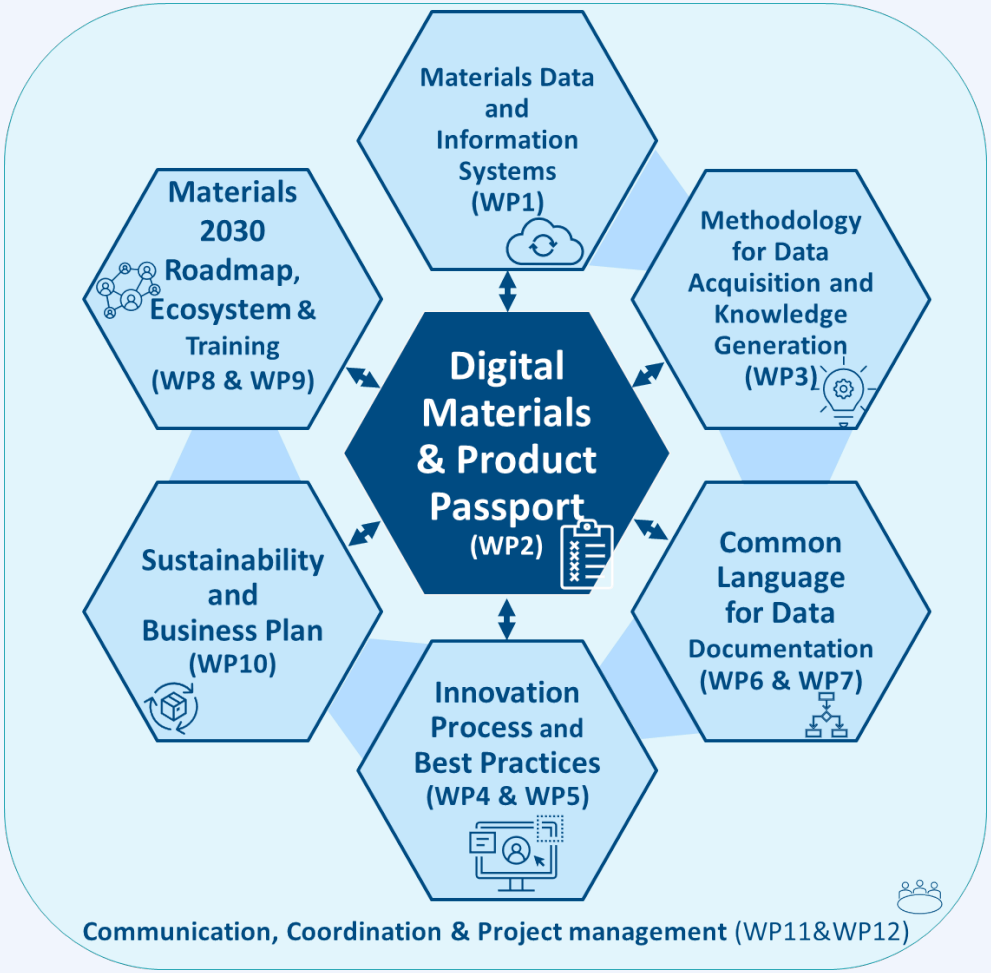


Digitalisering på Ås

DigiPass CSA: Developing the digital materials and product passport

DigiPass CSA

- O1: Enhance communication and cooperation among diverse communities.
- O2: Promoting the exchange of materials data and knowledge
- O3: Creation and utilization of Digital Product Passports
- O4: Demonstrate the projects developments and coordination actions
- O5: Establish collaborative digital skills training schemes
- O6: Elaborate the Business Plan



