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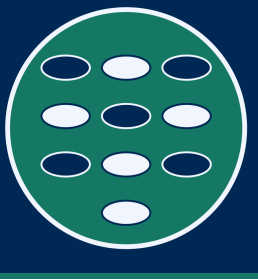

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Similarity, opacity, and unification in molecular thermodynamics

Designing AI systems that can work with thermodynamics domain knowledge

Paris, 17th May 2025
Global Centre for Advanced Studies

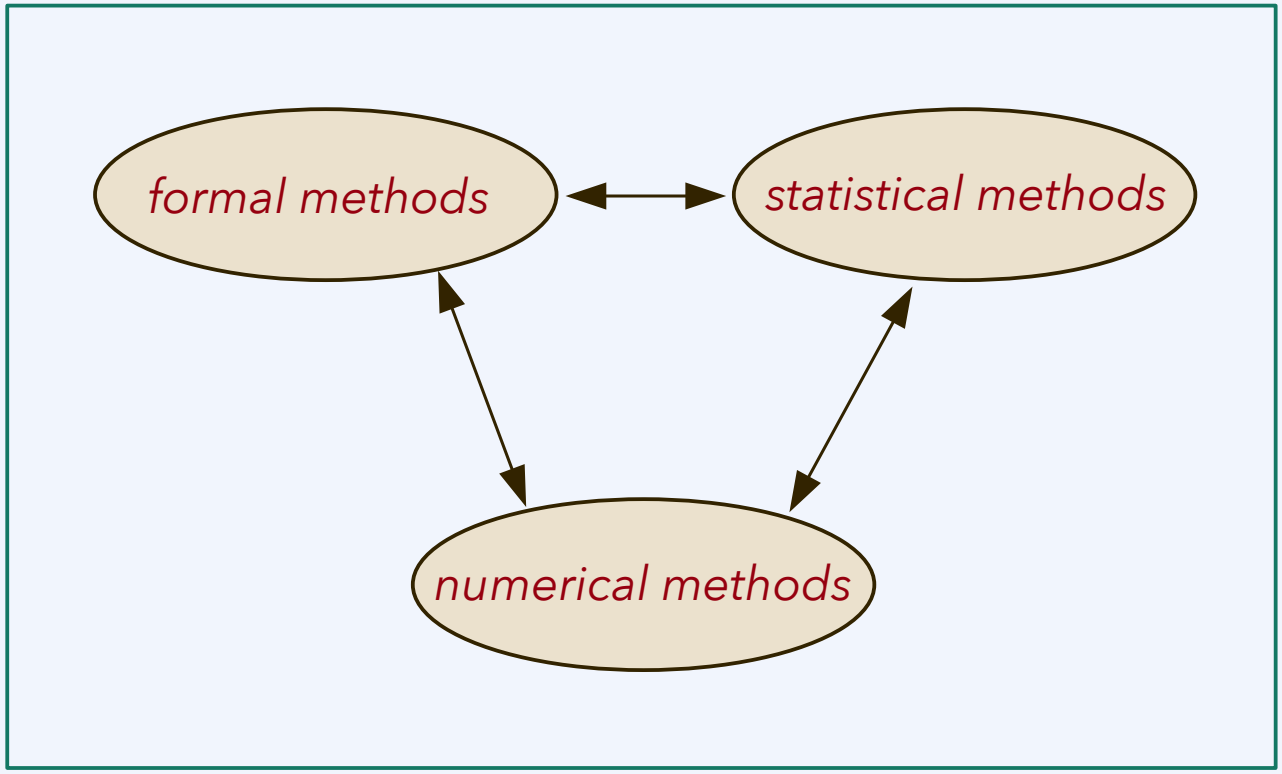
Fakultet for realfag og teknologi

Forskargruppe materialteori og -informatikk

Norwegian University of Life Sciences

What do we need to unify?

remit of **computational methods**



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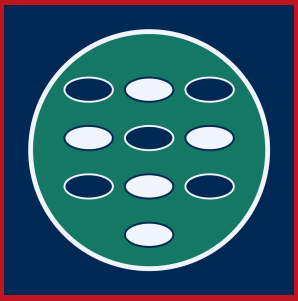

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1. **Similarity**
2. *Opacity*
3. *Unification*

There is only one ideal gas

Under the ideal gas approximation, for *pvT* behaviour, all gases are the same

$$p = \rho T.$$

They are not just "similar," but "the same," *i.e.*, there is only one ideal gas.

