Norges miljø- og biovitenskapelige universitet

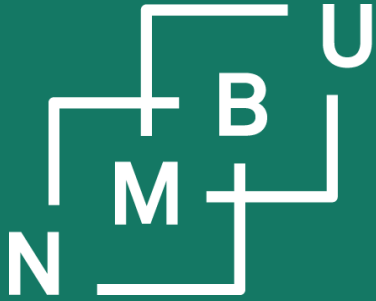# European recommendations for explainable-AI-ready (XAIR) data in materials modelling and characterization

M. T. Horsch,[1] F. Lønstad Bleken,[2] J. Friis,[3] H. A. Preisig[4]

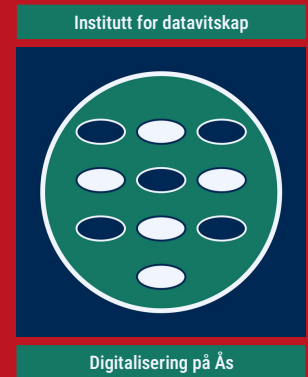[1]Norges miljø- og biovitenskapelige universitet, Institutt for datavitenskap
[2]SINTEF Industri, Avdeling prosessteknologi
[3]SINTEF Industri, Avdeling materialer og nanoteknologi
[4]Norges teknisk-naturvitenskapelige universitet, Institutt for kjemisk prosessteknologi
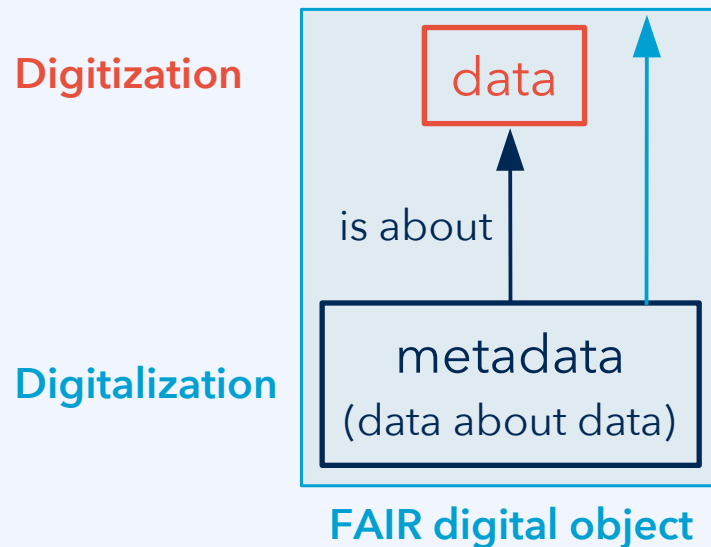
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1. **The need**
2. The state of the art
3. What are we proposing?

Epistemic opacity (Humphreys, 2011): A cognitive "process is **epistemically opaque** relative to a cognitive agent X at time t just in case X does not know at t all of the **epistemically relevant elements** of the process."

European AI Act proposal: "To address the **opacity** that may make certain AI systems **incomprehensible to or too complex for natural persons**, a certain degree of transparency should be required for high-risk AI systems. […] High-risk AI systems should therefore be accompanied by **relevant documentation**".

Digitization and digitalization

Metadata are "descriptive data about an object" (ISO 11179).

Digitization

Digitalization

FAIR digital object

Leiden 2022 Declaration for
FAIR digital objects:

https://www.fdo2022.org/site/fdo/
programme/leiden-declaration

The librarian:
– Focus on **archival** and **curation**
– **Help humans** use digital artefacts
– Focus on **provenance**, like for artefacts in a museum, so humans understand where they come from

The engineer:
– **Computers** must **understand** what the digital artefacts mean
– **Focus on knowledge**/meaning
– FAIR digital objects

Reproducibility and falsification

Research data infrastructures must accommodate mutually contradicting claims. They should also assist researchers at validating/falsifying each other's work.

