Norges miljø- og biovitenskapelige universitet

NORCORN

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Digitalisering på Ås

Data Science Lunch Meeting

Formal representation of the grounding and reproducibility of scientific claims:

What has been proposed – and obstacles.

IDV-lunsjmøte

24. november 2023

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1 Epistemic metadata

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."

Epistemic opacity

Epistemic opacity is a concept from the theory of physics-based modelling and simulation, but beyond this also became relevant to data-driven methods. It was introduced by **Humphreys** in *Extending Ourselves*[1] (2004), developed further in later work,[2] and gained traction with the hype in machine learning.

Humphreys (2004): «In many computer simulations, the dynamic relationship between the initial and final states of the core simulation is epistemically opaque because most **steps in the process** are **not open to direct inspection and verification**. This opacity can result in a loss of understanding».[1]

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**.

Norwegian University of Life Sciences

Epistemic opacity

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.[1] Users should be able to interpret the system output and use it appropriately. High-risk AI systems should therefore be accompanied by **relevant documentation**".

Beginning with the EC's **Battery Regulation**, **digital product passports** (DPPs) will become mandatory; first for batteries, later textiles, electronics, and for more and more products.

DIGIPASS CSA (from 2024)

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]Systems with "high risk" include all "safety components" related to "water, gas, heating, and electricity."

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

XAIR Data Initiative Ås

XAI: Explainable artificial intelligence

AIR: Artificial-intelligence ready

XAIR: Explainable AI-ready

Beginning with the EC's **Battery Regulation**, **digital product passports** (DPPs) will become mandatory; first for batteries, later textiles, electronics, and for more and more products.

DIGIPASS CSA (from 2024)

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

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

XAIR Data Initiative Ås

Our Mission

The Norwegian Reproducibility Network (NORRN) is a peer-led network that aims **to promote and enable rigorous, robust and transparent research practices in Norway**. We attempt to achieve this goal by establishing appropriate training activities, designing, and evaluating research improvement efforts, disseminating best practices, and working with stakeholders to ensure coordination of efforts across the sector. NORRN's activities span multiple levels, inɹding researchers, librarians, institutions, and other stakeholders (e.g., funders and public authorities).

Norwegian Reproducibility Network: https://www.norrn.no/

Researchers

We **support researchers** in educating themselves about open science practices, and founding local open science communities.

Initiatives

We **connect Reproducibility Initiatives** to a national network, and foster connections between them.

Institutions

We **advise institutions** on how to embed open science practices in their work.

Stakeholders

We **represent the open science community** toward other stakeholders in the wider scientific landscape.

XAIR Data Initiative Ås

Proposal to organize a Norwegian Reproducibility Network (NORRN) node for Campus Ås in form of the **XAIR Data Initiative Ås** as a **seminar**.

Fridays, every sixth week, 11.15 – 12.00.

Reserved TF-323b for seminar appointments as follows:

week 3	19th January 2024
week 9	1st March 2024
week 15	12th April 2024
week 21	24th May 2024
week 33	16th August 2024
week 39	27th September 2024
week 45	8th November 2024

Ontology development for 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**).

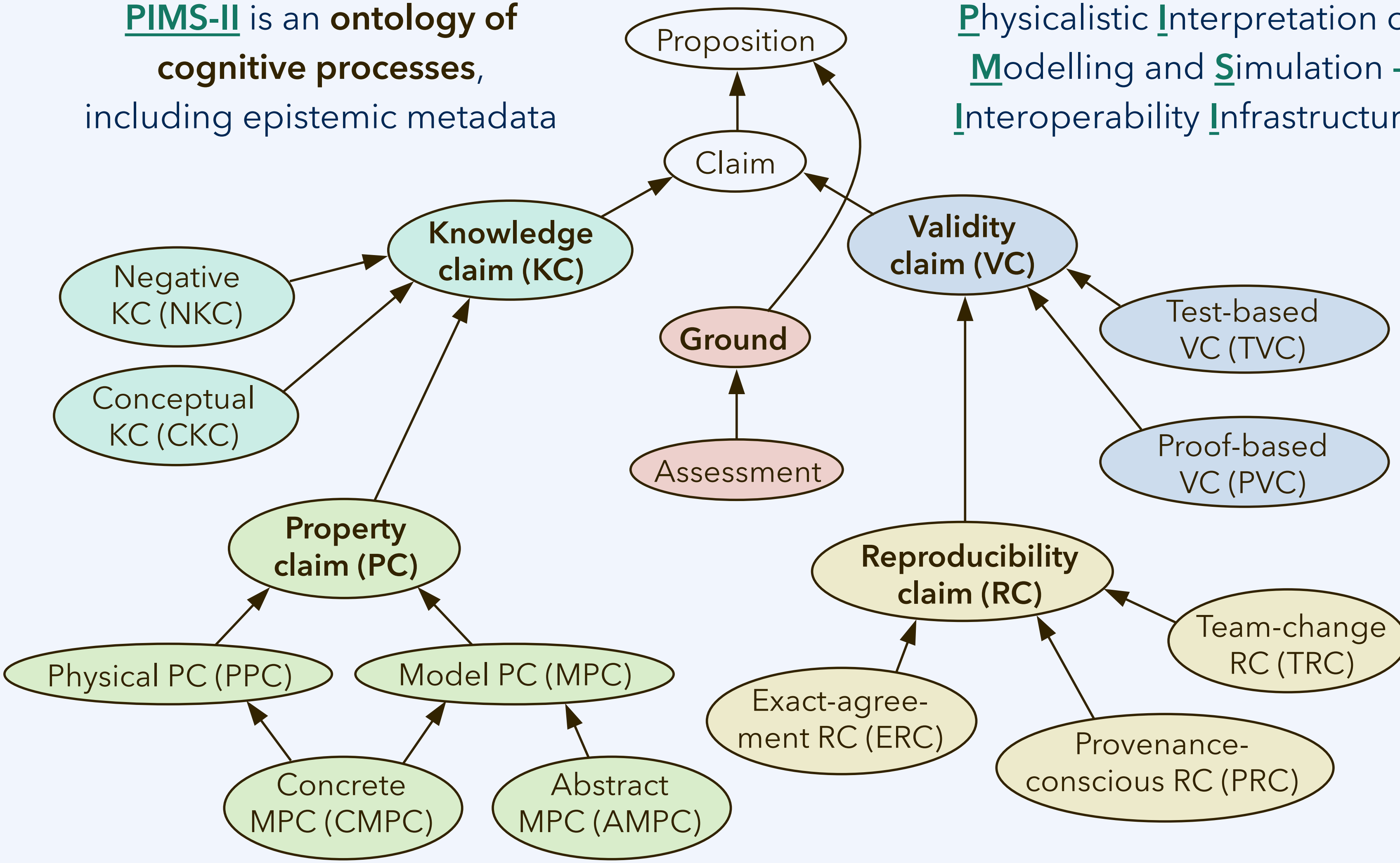
Key epistemic metadata items are the **knowledge claims** made based on data, their **provenance**, **validation** and **reproducibility**, and **epistemic grounding**.

[1]«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**.

Ontology development for epistemic metadata

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

Physicalistic Interpretation of Modelling and Simulation – Interoperability Infrastructure



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2 Case study

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

Case study in molecular thermodynamics

Epistemic metadata and their **documentation** were explored in molecular thermodynamics:

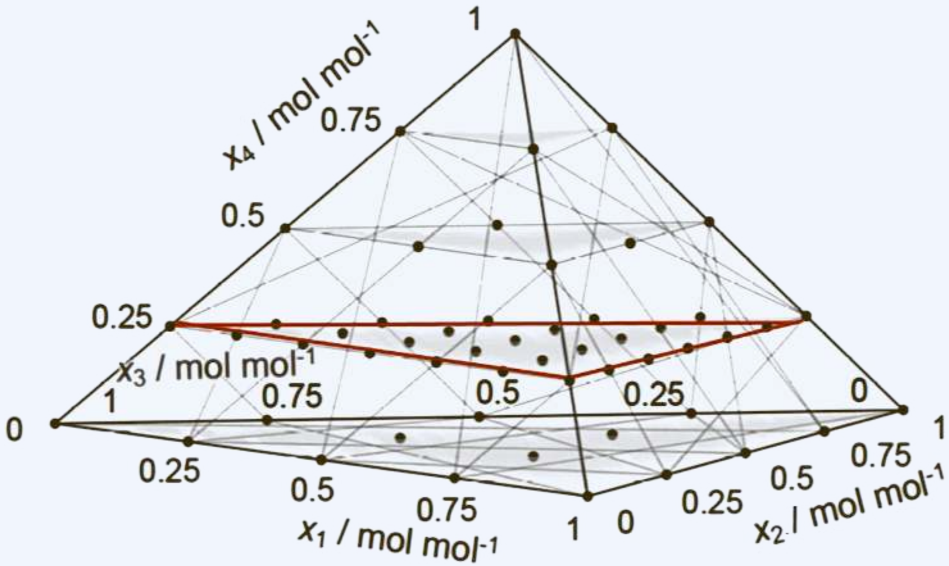
First stage report (10 cases), doi:10.5281/zenodo.7516532, **2023**.
Discussion of *five papers each* from *two research groups* (Berlin, London) without involving the papers' authors. Obtained a tentative **taxonomy for epistemic metadata** and explored the patterns of epistemic grounding.