This is "the ideal gas."

When working with it, we often don't need to say what atoms it consists of.

The nature of "the ideal gas" is that of an **idealized counterfeit object**.

It is more perfect (in a sense) than anything found in actual reality. For some purposes, this is not a shortcoming (*i.e.*, just an acceptable approximation), but desirable: A thought experiment more pure than any actual experiment.

Dilute real gases: Only one parameter

Under the ideal gas approximation, for *pvT* behaviour, all gases are the same

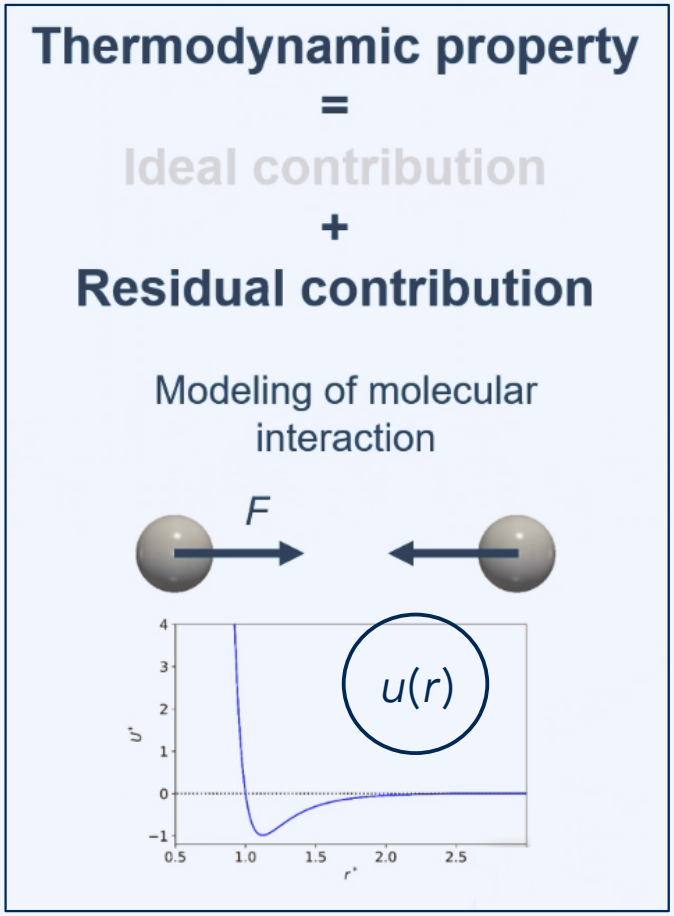
$$p = \rho T.$$

They are not just "similar," but "the same," *i.e.*, there is only one ideal gas.

The next best description for a dilute real gas is the 2nd order virial equation of state:

$$p = \rho T + \boldsymbol{B_2}(T)\,\rho^2 T + \ldots$$

Here we introduce one parameter for real gas behaviour. All gases with the same **2nd virial coefficient** are then also "the same."



Source: Simon Stephan

From sameness to similarity

Van-der-Waals fluid: $p(v, T) = T(v - \boldsymbol{b})^{-1} - v\boldsymbol{a}^{-2}$

Lennard-Jones fluid: $u(r) = 4\boldsymbol{\varepsilon}\,[(\boldsymbol{\sigma}/r)^{12} - (\boldsymbol{\sigma}/r)^{6}]$

The van-der-Waals fluid appears to have the parameters ***a*** and ***b***. The Lennard-Jones fluid appears to have the parameters ***σ*** and ***ε***.