Let us look into a "falsification" or "unsuccessful reproduction" of *a*'s work by *b*:

1) Reseacher *a* did *κ* and found *φ*.

2) Reseacher *b* did *γ*, which is very similar to *κ*, and found *ζ*, not very similar to *φ*.

3) Nobody disputes *a*'s integrity. Nobody disputes that "*a* did *κ* and found *φ*."

What is going on, what allows *b* to claim that this is some sort of falsification?

It is not just that *ζ* and *φ* are not the same. Sometimes that is OK.

Maybe the "very similar" phrases are important. What is the requirement there?
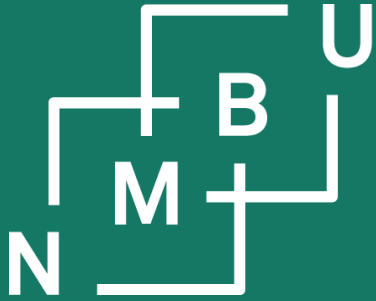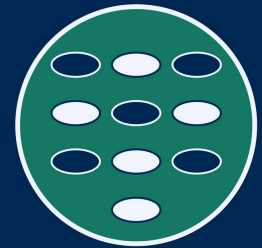
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EMMC-related development efforts from 2017 onward (stable release soon) have lead to a novel, radically physicalistic **top-level ontology**: The **Elementary Multiperspective Material Ontology** (EMMO). The EMMO includes a **Peircean semiotics** as a "perspective" on cognition.

The **European Materials Modelling Council (EMMC)** has advanced a CEN workshop agreement (CWA) for documenting **model data (MODA)** in table form, yielding the **CWA 17284** standard. The **European Models Characterization Council (EMCC)** did the same for **characterization data (CHADA)**, formalized through the **CWA 17815**.

