Automated metadata extraction and epistemic FAIRness in the engineering sciences

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Research Data Management and Dark Data

- Typically, data organized in filesystems is not FAIR
- This may leave lots of dark data
- However, a lot of (semi-structured) metadata is already available
  - In job or log files of simulation codes (e.g. nodes, version)
  - In non-standardized or standardized file formats (i.e. HDF5 or NetCDF)

```
[st_ac[redacted]@uc1n250 run]$ pwd
/home/st/st_st/st_ac[redacted]/itt_data/binary/educt_hexane/300_020_080/run
[st_ac[redacted]@uc1n250 run]$ ls -al
total 31596
drwxr-xr-x 2 st_ac108829 st_st     4096  5. Okt 13:44 .
drwxr-xr-x 9 st_a[redacted]9 st_st     4096 22. Aug 15:21 ..
-rw-r--r-- 1 st_a[redacted]9 st_st     2853 28. Aug 11:39 box.gro
-rw-r--r-- 1 st_a[redacted]9 st_st       58 17. Aug 15:44 foo.trr
-rw-r--r-- 1 st_a[redacted]9 st_st      358 15. Jan 2018  run0.job
-rw-r--r-- 1 st_a[redacted]9 st_st      423 15. Jan 2018  run.job
-rw-r--r-- 1 st_a[redacted]9 st_st 32314454 22. Jan 2018  run.log
-rw-r--r-- 1 st_a[redacted]9 st_st    12057 22. Jan 2018  run.mdp
```

Fig: Data organization in directory structures on filesystems. Sample from GROMACS

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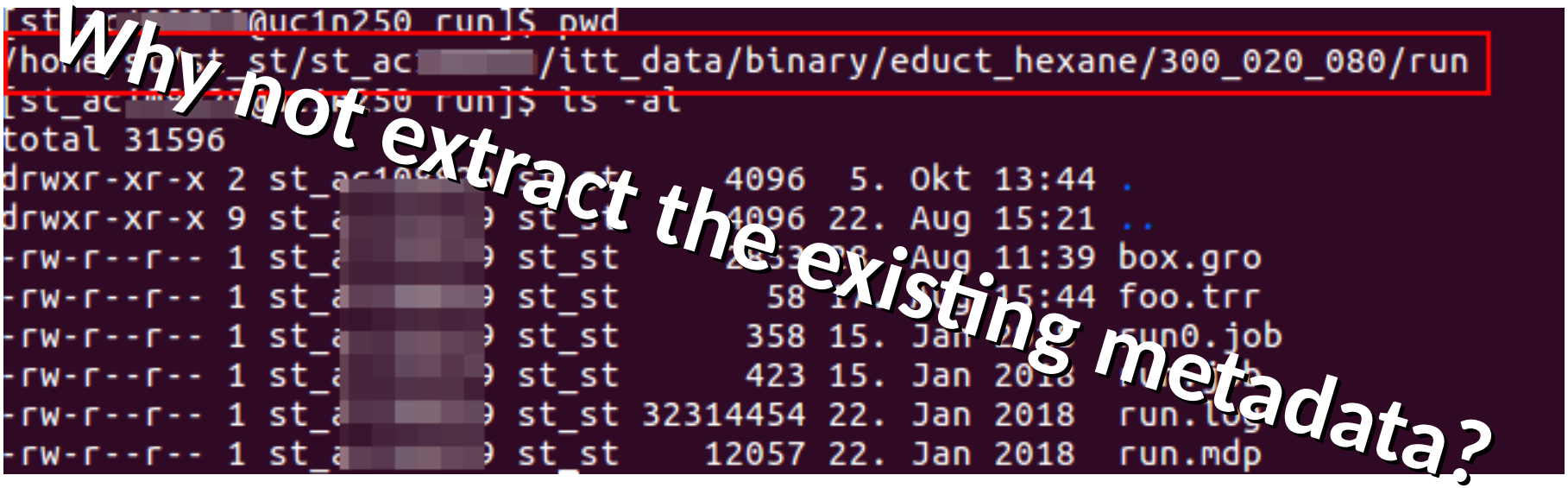


Fig: Data organization in directory structures on filesystems. Sample from GROMACS

ExtractIng metadata extraction tool

- Implemented in Java, published on GitHub (still a prototype though)[1]
- Native (Scanner API) and parallel (Apache Spark) version
- Generic: External configuration file based on the EngMeta convention
- Run of ExtractIng refers to a directory
- Data + metadata can then be ingested to a repository