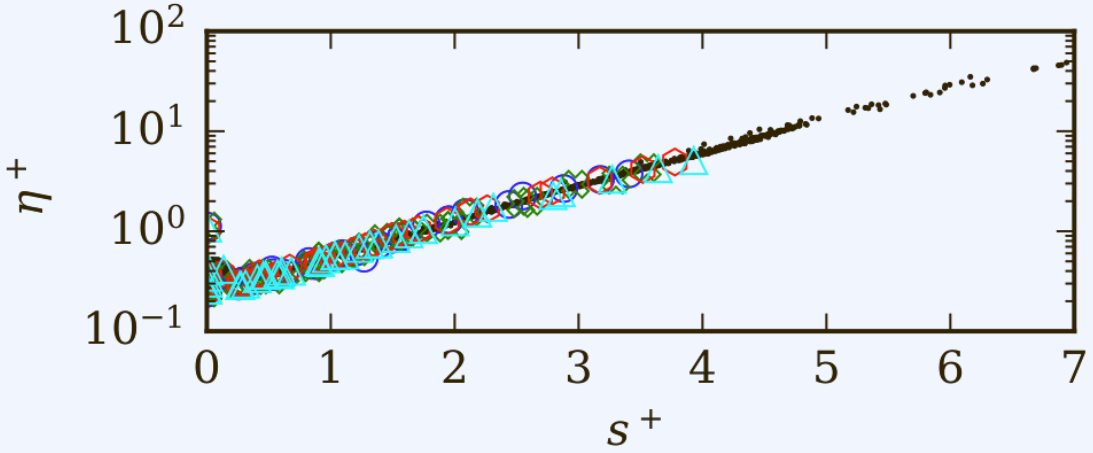
But the parameterizations are all similar. Similarity means that if rescaled, *i.e.*, if the characteristic length and energy scales are used for a system of units, they become the same.

Then there is only "the van-der-Waals fluid" and "the Lennard-Jones fluid."

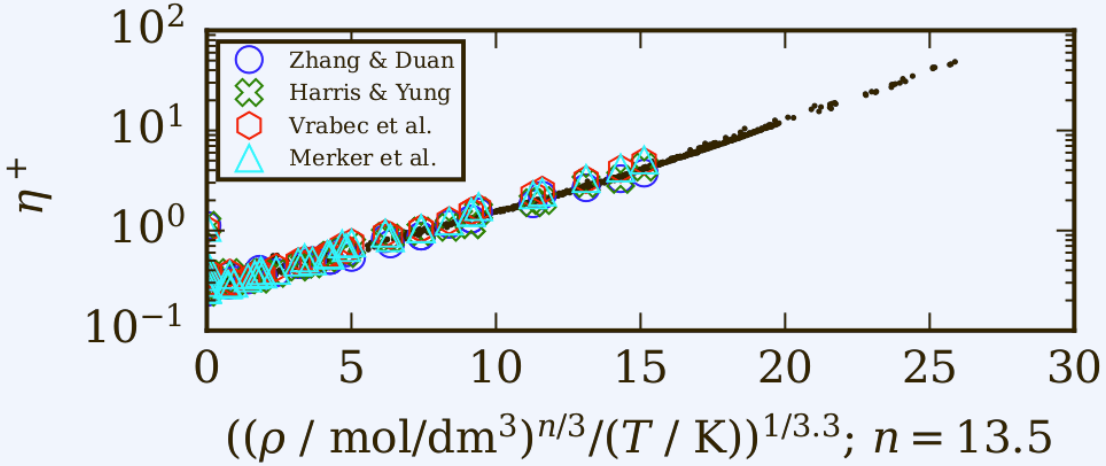
These are also abstract model fluids, *i.e.*, counterfeit objects of reference.

They *can* be used as models for actually exsiting fluids, like the ideal gas can. But they are also objects of investigation in their own right.

Similarity between thermodynamic properties[1]



Rescaled viscosity of CO_2 as a function of $s^+ = -s^r$, where is the residual entropy $s^r = s - s^{id}(v, T)$



Rescaled viscosity of CO_2 as a function of rescaled density and temperature, where n is the density scaling exponent.