RoMM (2017), MODA (2018), and CHADA (2021)
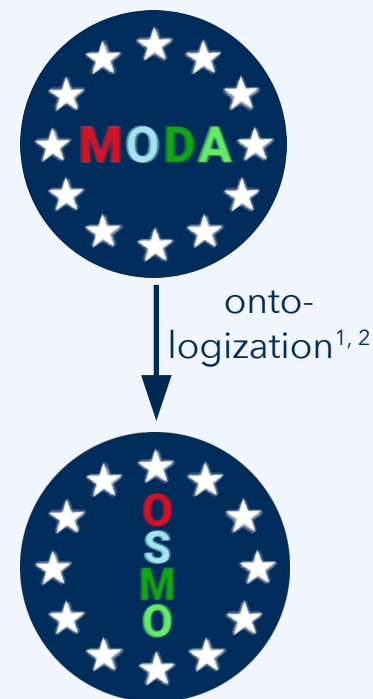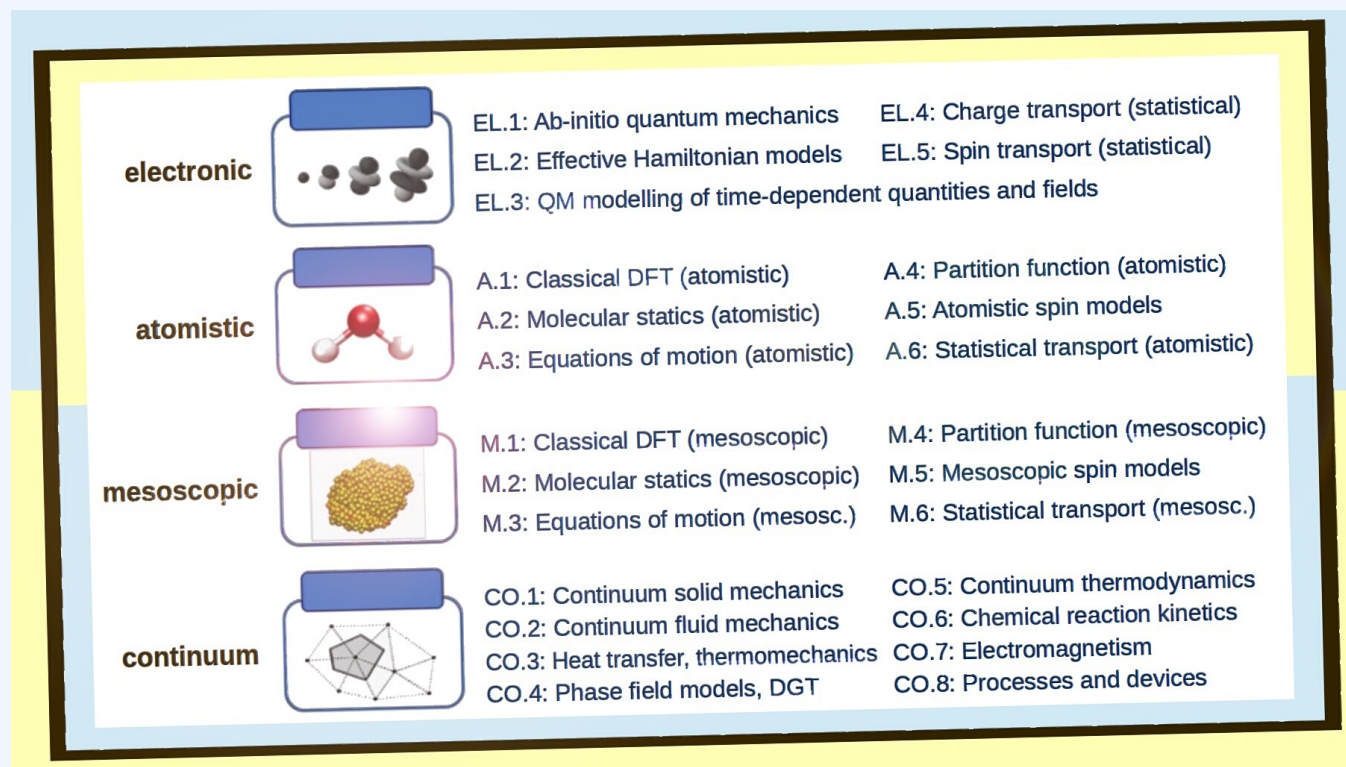
As an attempt at metadata standardization, RoMM/MODA resulted in a closed episte-mic space with a rigid categorization of modelling methodologies. MODA/CHADA docu-mentations are hard to create and **hard to use by humans, but not machine-actionable**.


electronic
- EL.1: Ab-initio quantum mechanics
- EL.2: Effective Hamiltonian models
- EL.3: QM modelling of time-dependent quantities and fields
- EL.4: Charge transport (statistical)
- EL.5: Spin transport (statistical)

atomistic
- A.1: Classical DFT (atomistic)
- A.2: Molecular statics (atomistic)
- A.3: Equations of motion (atomistic)
- A.4: Partition function (atomistic)
- A.5: Atomistic spin models
- A.6: Statistical transport (atomistic)

mesoscopic
- M.1: Classical DFT (mesoscopic)
- M.2: Molecular statics (mesoscopic)
- M.3: Equations of motion (mesosc.)
- M.4: Partition function (mesoscopic)
- M.5: Mesoscopic spin models
- M.6: Statistical transport (mesosc.)

continuum
- CO.1: Continuum solid mechanics
- CO.2: Continuum fluid mechanics
- CO.3: Heat transfer, thermomechanics
- CO.4: Phase field models, DGT
- CO.5: Continuum thermodynamics
- CO.6: Chemical reaction kinetics
- CO.7: Electromagnetism
- CO.8: Processes and devices

onto-logization[1,2]

MODA → OSMO

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

[2]M. T. Horsch *et al.*, in *Proc. JOWO 2021*, CEUR *vol.* **2969**: *p.* 47 (FOIS ontology showcase), **2021**.