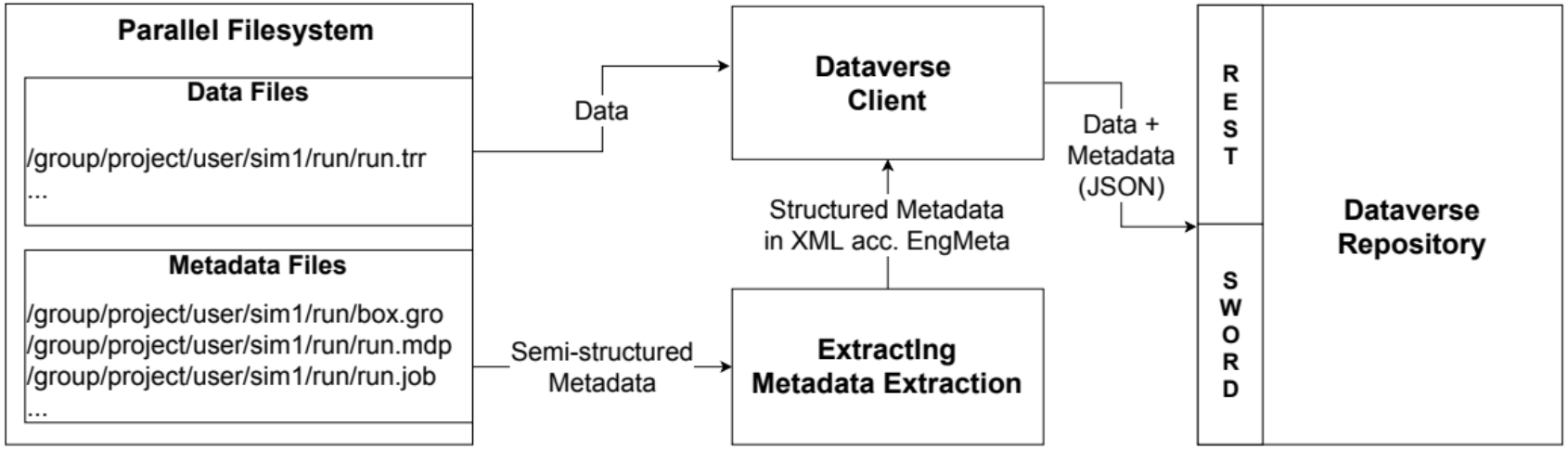


Fig: Workflow of the Metadata Extraction

[1] https://github.com/bjschembera/ExtractIng

Outcome: Extractable metadata

- Extractability of the metadata strongly related to
  - The type of metadata (technical, process, ...)
  - Also related to the simulation code output
- Evaluation with the following simulation codes output
  - GROMACS (molecular dynamics)
  - EAS3 (aerodynamics)
  - CCSM (climate modelling, in NetCDF conventions)

Type of metadata	Extractability
Technical metadata	high, as available via file attributes
Process metadata	medium, as available in log-, job- or system files
Domain-specific metadata	medium, as available in log- or output files
Descriptive metadata	poor, as it's a description from a higher level

Table: Extractability of the different metadata categories. It is strongly dependent on the field of science.

Schembera, B. Like a rainbow in the dark: metadata annotation for HPC applications in the age of dark data. J Supercomput (2021). https://doi.org/10.1007/s11227-020-03602-6

Automated extraction of data provenance information

- Provenance information/metadata is key for FAIR data.
- For GROMACS, the tool can extract lots of this provenance information:

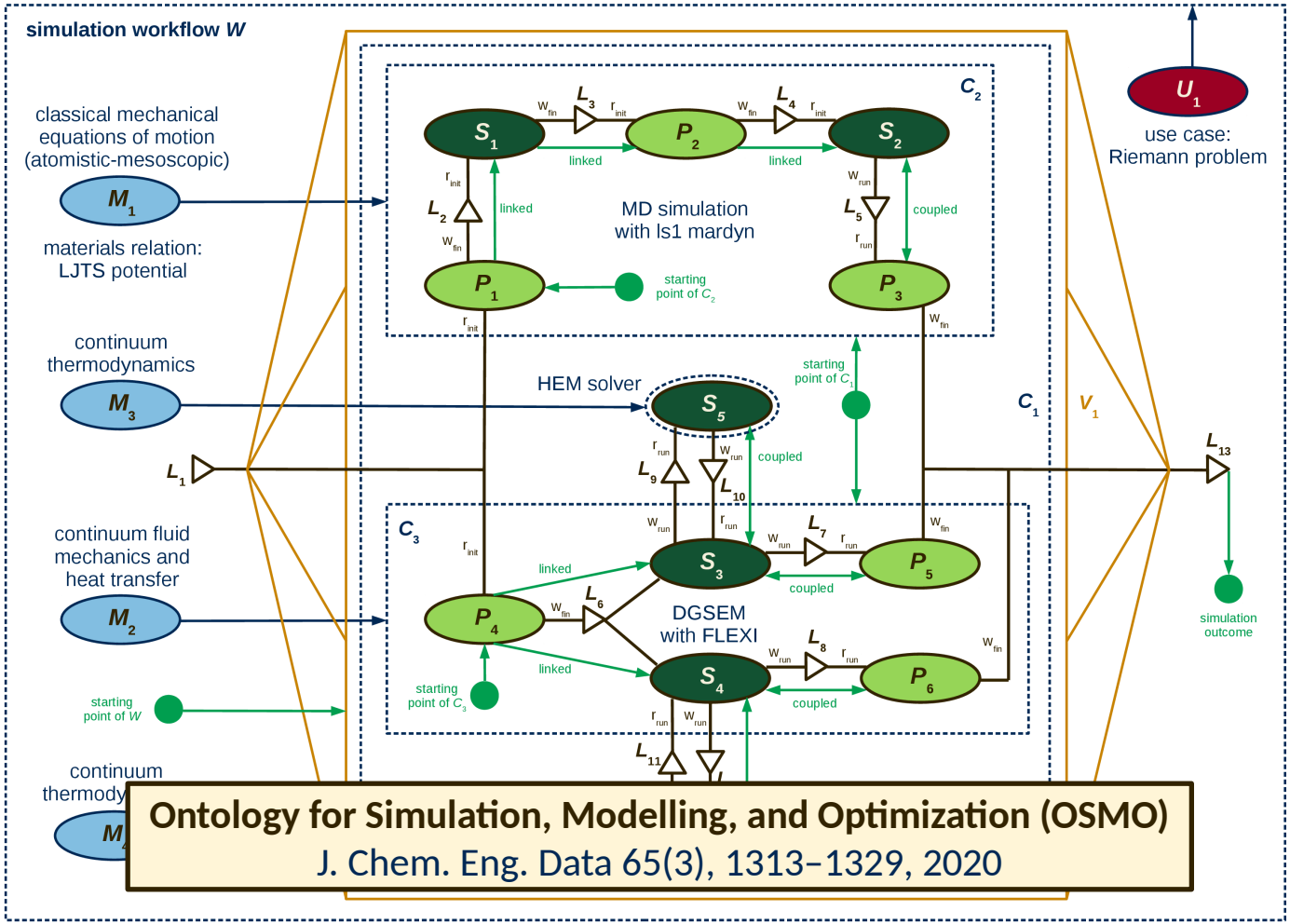
processingStep.tool.name	*.log	GROMACS
processingStep.tool.softwareVersion	*.log	GROMACS version
processingStep.tool.operatingSystem	*.log	Build OS/arch
processingStep.executionCommand	*.log	gmx_mpi mdrun
processingStep.executionCommand	*.log	gmx_mpi grompp
processingStep.environment.compiler.name	*.log	C++ compiler
processingStep.environment.compiler.flags	*.log	C++ compiler flags
processingStep.environment.compiler.name	*.log	C compiler
processingStep.environment.compiler.flags	*.log	C compiler flags
processingStep.environment.nodes	*.job	nodes
processingStep.environment.ppn	*.job	ppn
processingStep.environment.cpu	*.log	Build CPU brand