[1]I. Bell *et al.*, *J. Chem. Phys.* **157**: 074501, doi:10.1063/5.0097088, **2022**.

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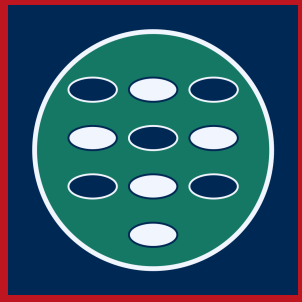

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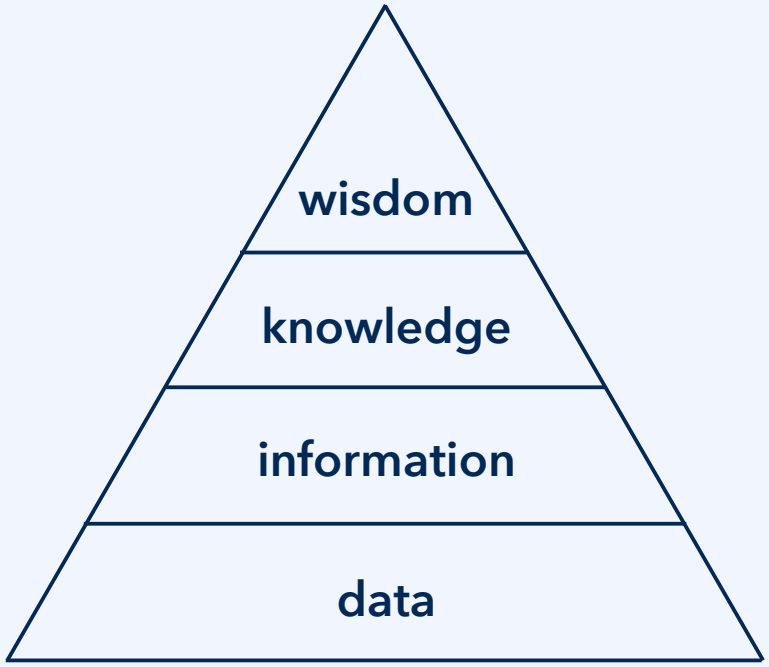
1. Similarity
2. **Opacity**
3. *Unification*

DIKW: Data, information, knowledge, and wisdom



Hierarchy of data, information, knowledge, and wisdom (**DIKW pyramid**[1, 2]).

[1]J. Rowley, *J. Inform. Sys.* **33**: 163–180, doi:10.1177/0165551506070706, **2009**.

[2]B. Schembera, in *Proc. DCLXVI 2024*, *pp.* 122–132, Springer, doi:10.1007/978-3-031-89274-5_9, **2025**.

Pragmatic competency and interoperability, including agreed good practices.

Epistemic metadata documentation: Establish the knowledge status.

Semantic interoperability: Data become information if their meaning is agreed.

Syntactic interoperability: Data exchanged in an agreed format.

Definition of epistemic opacity

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]