EMMO[1] and Peircean semiotics

Peircean semiotics: By using a sign (1st) for an object (2nd), a "Third" is created.

the representation re-
lation is grounded
in a **real causal
connection**
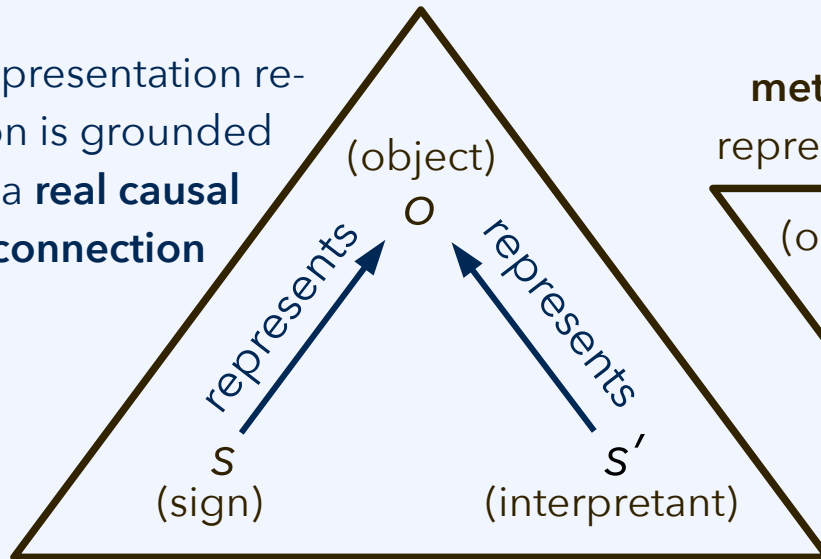
(object)

O

represents   *represents*

S S'
(sign)   (interpretant)

semiosis, a process by which a new
representamen, the interpretant, is created

metonymization, a process by which a
representamen is assigned a new referent

(old referent)   (new referent)

O O'

represents   *represents*

S
(sign)

Elementary Multi-
perspective Material
Ontology (EMMO)
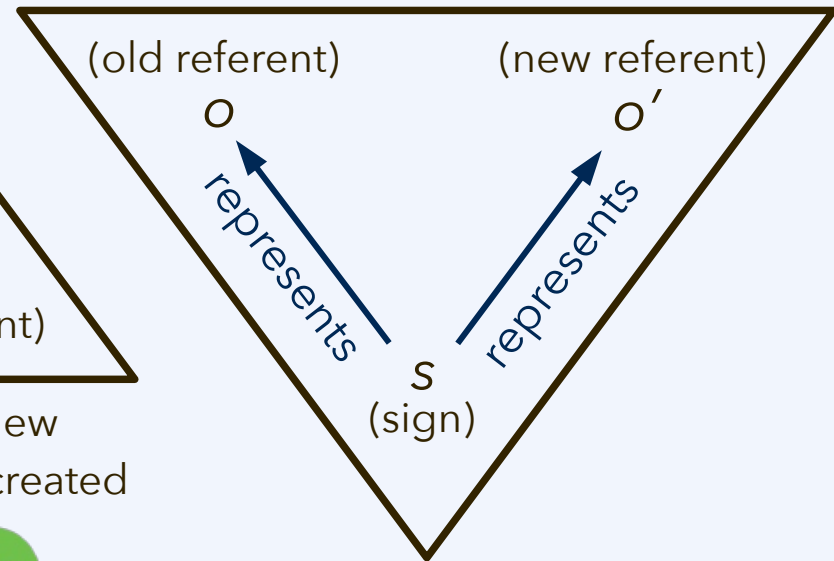
C. S. Peirce

The EMMO[1] combines this with
mereotopology – foundational
ontology as **mereosemiotics**.

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Peircean semiotics: Provenance

Peircean semiotics

the representation relation is grounded in a "real causal connection"

(object) *o*

represents *represents*

s (sign) *s'* (interpretant)

the semiosis, a process by which a new representamen, the interpretant, is created

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*.