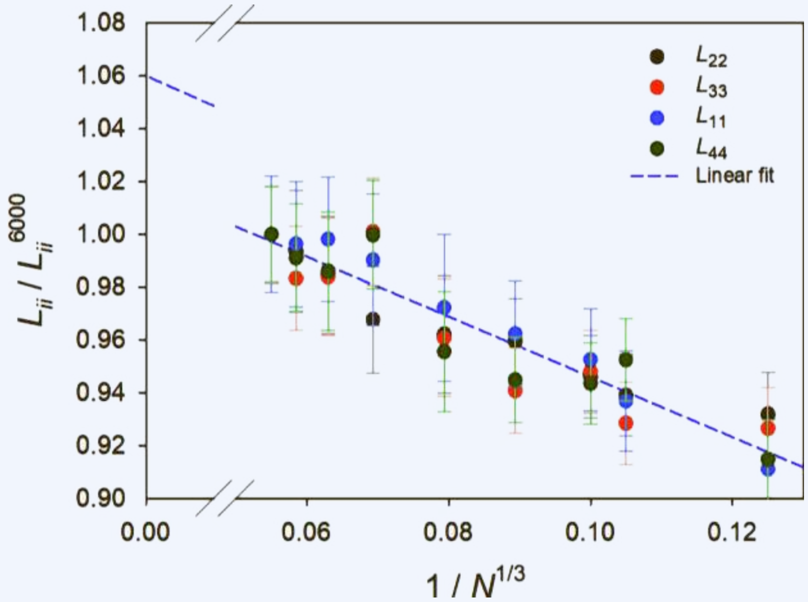
Second stage report (12 claims), doi:10.5281/zenodo.7608074, **2023**.
Discussion of *two claims each* from *six papers*, with two papers each from three research groups (Berlin, Kaiserslautern, London), involving the papers' authors. **Ontology of epistemic metadata** implemented.

Good data documentation standards give researchers freedom to say what they want. They **provide a language**, but **don't micromanage** researchers' self-expression. (Morton: Ontology should not be "object police.")

Guevara *et al.* (2020) paper:[1] First-stage analysis[2]

Example: The work by Guevara *et al.*[1] (2020) was considered at both stages.[2, 3]





[1]G. Guevara Carrión, R. Fingerhut, J. Vrabec, «Fick diffusion coefficient matrix of a quaternary liquid mixture by molecular dynamics», *J. Phys. Chem. B* **124**(22): 4527–4535, doi:10.1021/acs.jpcb.0c01625, **2020**.

[2]M. T. Horsch, B. Schembera, «Epistemic metadata in molecular modelling: First-stage case-study report (10 cases)», Inprodat technical report 2023–A, doi:10.5281/zenodo.7516532, **2023**.

[3]M. Horsch, S. Chiacchiera, G. Guevara, M. Kohns, E. Müller, D. Šarić, S. Simon, I. Todorov, J. Vrabec, B. Schembera, «Epistemic metadata in molecular modelling: Second-stage case-study report (12 claims)», Inprodat technical report 2023–B, doi:10.5281/zenodo.7610237, **2023**.

Guevara *et al.* (2020) paper:[1] First-stage analysis[2]

Question: What is a good methodology for obtaining Fick diffusion coefficients in multicomponent mixtures by [equilibrium molecular dynamics] simulation?

Object of research: The object of research is the Fick diffusion coefficient matrix as such.

Knowledge claim: […] methodology […] first, the explicit inclusion of a finite-size correction, where it is specifically novel that this correction is applied to the Onsager coefficients, and second, obtaining the Darken correction from [Kirkwood-Buff] integrals.

Grounding: KB part […] validated against "the Wilson excess Gibbs energy model […]" […] not clear what should make us accept the finite-size methodology […]. It yields a correction of 6% […] whereas the "[…] following Yeh and Hummer would have led to corrections of around 15%." It is based on a linear regression in $N^{-1/3}$ […] ad hoc fit.

[1]G. Guevara Carrión, R. Fingerhut, J. Vrabec, «Fick diffusion coefficient matrix of a quaternary liquid mixture by molecular dynamics», *J. Phys. Chem. B* **124**(22): 4527–4535, doi:10.1021/acs.jpcb.0c01625, **2020**.

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[3]M. Horsch, S. Chiacchiera, G. Guevara, M. Kohns, E. Müller, D. Šarić, S. Simon, I. Todorov, J. Vrabec, B. Schembera, «Epistemic metadata in molecular modelling: Second-stage case-study report (12 claims)», Inprodat technical report 2023–B, doi:10.5281/zenodo.7610237, **2023**.

Guevara *et al.* (2020) claims:[1] Second-stage analysis[2]

Interviews were done with the authors; *e.g.*, on 24th January 2023, two papers, among them Guevara *et al.*[1] (2020) were discussed in a 70-minutes meeting. Two of the three authors participated (Gabriela Guevara and Jadran Vrabec).

«**Why is it knowledge?**

- Yeh & Hummer instead use a semiempirical correlation, relying on all sorts of properties, working with the end result which *D*.
- The new method is formally much simpler, relying only on *N*, and it works with the underlying quantity *L* which is more fundamental, rather than with the end outcome *D*.
- Also, linear behaviour of *D* in $1/N^3$ was already claimed before by others, and not only for *D*, it is something like "community shared understanding". In particular, Yeh-Hummer also has $1/N^3$ in it.

Validation:

- Is it better than Yeh-Hummer? Really such a validation still needs to be done.»

[1]G. Guevara Carrión, R. Fingerhut, J. Vrabec, «Fick diffusion coefficient matrix of a quaternary liquid mixture by molecular dynamics», *J. Phys. Chem. B* **124**(22): 4527–4535, doi:10.1021/acs.jpcb.0c01625, **2020**.

[2]M. Horsch, S. Chiacchiera, G. Guevara, M. Kohns, E. Müller, D. Šarić, S. Simon, I. Todorov, J. Vrabec, B. Schembera, «Epistemic metadata in molecular modelling: Second-stage case-study report (12 claims)», Inprodat technical report 2023–B, doi:10.5281/zenodo.7610237, **2023**.

Guevara *et al.* (2020) claims:[1] Second-stage analysis[2]

Interviews summarized in the second-stage report,[2] with two claims per paper.

Selected knowledge claims from the paper:

1. A novel finite-size correction methodology for the phenomenological diffusion coefficient matrix $\mathbf{L}$ based on linear extrapolation over $1/N^3$ to the limit $1/N^3 \to 0$ is proposed and successfully used to calculate $\mathbf{D}$.
2. The Fick diffusion coefficient matrix $\mathbf{D}$ of the considered mixture has the values given in Table 1 of the paper under the conditions specified there.

d The novel method looks preferable or more plausible as it exhibits what is typically seen in the community as theoretical virtues: *First*, Yeh and Hummer [21] use a semiempirical correlation relying on multiple properties, while the novel method is formally much simpler, relying only on N. *Second*, the Yeh-Hummer method operates on the end result $\mathbf{D}$, whereas the novel method operates on the intermediate result $\mathbf{L}$ that directly experiences the finite-size limitation in the molecular simulation.

[1]G. Guevara Carrión, R. Fingerhut, J. Vrabec, «Fick diffusion coefficient matrix of a quaternary liquid mixture by molecular dynamics», *J. Phys. Chem. B* **124**(22): 4527–4535, doi:10.1021/acs.jpcb.0c01625, **2020**.

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3 Metadata documentation

Reproducibility claim

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

Documenting a reproducibility claim

reproducibility

There are many definitions of reproducibility and replicability; see the review by Hans Ekkehard Plesser.[1]

1) Researcher *a* did κ and found φ.