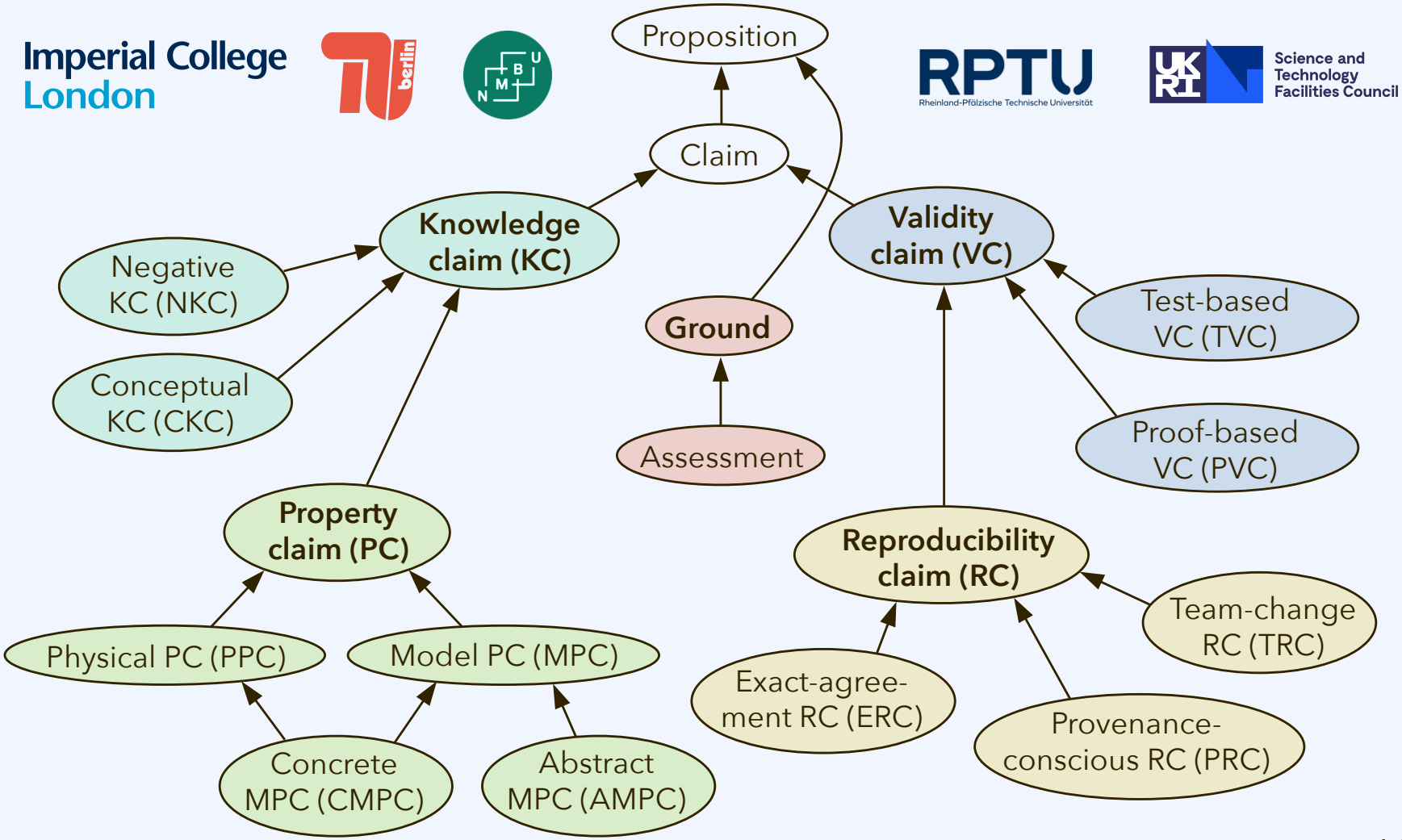
> **Epistemic opacity** (Humphreys, 2011): A «process is **epistemically opaque** relative to a cognitive agent *X* at time *t* […if …] *X* does not know at *t* all of the **epistemically relevant elements**»[2]

[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**.

Taxonomy of claims developed in a case study



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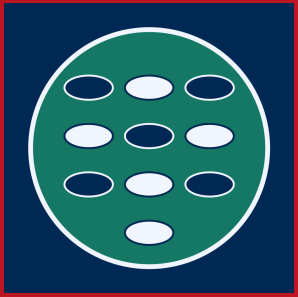