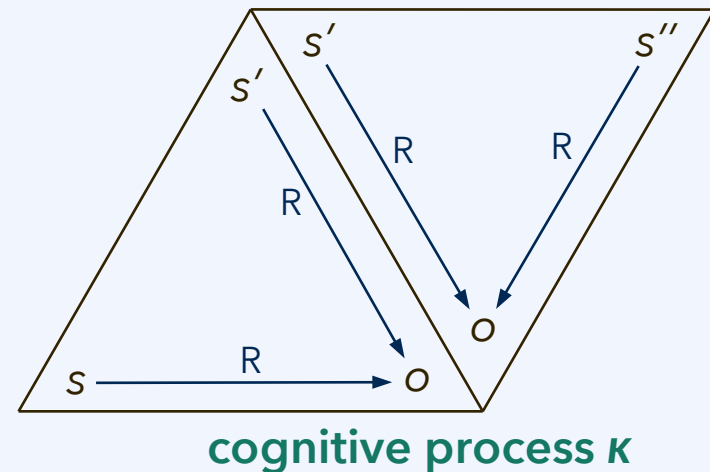**Cognitive process (example):**

- 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*).
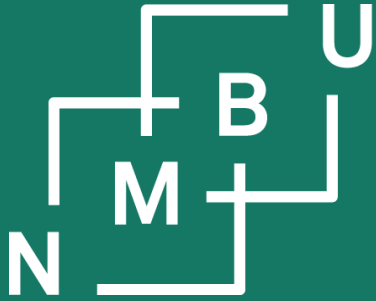
Research workflows as cognitive processes:[1]

cognitive process κ

[1]M. T. Horsch, in *Proc. JOWO 2021*, CEUR *vol.* **2969**: *p.* 3 (FOUST), **2021**.

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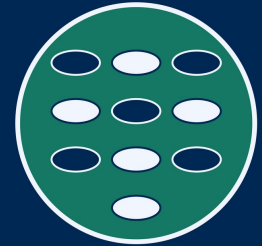
1. The need
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The **CWA 17960 ModGra** is a new community standard for **process model topologies**. The **PIMS-II mid-level ontology** implements a data documentation strategy based on **epistemic metadata**, with a focus on **knowledge claims** and their assessment, in particular, through **reproducibility claims**.

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.