2) Researcher *b* did γ (similar enough to κ) and found ζ (not similar enough to φ).

3) If ζ was similar enough to φ, it would still contradict φ, but not be a falsification.
The literal claim of *a*, "I carried out process κ and found φ" is not contradicted.

Reproducibility claim

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

[1]H. E. Plesser, *Frontiers Neuroinform.* **11**: 76, doi:10.3389/fninf.2017.00076, **2018**.

Documenting a reproducibility claim

NOR RN

The scientific process can benefit from making reproducibility claims explicit.

In this way, other researchers know what exactly they need to comply with when attempting to replicate and validate or falsify others' work.

1) Researcher *a* did κ and found φ.

   Here, *a* also made a **positive reproducibility claim ψ**.

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

   Here, *b* made the **negative reproducibility claim $\neg\psi$**.

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

provenance metadata κ
provenance paradata κ'

---

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

«repeat κ, but no need to retain κ'»

knowledge claim metadata φ
knowledge claim paradata φ'

---

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

«obtain φ again, except for φ' maybe»

Documenting a reproducibility claim

The scientific process can benefit from making reproducibility claims explicit.

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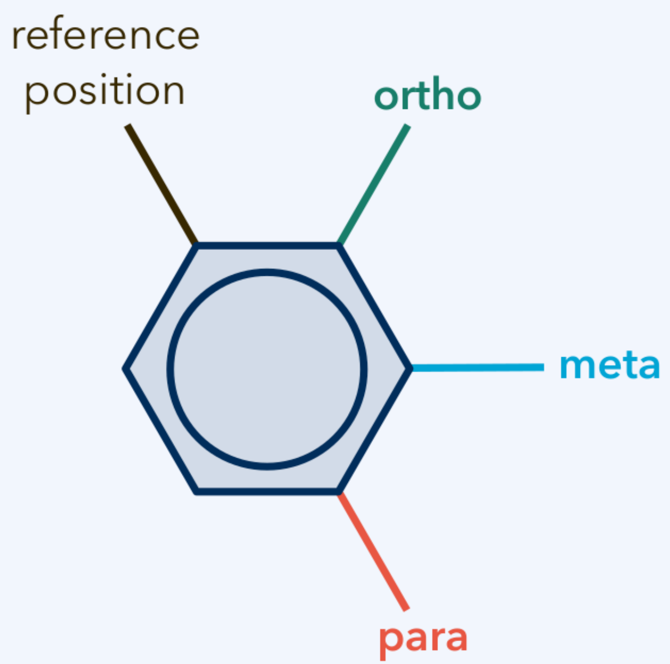
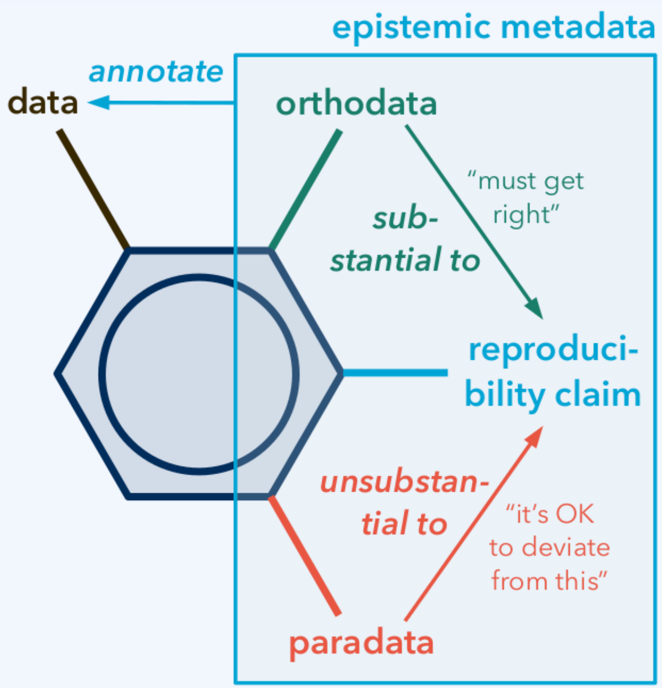




«repeat κ, but no need to retain κ'»

«obtain φ again, except for φ' maybe»

Logical subtraction and subject matter (*i.e.*, topic)

Logical subtraction is a concept from analytic philosophy.[1-3]

Its formalization is closely connected to the theory of **subject matter**.[2, 3]

Could you try to **replicate my old simulation result**? Just do the same as I did.
Except that you of course log in with your user account, not mine.
Your result was off by 0,5%? **Don't worry**, that is totally normal.

Our **simulation of object *o*** confirms theory *s*.
Except that theory *s* deals with physical reality, and *o* is so simplified
that **we know it cannot exist** or be built exactly in physical reality.

[1]R. A. Jaeger, *Philos. Rev.* **82**(3): 320–329, doi:10.2307/2183898, **1973**.
[2]K. Fine, *J. Philos. Log.* **46**: 675–702, doi:10.1007/s10992-016-9419-5, **2017**.
[3]S. Yablo, *Aboutness*, Princeton Univ. Press (ISBN 978-0-691-14495-5), **2014**.

Logical subtraction and subject matter (*i.e.*, topic)

Following Yablo,[1] the **subject matter** of a knowledge claim and/or associated research data is given by the **research question that is being answered**, or by the «equivalence relation over logical space» with respect to that question.

Proposition: "A is the factually correct answer to question Q."
Subject matter of the proposition: Q.

PIMS-II distinguishes two ways of **combining topics**. Related topics q_1 and q_2 form a **topical product** $q_1 q_2$ where the partitioning of logical space by $\equiv_{q1q2}$ is the *product of the sets of equivalence classes* with respect to $\equiv_{q1}$ and $\equiv_{q2}$.

However, long papers *etc.* can also be about many topics that are not closely related. They stand side by side. We call this a **topical sum** $q_1 + q_2$, e.g.,

q_1 = a theoretical research question from statistical mechanics,
q_2 = topic of a concrete series of simulations from the same paper.

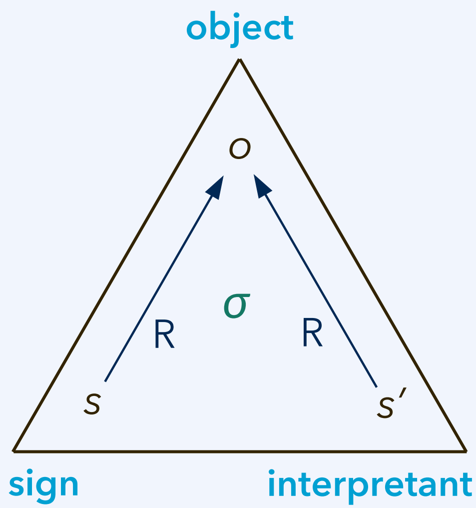
[1]S. Yablo, *Aboutness*, Princeton Univ. Press (ISBN 978-0-691-14495-5), **2014**.

Knowledge graph patterns (PIMS-II ontology)

Step in a cognitive process:

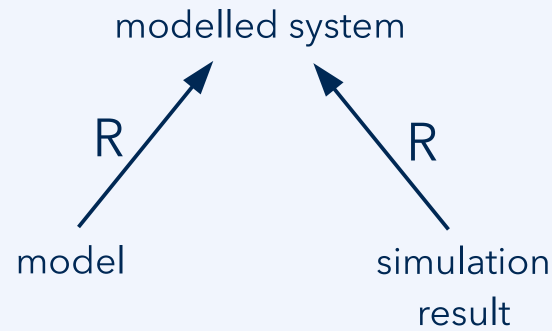
First, shown in triadic notation as a Peircean semiosis.