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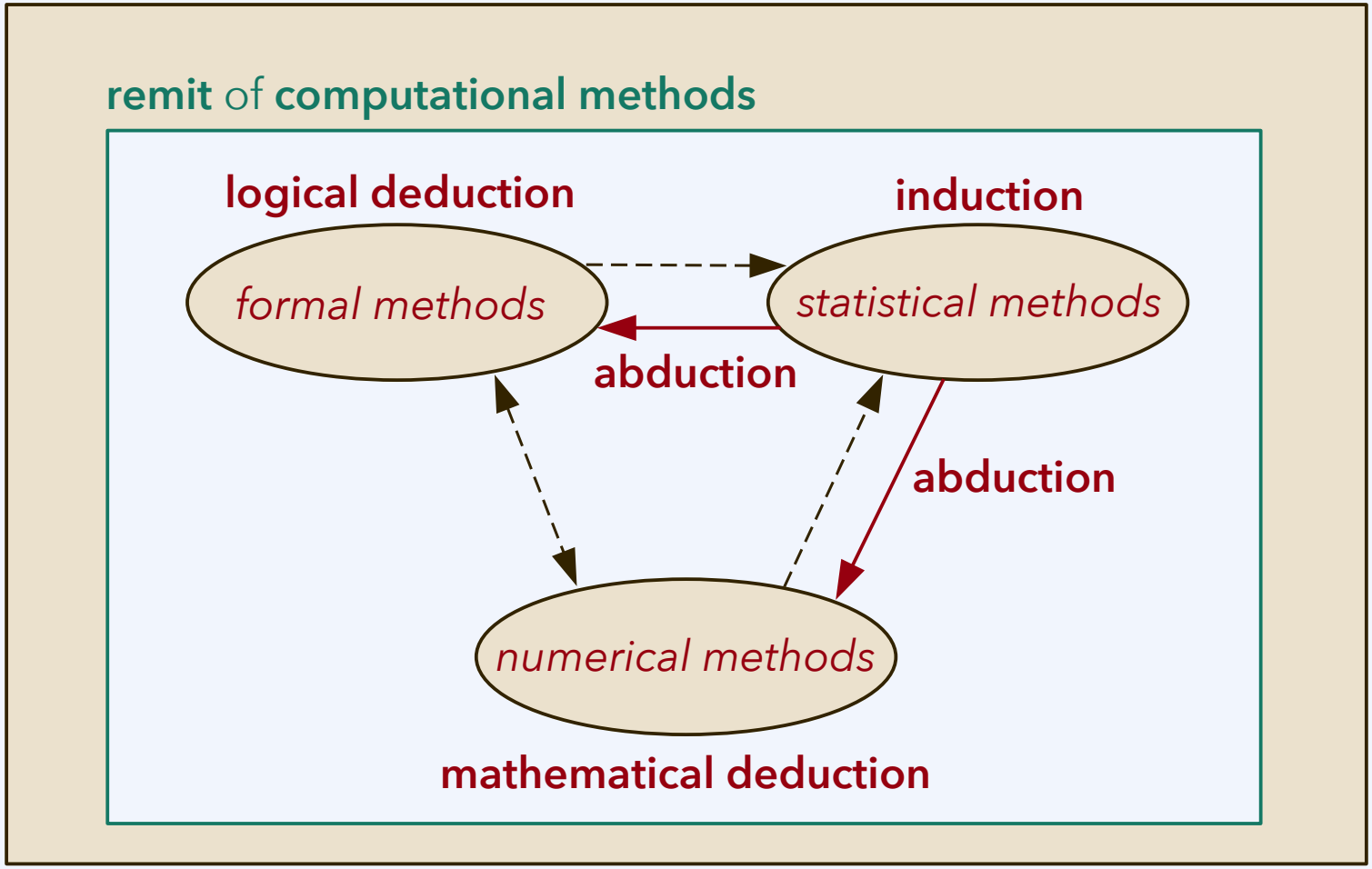
2. Opacity
3. **Unification**

Reasoning by abduction, deduction, and induction



human cognition employing **abduction**, **deduction**, and **induction**

Domain knowledge: How not to do it

Interpretation of Popper's classical example: Before people knew black swans, they may have had an "ontology representing the domain knowledge" such as

- Under such and such conditions (not mentioning feathers), *x* is a swan;
- Falsifiable scientific claim φ: All swans have white feathers.

So the claim is that being a swan logically entails having white feathers.

Now we discover one black swan somewhere. The claim φ is falsified.