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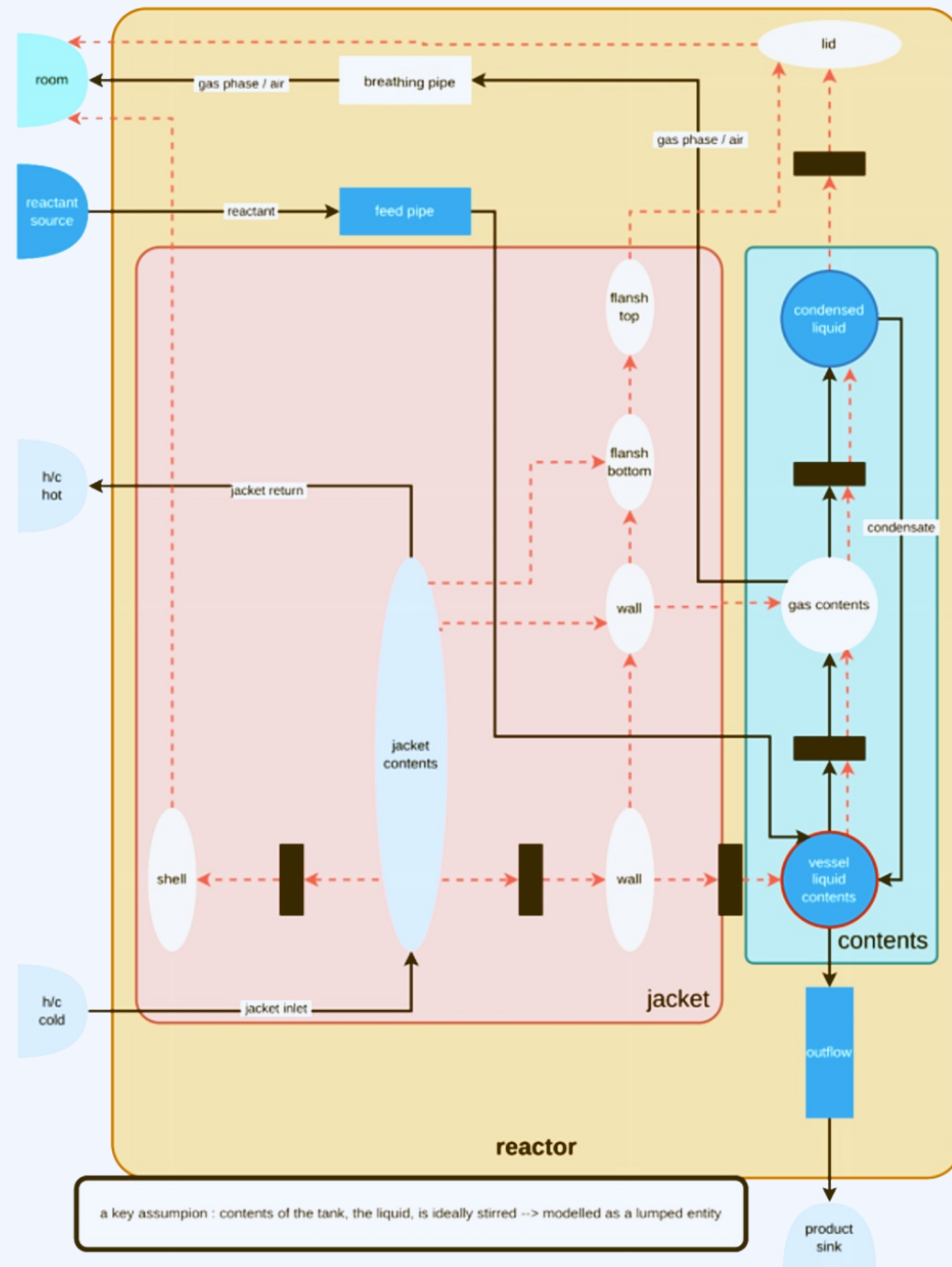
Epistemic metadata

Metadata are "descriptive data about an object" (ISO 11179).

Epistemic metadata are those that help establish the knowledge status of data.[1]

> **Epistemic metadata in the PIMS-II mid-level ontology:**
>
> **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**).