Automated extraction and metadata standardization of data provenance information

After the extraction run, provenance information is extracted and structured according to the EngMeta metadata standard (in a subdirectory *.metadata* as XML):

```
[[redacted]@nid00030 .metadata]$ pwd
/mnt/lustre/[redacted]/itt_data/binary/educt_hexane/300_020_080/run/.metadata
[[redacted]@nid00030 .metadata]$ ls -alrt
total 20
drwxr-xr-x 2 [redacted] s29931 4096 Jan 29 15:39 .
-rw-r--r-- 1 [redacted] s29931 1520 Feb  6 11:46 metadata.txt
-rw-r--r-- 1 [redacted] s29931 2717 Feb  6 11:46 engMeta.xml
-rw-r--r-- 1 [redacted] s29931  630 Feb  6 11:46 atom.xml
drwxr-xr-x 3 [redacted] s29931 4096 Feb 13 11:49 ..
[[redacted]@nid00030 .metadata]$ tail engMeta.xml
                    <flags>-mavx     -O3 -DNDEBUG -funroll-all-loops -fexcess-precision=fast</flags>
                </compiler>
                <nodes>1</nodes>
                <ppn>8</ppn>
                <cpu>Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz</cpu>
            </environment>
        </step>
    </provenance>
    <size>58</size>
</dataset>
[[redacted]@nid00030 .metadata]$
```

Metadata standardization for research data provenance



Ontology for Simulation, Modelling, and Optimization (OSMO)
J. Chem. Eng. Data 65(3), 1313–1329, 2020

OSMO-based **provenance description** as an extension of the MODA workflow meta-data standard:

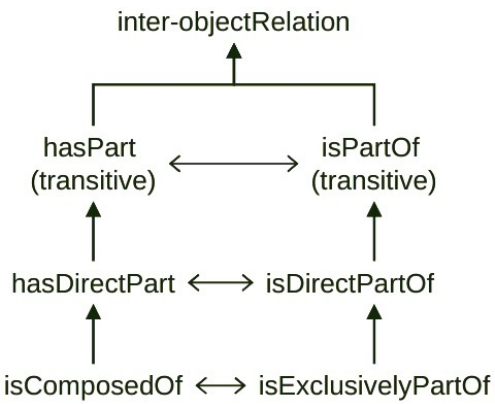
For all elements of the graph notation, there are corresponding concepts and relations from the ontology OSMO.

Metadata standardization based on top-level ontologies

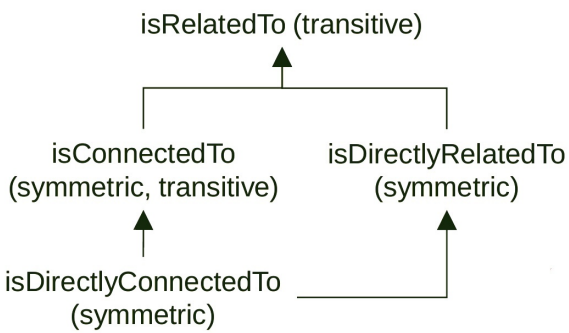
NFDI4Cat uses OntoCAPE,[1] the ontology for the CAPE-OPEN interface standard.

„CAPE“ = „computer-aided process engineering“

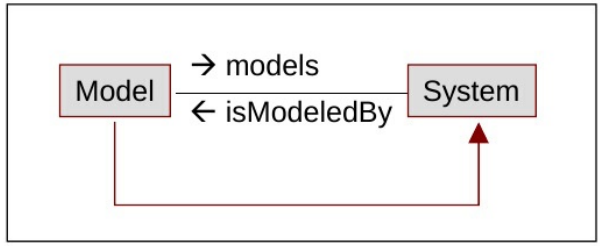
OntoCAPE combines domain-specific and **top-level conceptualizations**.



mereology



topology of systems

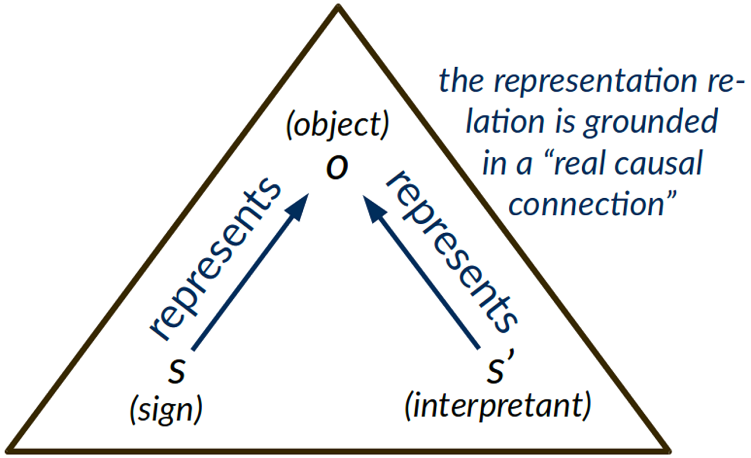


representation by **models**

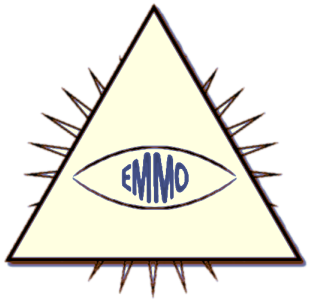
[1]Morbach *et al.*, Technical Reports LPT-2008-24 & LPT-2008-25, RWTH Aachen, **2008**.