"This is how science works." Zoologists had made claim φ, but then they learnt it was false by seeing one black swan.

Domain knowledge: How not to do it

But in reality:

- Nobody claimed that being a swan "logically entails" having white feathers. That is only what we get by artificially enforcing "ontology form."
- Also, zoologists only extended their taxonomy because there was *a whole species* of black swans, not just one, two or three of them.

In our domain, we deal with conflicting claims. If we accept them and enforce logical reasoning, we get contradictions.

A measured 106 kPa for a uniquely defined quantity, *B* measured 107 kPa. With the "ontology encoding domain knowledge," it entails 106 kPa = 107 kPa.

The pragmatist view

Following *e.g.* Davidson and Øfsti:

Two conceptual schemes cannot be incommensurable and at the same time be about the same things.

Where commensurable, they can be mapped to / aligned with each other.

At a certain point, a conceptual scheme or language becomes "**complete**." Øfsti: The reference object for what constitutes a complete knowledge representation formalism is *the Norwegian language*.

«et språk er **a-komplett** *[...] når det er tilstrekkelig rikt strukturert til å være transcendentalt ekvivalent med norsk»* (s. 61)

The Norwegian view

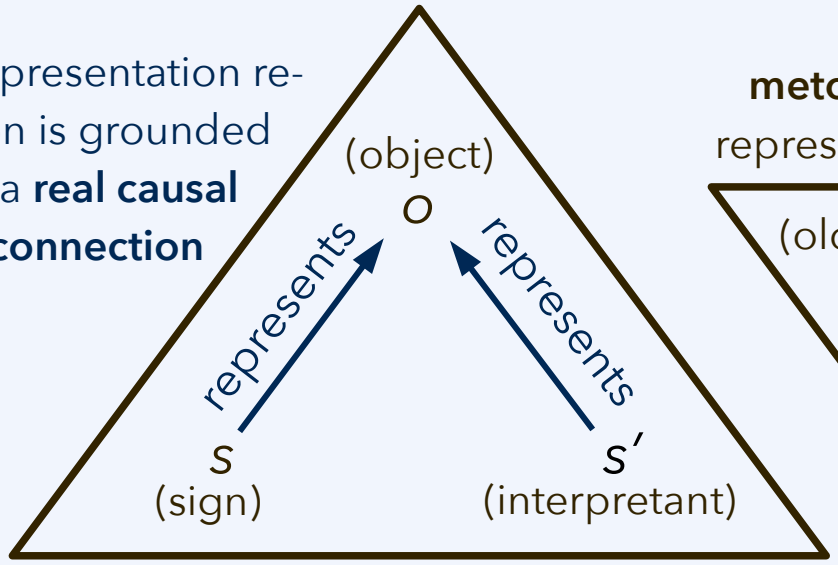
At a conceptual scheme or language becomes "**complete**." Øfsti: The reference object for what constitutes a complete knowledge representation formalism is *the Norwegian language*.

«et språk er **a-komplett** *[...] når det er tilstrekkelig rikt strukturert til å være transcendentalt ekvivalent med norsk»* (s. 61)

Unification: Semiotic perspective

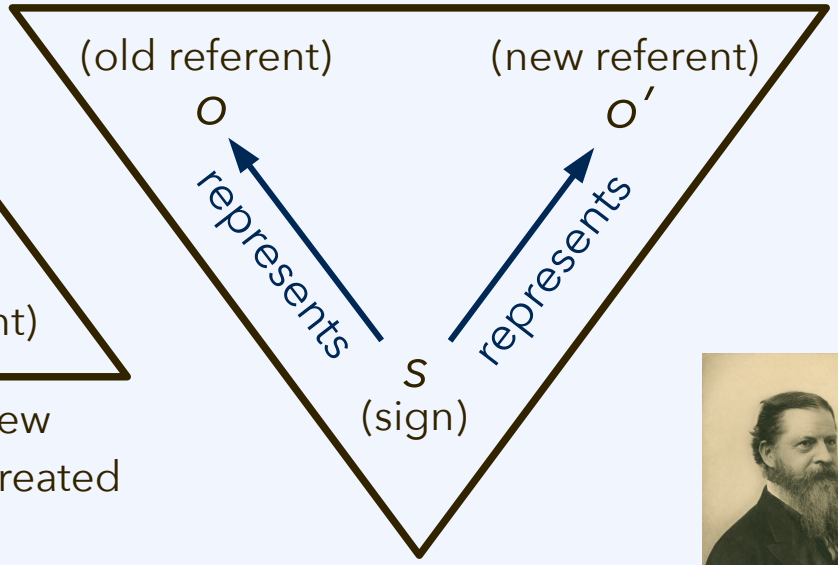
Peircean semiotics: By using a sign (1st) for an object (2nd), a "Third" is created.