C. S. Peirce



Semiosis
(following C. S. Peirce)

cognitive step

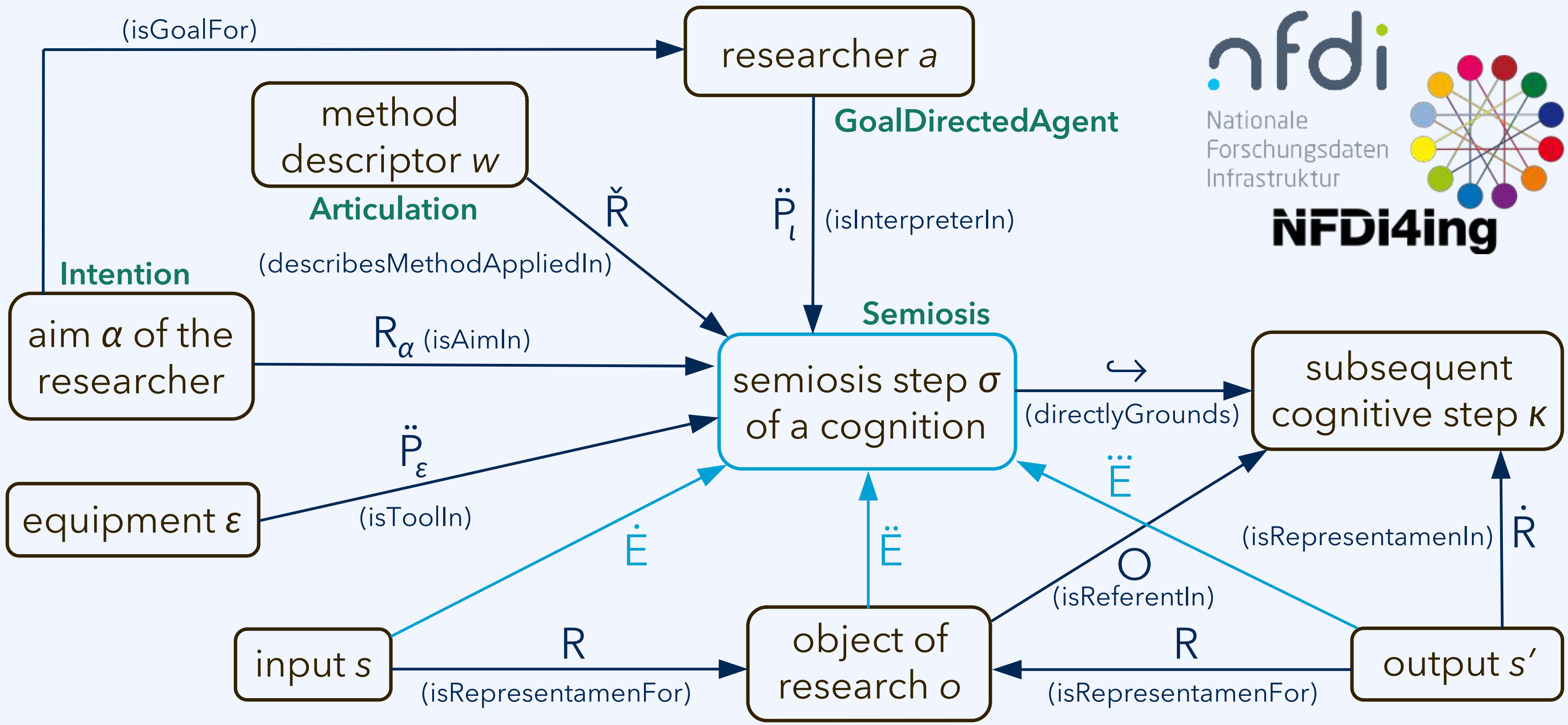


example

Next, construct a knowledge graph pattern for documenting the semiosis.

Knowledge graph patterns (PIMS-II ontology)

Step in a cognitive process (called «processing step» by Metadata4Ing).
The knowledge graph pattern is 1:1 aligned between PIMS-II and Metadata4Ing.



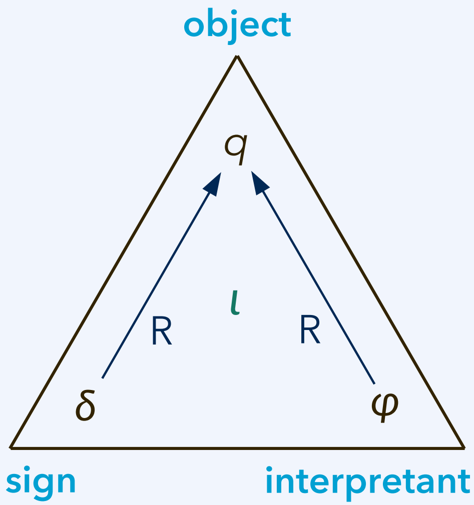
NFDI4ing — Nationale Forschungsdaten Infrastruktur

knowledge graph pattern

Knowledge graph patterns (PIMS-II ontology)

Consider the following scenario, in which a dataset is analysed, yielding a claim:

- 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**.



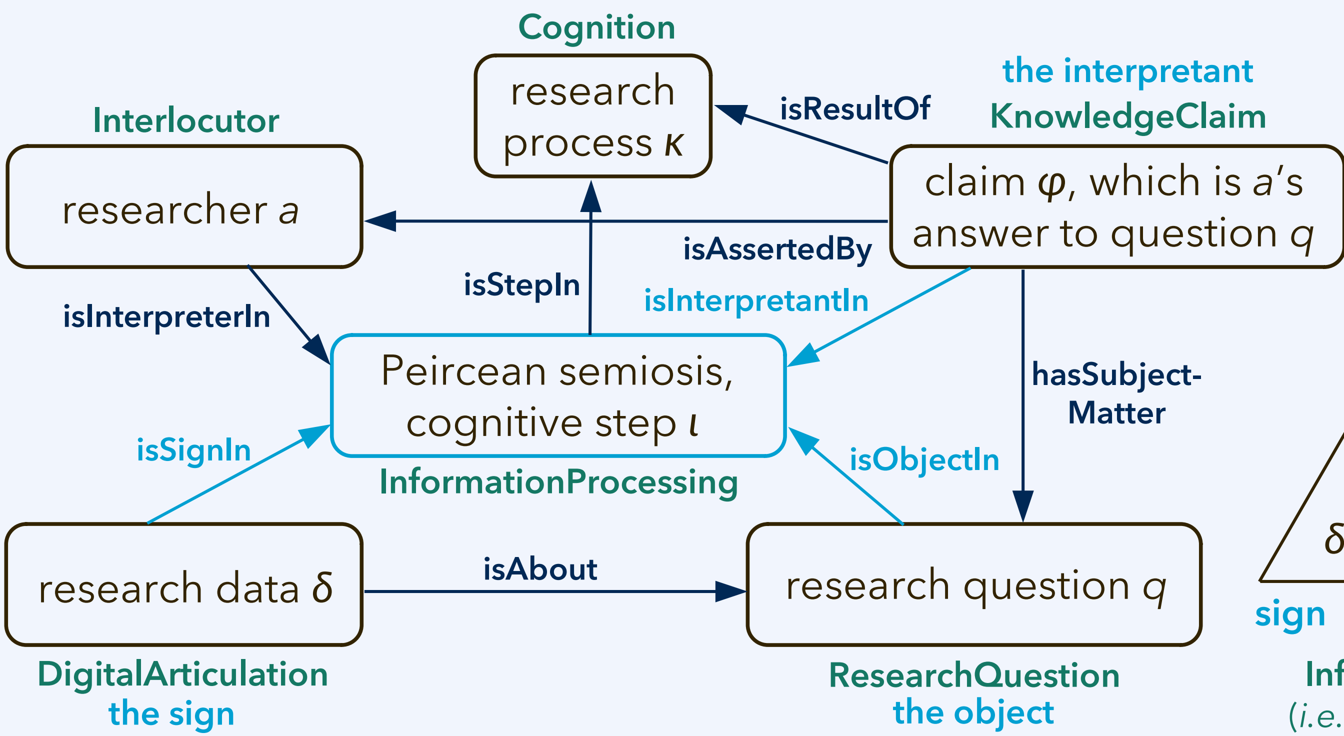
InformationProcessing
(*i.e.*, a Peircean semiosis)

cognitive step

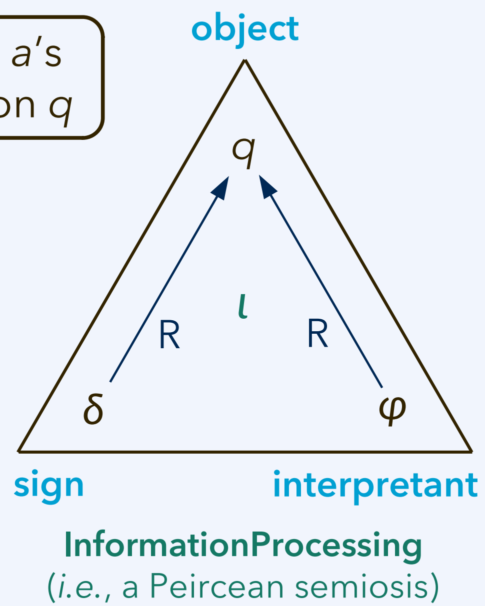
Knowledge graph patterns (PIMS-II ontology)

Knowledge claim (KC), including the provenance

«Researcher *a* did *κ* and found *φ* (and thus claims to know *φ*).»
→ Therefore, when research process *κ* is carried out, it <u>can</u> lead to outcome *φ*.