Metadata standardization based on top-level ontologies

Peircean semiotics



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



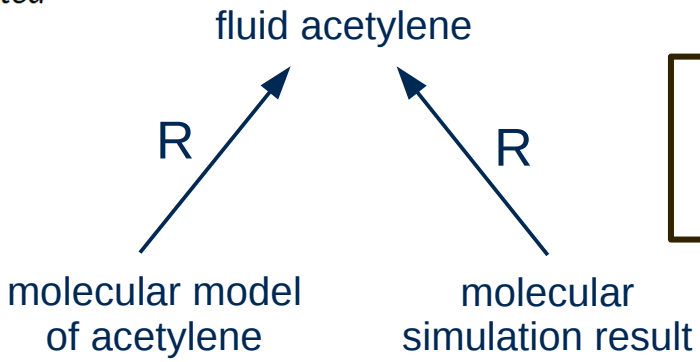
C. S. Peirce

European Materials and Modelling Ontology

1) **Taxonomy**:
   Conceptual hierarchy (subclass relation)

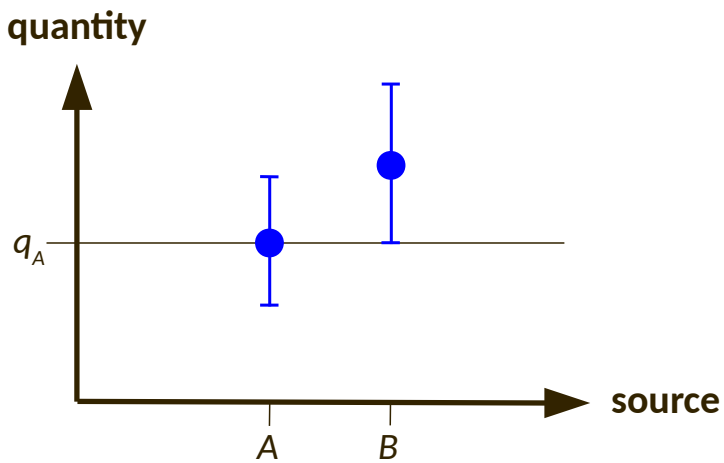
2) **Mereotopology**:
   Spatiotemporal parthood and connectivity

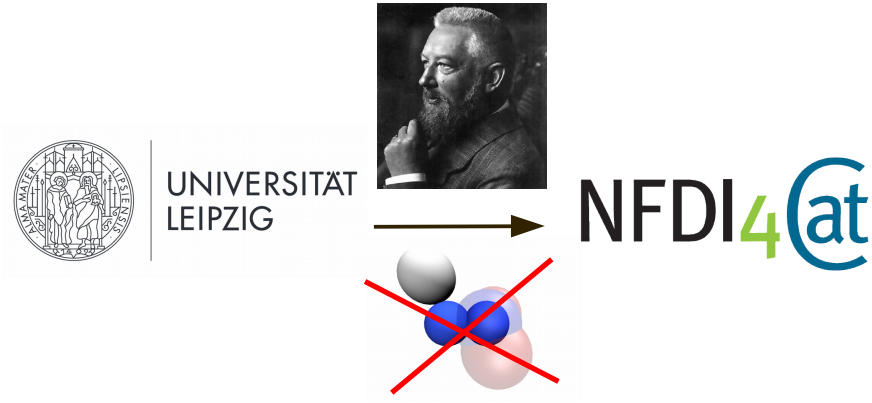
3) **Semiotics**:
   Representation of physical entities by signs