Case study from molecular thermodynamics
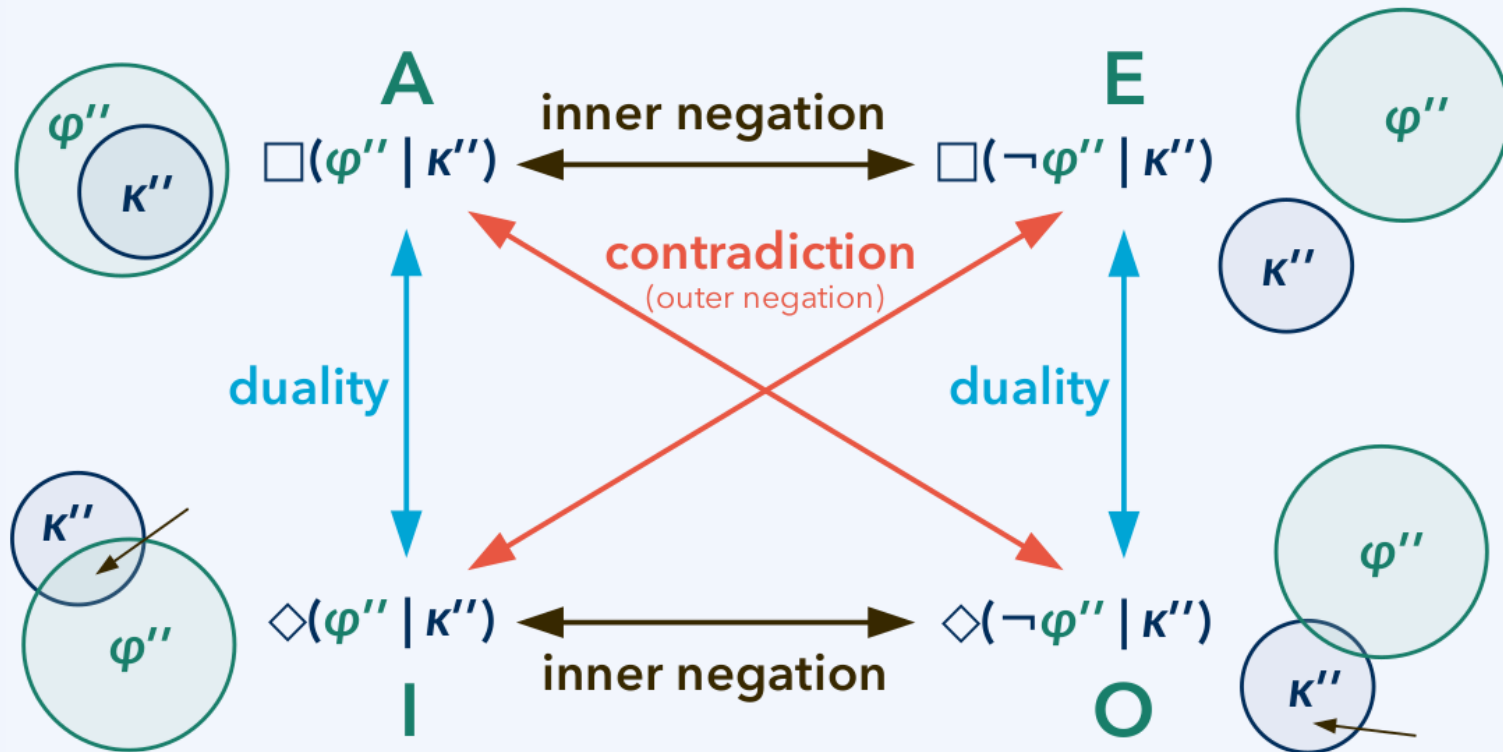
- First stage, evaluating ten journal articles, doi:10.5281/zenodo.7516532.
- Second stage, discussing twelve claims, doi:10.5281/zenodo.7608074.

[1]M. T. Horsch, B. Schembera, in *Proc. JOWO 2022*, CEUR *vol.* **3249**: *p.* 2 (CAOS), **2022**.

Reproducibility claims

If the research process conforms with κ'', the outcome **must conform** with φ''.

If the research process conforms with κ'', the outcome **must not conform** with φ''.

A
$\Box(\varphi'' \mid \kappa'')$

inner negation

E
$\Box(\neg\varphi'' \mid \kappa'')$

contradiction
(outer negation)

duality

duality

$\Diamond(\varphi'' \mid \kappa'')$

inner negation

$\Diamond(\neg\varphi'' \mid \kappa'')$

I

O

If the research process conforms with κ'', the outcome **can conform** with φ'' (and it is possible to conform with κ'').

If the research process conforms with κ'', the outcome **can disagree** with φ'' (and it is possible to conform with κ'').

Reproducibility claims 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»
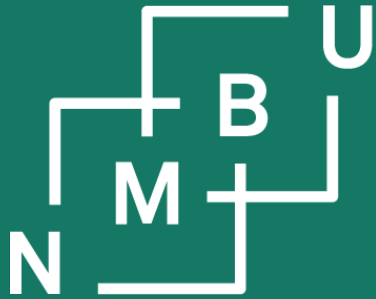
Institutt for datavitenskap

Digitalisering på Ås

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Fakultet for realfag og teknologi   Institutt for datavitenskap