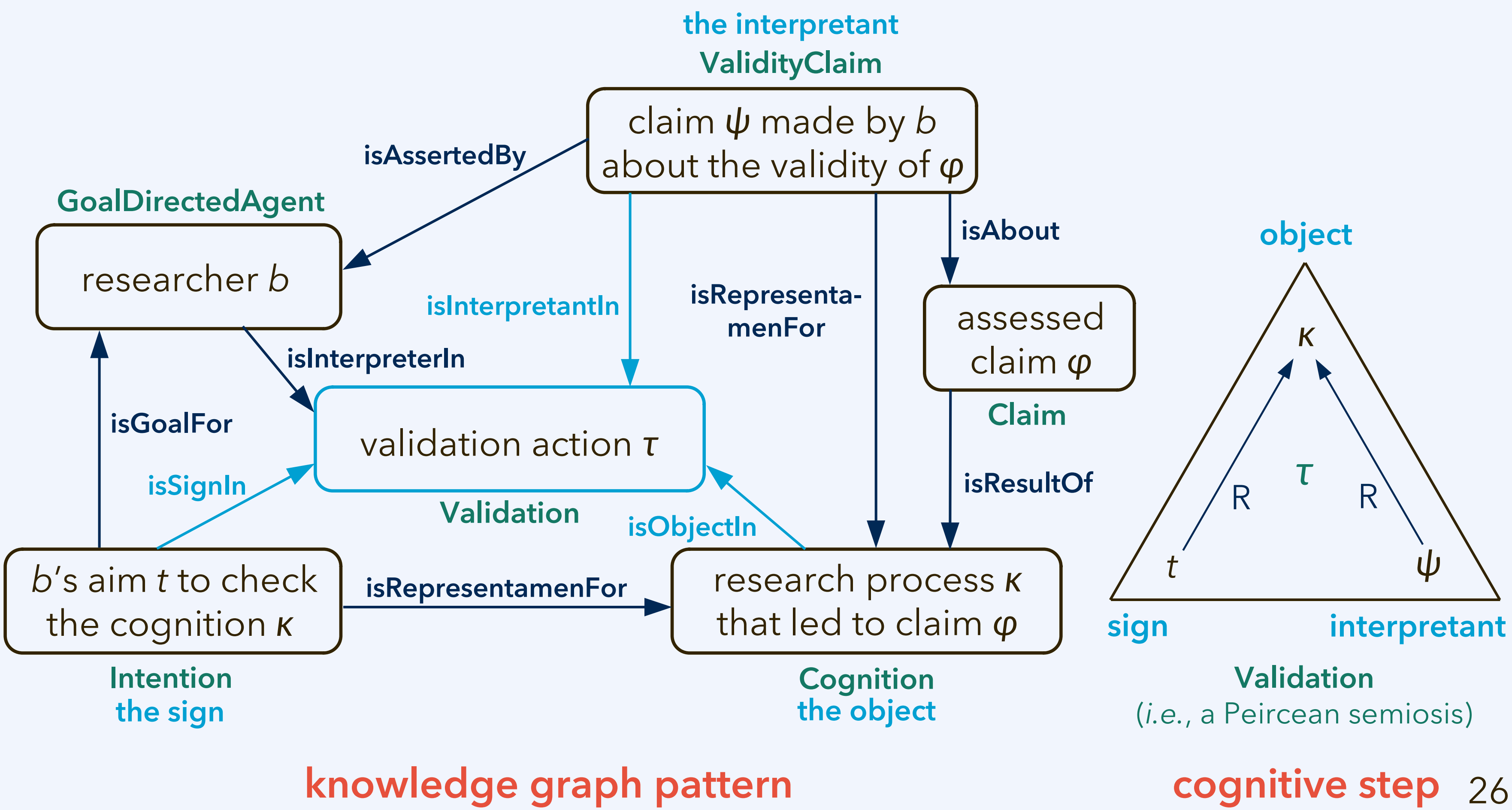
knowledge graph pattern



cognitive step

Knowledge graph patterns (PIMS-II ontology)

A **validation** is an evaluation (special type of semiosis) where the evaluated object is a cognitive action and the interpretant is a **validity claim**.



NMBU

The epistemic grounding of a research outcome is an explanation for **why** the scientific community accepts that result as **knowledge**; *i.e.*, a rationale for why it should be accepted as knowledge.

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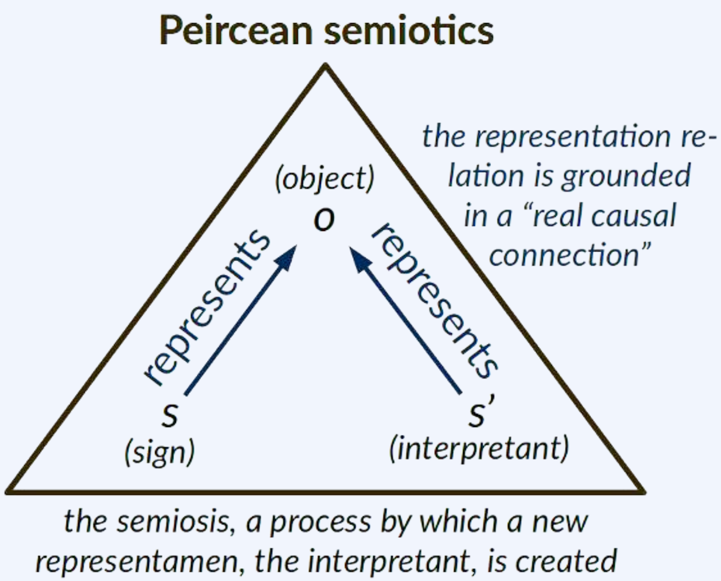
4 Epistemic grounding

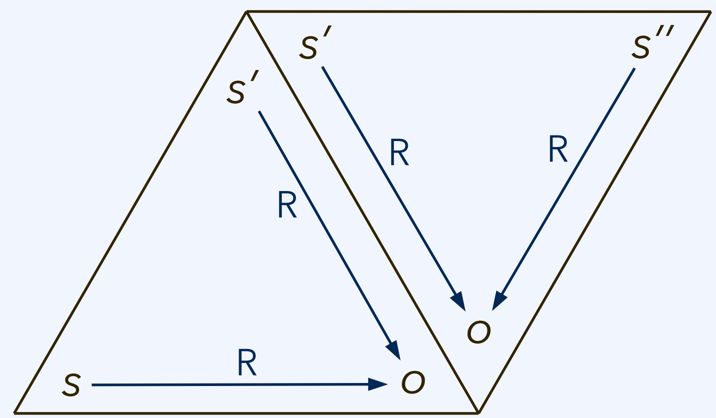
Grounding in multi-stage cognitive processes



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]



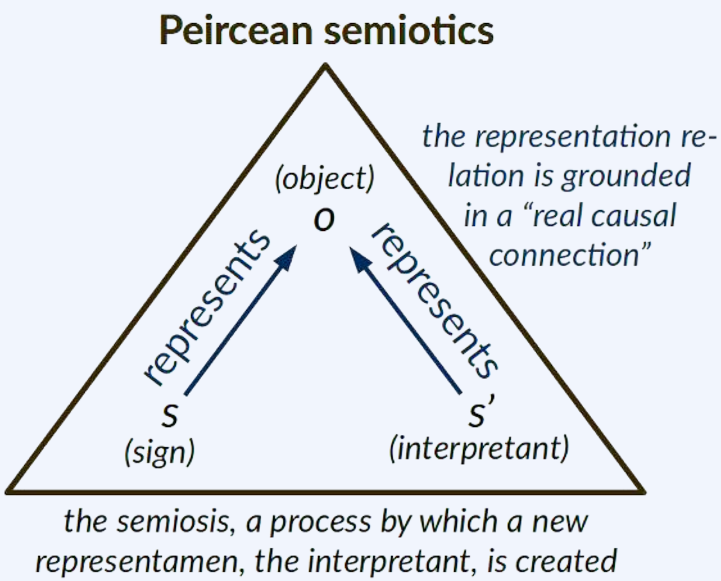
cognitive process κ

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

Grounding in multi-stage cognitive processes



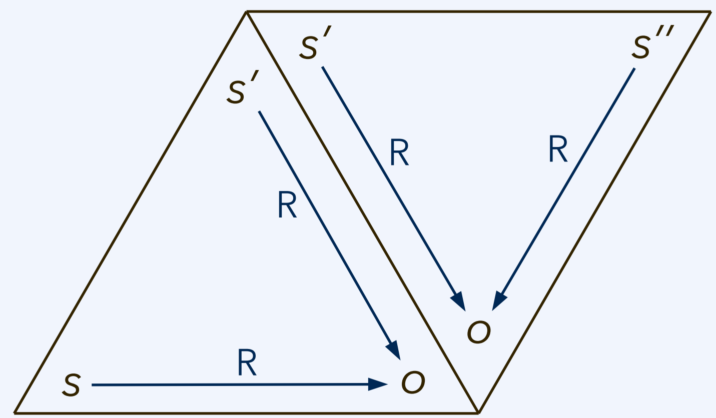
Cognitive process (example):

- 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, $Rs''o$.