DigiPass CSA

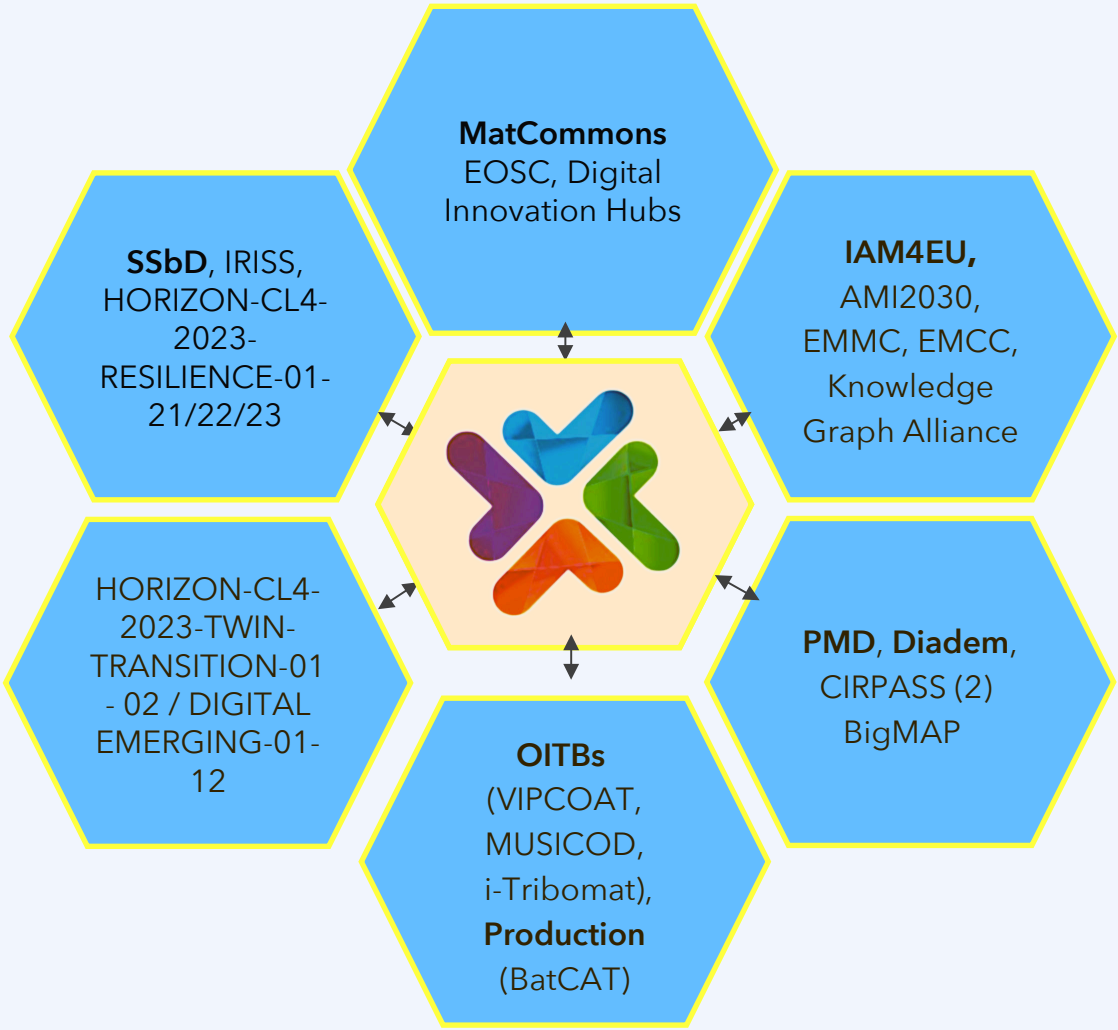
Four demonstrators:

Case 1:
Advanced composites

Case 2:
Advanced materials for renewable energy sources

Case 3:
Health and safety when using nanomaterials

Case 4:
Pre-painted metals



DigiPass CSA

WP7: Semantic interoperability and data spaces

Fraunhofer ITWM

WP2: Digital materials and product passport

WP10: Sustainability and business plan

NTNU

WP6: Metadata standardization

IRES

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

ARISTOTLE UNIVERSITY OF THESSALONIKI

Demonstration case: Pre-painted metals supply cain

ecca prepaintedmetal.eu

WP1: Materials data and information systems

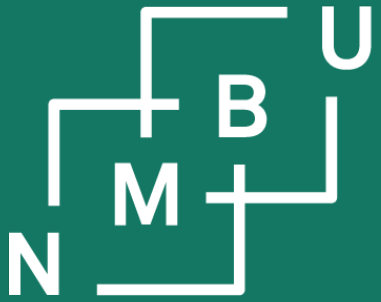
LIST

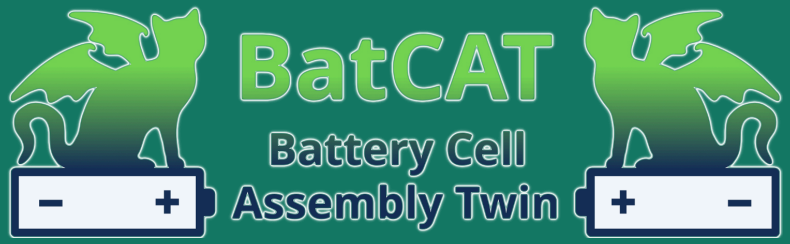
WIKKI

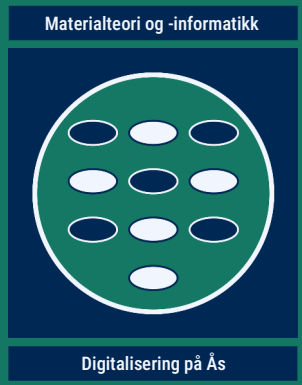
WP5: Innovation process

Demonstration case: Advanced materials for renewable energy sources

oet







BatCAT has received funding from the European Union's **Horizon Europe** research and innovation programme under **grant agreement no. 101137725**. Views and opinions expressed are however those of the author only and do not necessarily reflect those of the project, the European Climate, Infrastructure and Environment Executive Agency (CINEA), or the European Union. Neither BatCAT nor the CINEA or the EU can be held responsible for them.

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BatCAT Battery Cell Assembly Twin

DigiPass Know your products!

EUMINE

Moving from FAIR data principles to XAIR

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Norwegian University of Life Sciences

CAPE-OPEN Annual Meeting
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