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



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

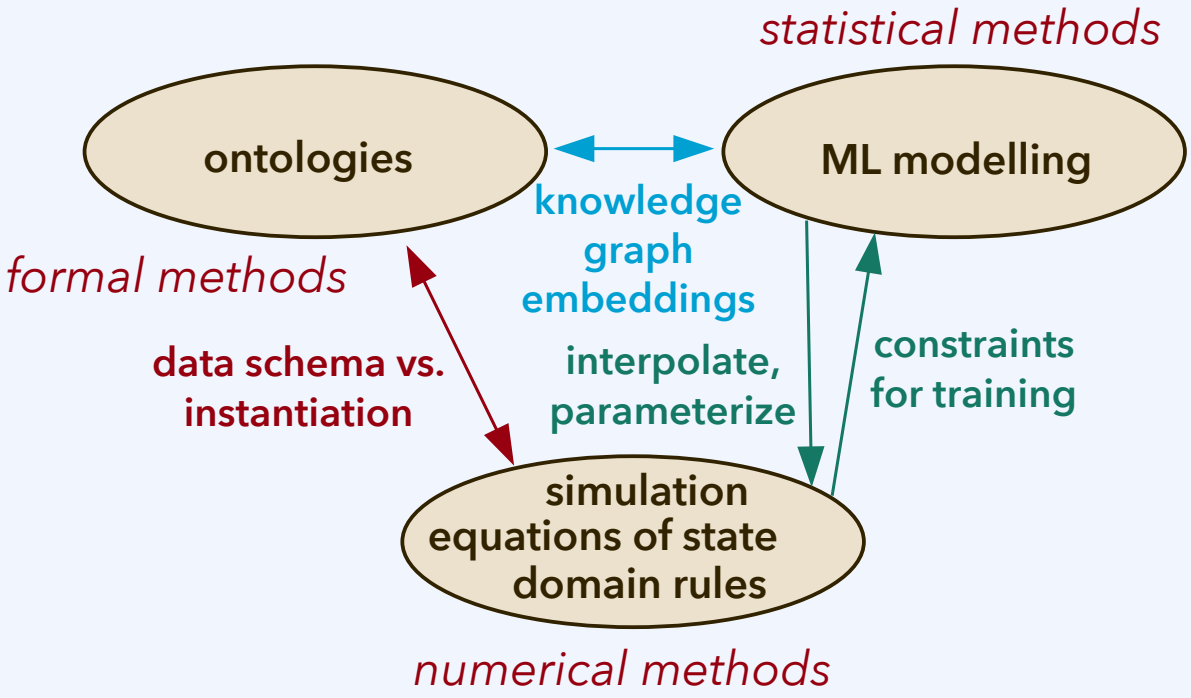
metonymization, a process by which a representamen is assigned a new referent



C. S. Peirce

Unification: Technical perspective

Logical deduction, numerical deduction, machine-learning induction, and theory building by abduction are different modes of reasoning. They are central in different practices, but these practices *can* be brought together.



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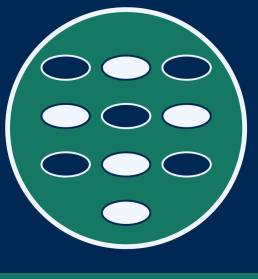

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