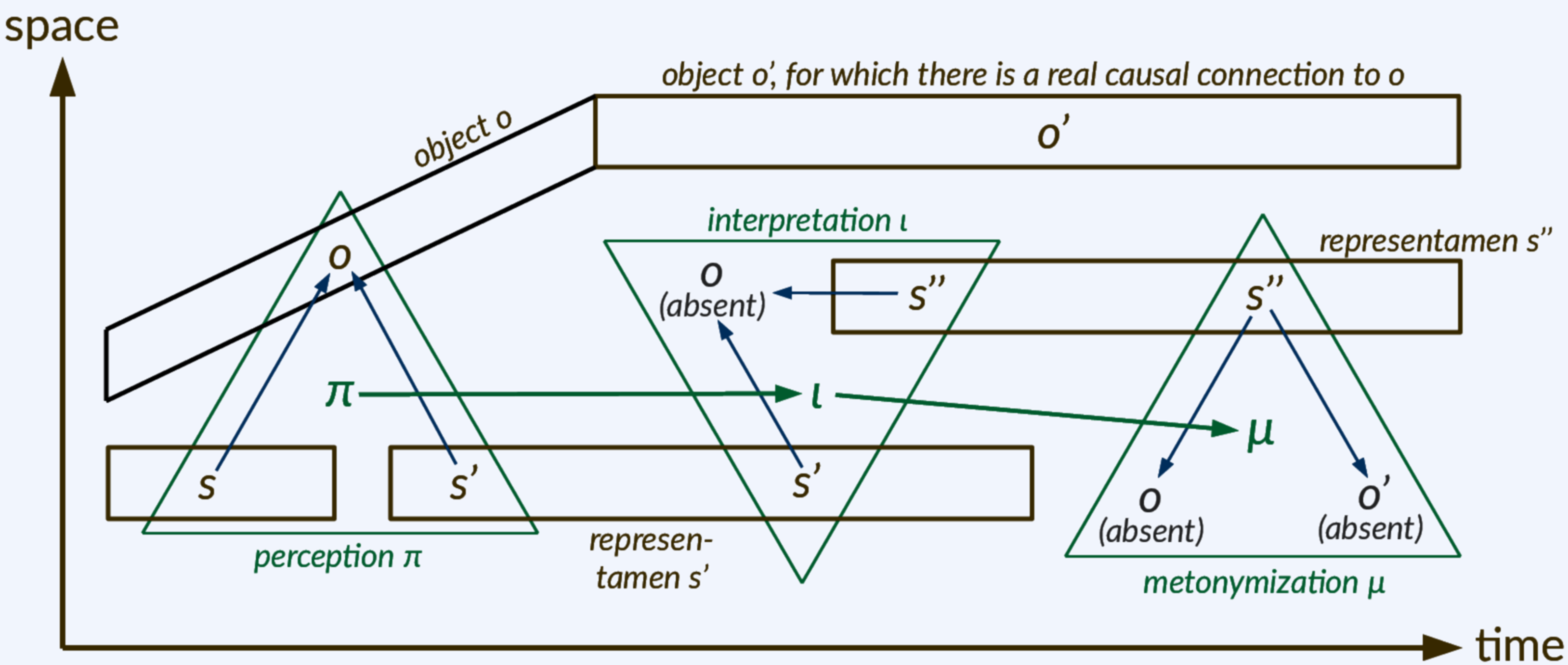
cognitive process κ

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

Grounding in multi-stage cognitive processes

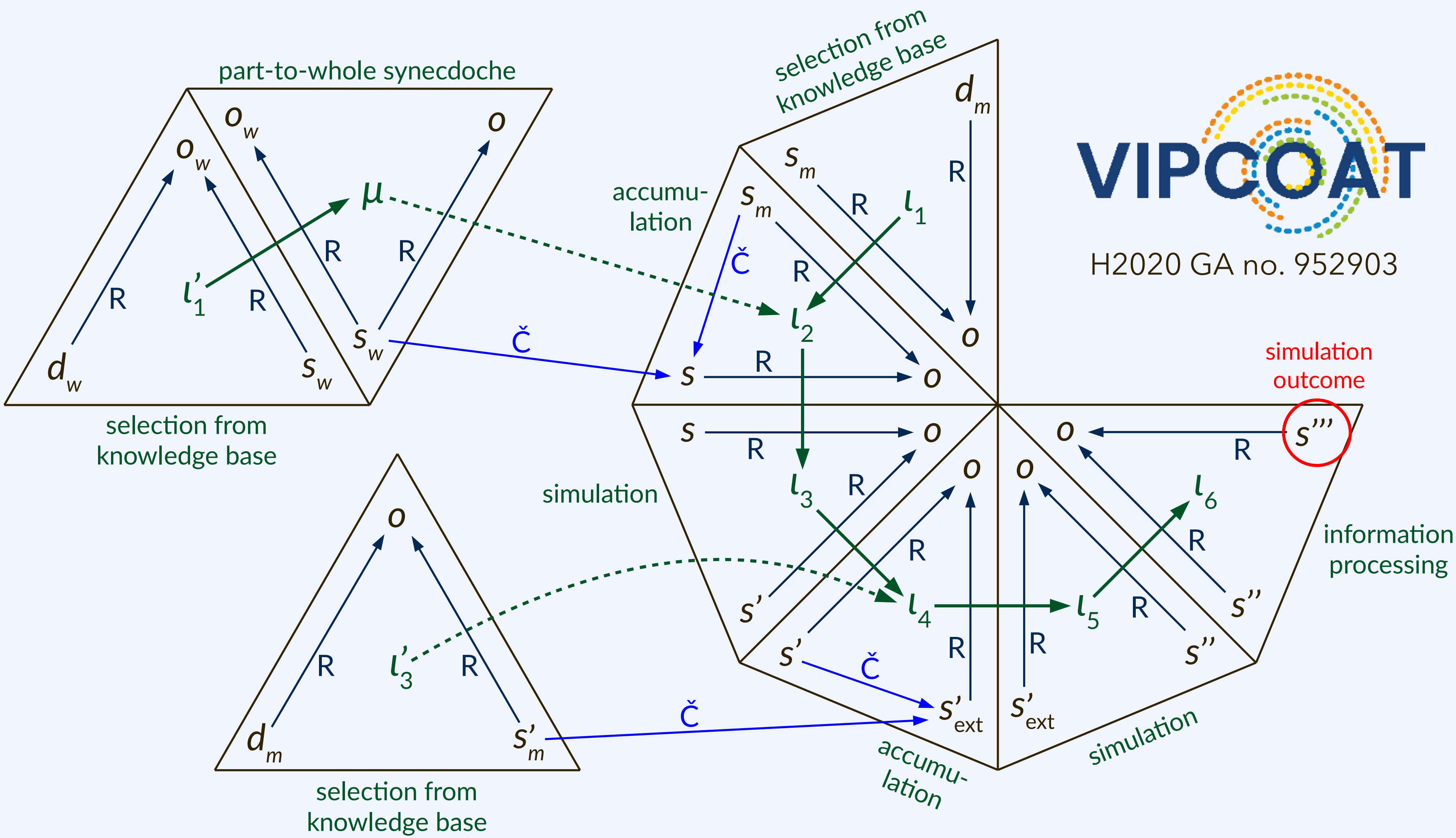
PIMS-II mid-level ontology:[1, 2] http://www.molmod.info/semantics/pims-ii.ttl

Mereosemiotics:[1-3] Combination of mereotopology and Peircean semiotics



[1]M. T. Horsch, no. 3 in *Proc. JOWO 2021*, **2021**. [2]P. Klein *et al.*, no. 26 in *Proc. JOWO 2021*, **2021**.
[3]M. T. Horsch, S. Chiacchiera, B. Schembera, M. Seaton, I. T. Todorov, in *Proc. ECCOMAS 2020*, **2021**.

Grounding in multi-stage cognitive processes



H2020 GA no. 952903

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

Types of epistemic grounding

Distinction between Type-1 and Type-2 grounding inspired by Marr.[1, 2]

Type-1 The **results** explain (or are **presented** in a way to explain) why they are valid.	*Example:* **Mathematical proof** in statistical mechanics for a theoretical framework with widely accepted definitions and axioms.	
Type-2 The **provenance** of the results tells that they are valid.		*Example:* We used a **model**, **method**, and **simulation code** validated in the past and – usually – very accurate.

[1]D. Marr, *Artificial Intelligence* **9**(1): 37–48, doi:10.1016/0004-3702(77)90013-3, **1977**.

[2]«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**.

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Distinction between Type-1 and Type-2 grounding inspired by Marr.[1, 2]

Type-1 The **results** explain (or are **presented** in a way to explain) why they are valid.	*Example:* **Mathematical proof** in statistical mechanics for a theoretical framework with widely accepted definitions and axioms.
Type-2 The **provenance** of the results tells that they are valid.	**Reliability** of process m means that «If S's believing p at t results from m, then S's belief in p at t is **justified**».[3] *Example:* We used a **model**, **method**, and **simulation code** validated in the past and – usually – very accurate. (**process reliabilism**)

[1] D. Marr, *Artificial Intelligence* **9**(1): 37–48, doi:10.1016/0004-3702(77)90013-3, **1977**.

[2] «Documentation of epistemic metadata by a mid-level ontology of cognitive processes», in *Proc. JOWO*, **2022**.

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

Types of epistemic grounding

Distinction between Type-1 and Type-2 grounding inspired by Marr.[1]

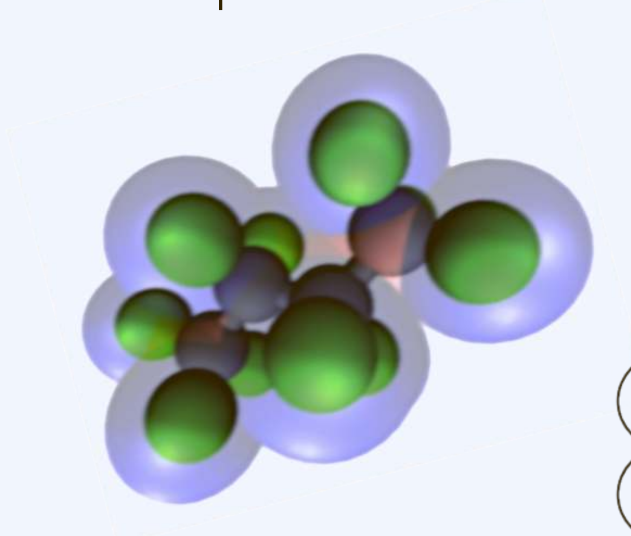
	authority or **trust**	**reliabilism**
Type-1 The **results** explain (or are **presented** in a way to explain) why they are valid.	*Example:* Mathematical proof in statistical mechanics for a theoretical framework with widely accepted definitions and axioms.	*Example:* The new theory is better because it is simpler, has fewer parameters, or "looks more" like reality. (**virtue reliabilism**)
Type-2 The **provenance** of the results tells that they are valid.	*Example:* We validated the artificial neural network as specified by the ISO 24029 norm, and established its prediction error accordingly.	*Example:* We used a model, method, and simulation code validated in the past and – usually – very accurate. (**process reliabilism**)

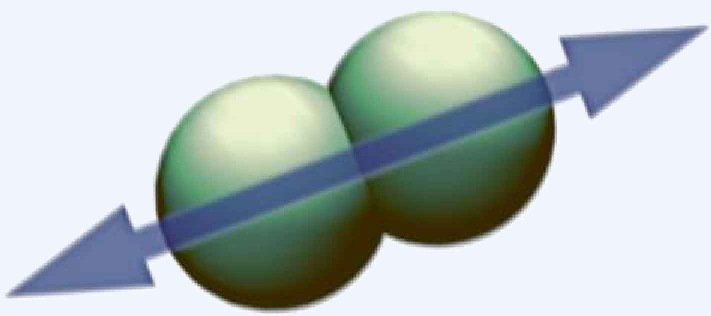
Distinction between "**moral grounds**" and grounding by **appeal to reliability**.

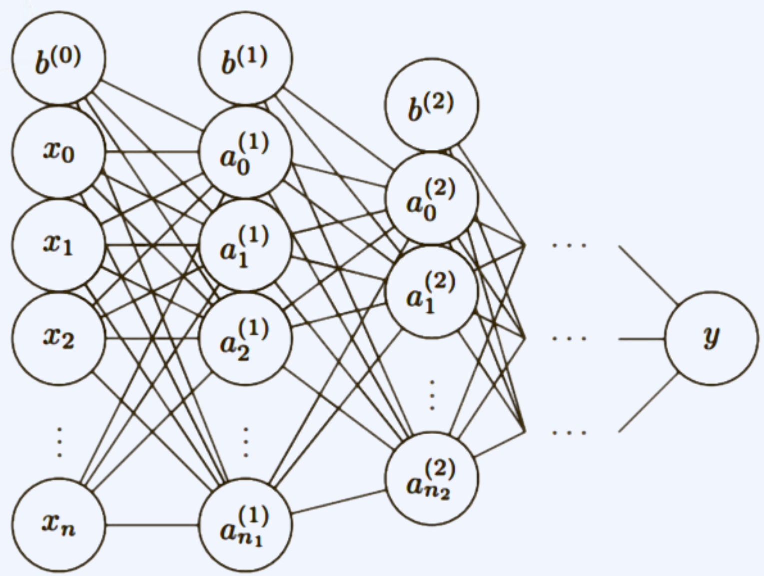
[1]D. Marr, *Artificial Intelligence* **9**(1): 37–48, doi:10.1016/0004-3702(77)90013-3, **1977**.

Epistemic virtues

Which of these models of perfluorobutane would you trust most?[1]







[1]Figure sources: MolMod DB and Anna Jenul's doctoral thesis.

Epistemic virtues

Problems related to epistemic virtues:

- Epistemic virtues often oppose each other.
  - **Simplicity** favours few elements and few adjustable parameters.
  - **Faithfully representing** the object (physics) does the opposite.
    - However, they are aligned in that neural networks lack any virtue.
- It is hard to differentiate between grounding in virtues or in reliabilism.
  - «Model x is better than y. It is equally accurate with fewer parameters,
    - … so we should prefer it because it is **more simple**» (virtue).
    - … so, from our experience, its extrapolations are **more reliable**.»
      - » Nobody writes either of the above explicitly.
      - » Then, any mode of grounding can be attributed to authors.

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1 Epistemic metadata

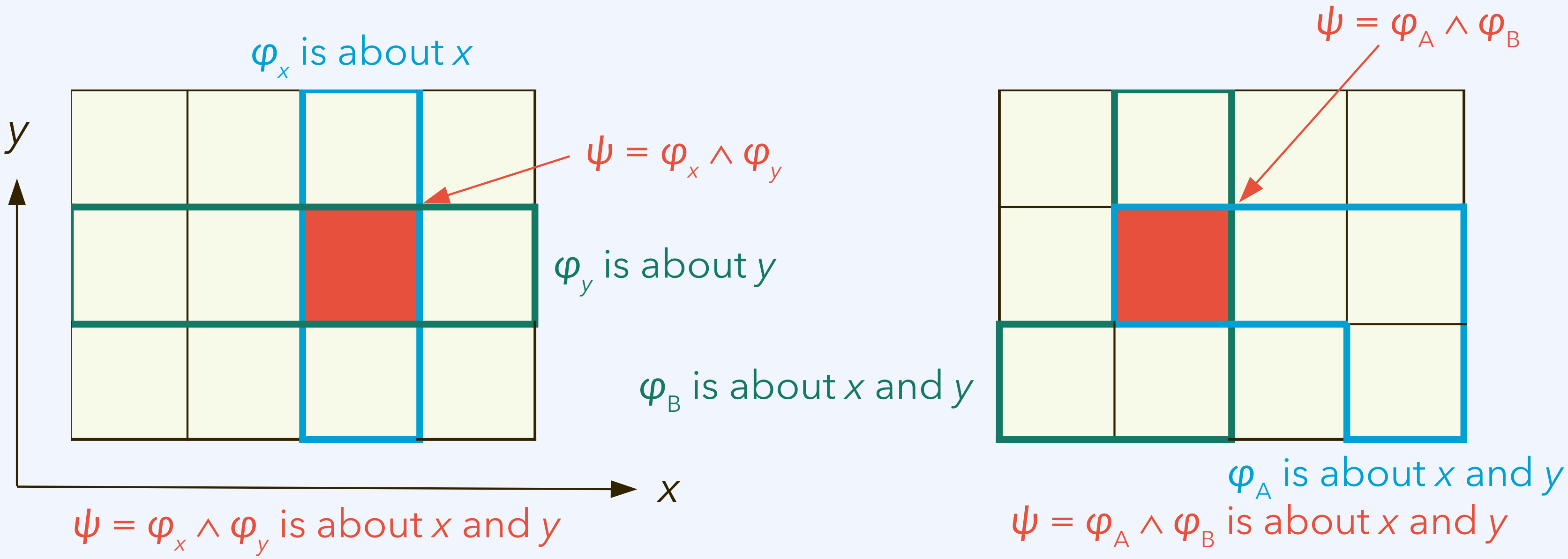
2 Case study

3 Metadata documentation

4 Epistemic grounding

5 Logical subtraction

Logical subtraction



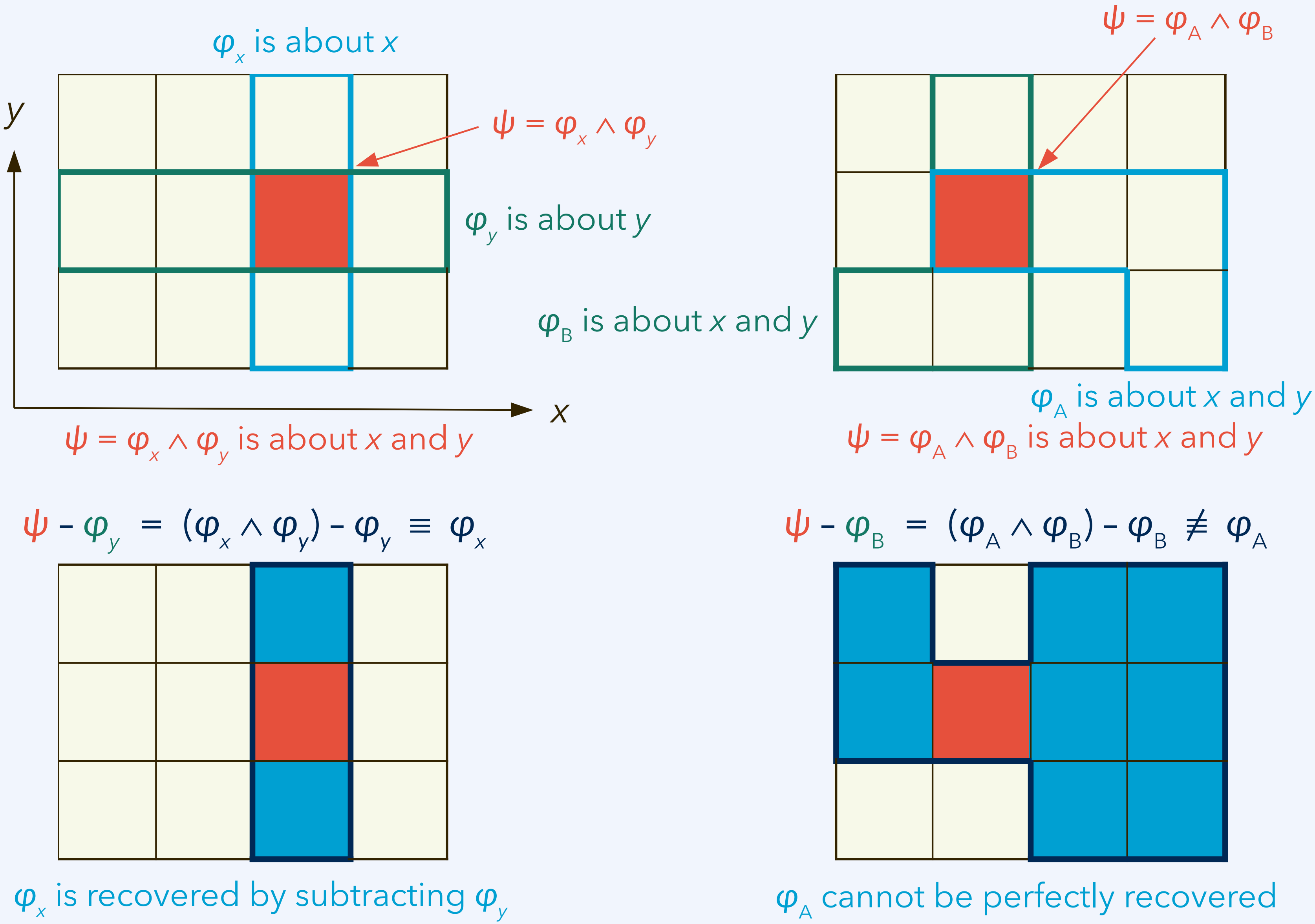
System with two separate elementary **topics** / **subject matters**: x and y.

There are four possible values for x and three possible values for y.

Conjunction of two unrelated formulas = **addition** of information content.

Logical subtraction is meant to be the opposite of such an addition.

Logical subtraction



Metadata - Paradata = Orthodata

Blue: **Orthodata**. Red: **Paradata**.

Reproducibility claims that could be formulated from modelling and simulation:

If you use the same **model**, **method**, **solver** code (& version), and **execution environment**, …	You will find the same **value** for the property, within a margin of **2%**. The **runtime** will be the same within **40%**.
If you use the same **model** and **method** (but any **code** and **execution environment**), …	You will find the same **value**, within **5%**, except for errors due to *your* **code**, *etc.* (No claim on **computational resources**.)
If you apply any **method** (including experiment) to the problem …	You will find the same **value**, within **20%**, except for errors due to *your* **methods**. (No claim on **computational resources**.)
«repeat κ, but no need to retain κ'»	«obtain φ again, except for φ' maybe»

Metadata - Paradata = Orthodata

Easy:

"The computing time will be x and the computed value will be y."

- "The computing time will be x."

= "The computed value will be y."

Challenge 1: Can the following really be done?

"The computing time will be x and the computed value will be y."

- φ'

= "The computed value will be y, within Δy."

Challenge 2: How would we apply the orthodata/paradata distinction to workflows expressed in terms of Peircean semiotics?

Simulation as fiction

> Simulation is a kind of **fiction**.
> We must **suspend our disbelief** to accept the scenario.
> Can this suspension be understood as **subtraction**?

Naive view: The simulation **represents** a real physical process, the model represents a real physical system.

Actual practice:

The simulated process is almost always **fictitious**; often, it is **impossible** – it cannot technically occur.

While models legitimately represent real systems, they simplify them. Often, simulations really aim at **characterizing the model** as such, not a real system.

counterfeit objects

Simulation as fiction

Simulation is a kind of **fiction**.
We must **suspend our disbelief** to accept the scenario.
Can this suspension be understood as **subtraction**?

model represents a fictitious entity *o*, but it is "**not about** whether *o* can exist."

Our **simulation of object *o*** confirms theory *s*.
Except that theory *s* deals with physical reality, and *o* is so simplified
that **we know it cannot exist** or be built exactly in physical reality.

Simulation as fiction

Modelling and simulation has a **figurative/metaphorical aspect**: In the virtual reality of a simulation, there are *p*, *T*, *etc.*, and in physical reality, there are also *p*, *T*, *etc.*, but despite the same symbols, these are very different quantities.

But to be productive, this mechanism also requires an **aspect of fiction**. The model represents a fictitious entity *o*, but it is "**not about** whether *o* can exist."

Our **simulation of object *o*** confirms theory *s*.

Except that theory *s* deals with physical reality, and *o* is so simplified that **we know it cannot exist** or be built exactly in physical reality.

Searle, *The logical status of fictional discourse:*[1]

- "the **difference between fictional and serious** utterances [...] is not [...] the **difference between figurative and literal** utterances, which is another distinction"
- "work[s] of fiction are made possible by [...] a set of conventions which **suspend** the normal operation of the **rules relating illocutionary acts and the world**"

[1]In J. R. Searle, *Expression and Meaning:* Chapter 3, Cambridge Univ. Press, **1979**.

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Data Science Lunch Meeting

Formal representation of the grounding and reproducibility of scientific claims:

What has been proposed – and obstacles.

IDV-lunsjmøte

24. november 2023