"represents" or **"is sign for"** is here abbreviated by **R**

Research data infrastructures and scientific knowledge





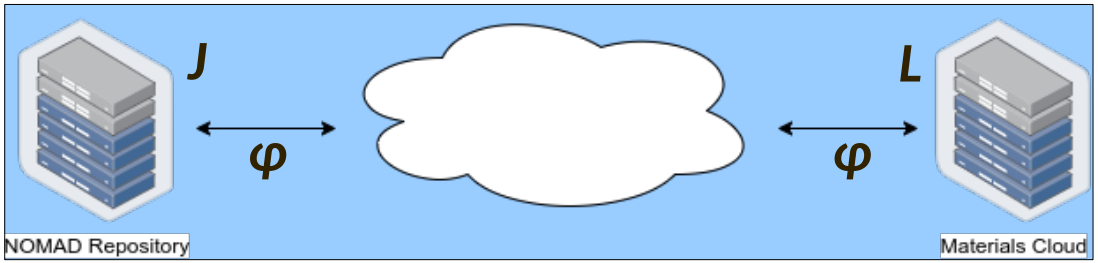
Averroes[1]
(Bidayat al-Mujtahid)
al-Sulami
(*Book of the Jihad*, 1106)

Pope Urban II
(in *Proc. Council Clermont*, 1059)
Augustine (*Civitas Dei*, 426)

[1]Research data infrastructure on Averroes' works: https://averroes.uni-koeln.de/

Digital infrastructures and communication of knowledge

Scientific knowledge is a kind of knowledge (or else, little will qualify as knowledge). Research data infrastructures store and exchange scientific knowledge.



Scenario requiring epistemological formalization:

- "The scientific knowledge φ is communicated by knowledge base J to L."
- φ is a justified tenable assertion, by standards applied to its source. But it would be inappropriate to require every φ to be a justified true belief.

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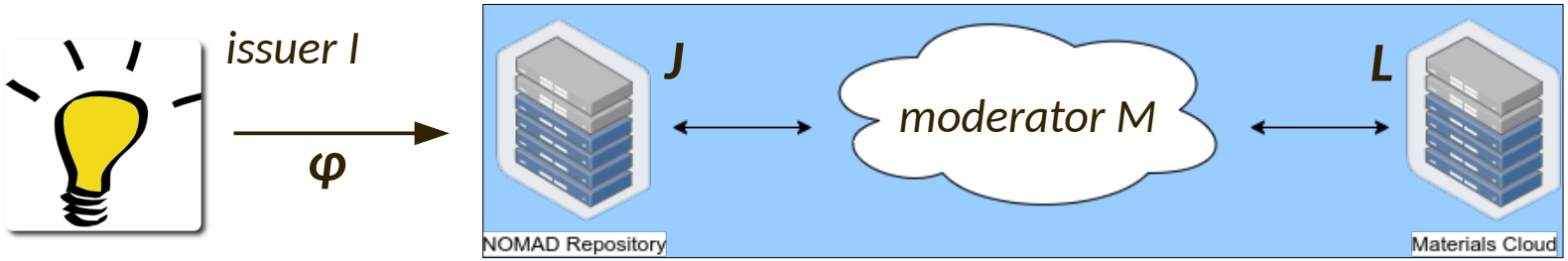
Scientific knowledge is a kind of knowledge (or else, little will qualify as knowledge). Research data infrastructures store and exchange scientific knowledge.



Scenario requiring epistemological formalization:

- "*M* asserts and approves *φ*'(*I*, *J*, *L*, *φ*)," where *φ*'(*I*, *J*, *L*, *φ*) is given by:
- "The scientific knowledge *φ*, previously issued by a source *I*, has been communicated by the knowledge base *J* to the knowledge base *L*."
- *J*, *L*, and *M* have a justified true belief in *φ*'.
- *φ* is a justified tenable assertion, by the standards applied to *I* by *M*.

User stories: Representative research workflows

user story 3: CO_2 methanation

user story 2: synchrotron QEXAFS experiments

user story 4: biocatalysis & multiphase flow

user story 1: photocatalytic water splitting

user story 5: CO_2 electrolysis

user story 6: metal-organic frameworks

user story 7: nanoparticle & SILP catalysts

user story 8: selective NOx reduction

User stories: Representative research workflows

user story 11: coupled in-situ and offline analytics

user story 10: Fischer-Tropsch process

user story 12: syngas-to-ethanol catalyst characterization

TECHNISCHE UNIVERSITÄT DARMSTADT

Catalysis Leibniz-Institut für Katalyse e.V.

user story 9: photocatalytic CO_2 reduction

user story 13: syngas-to-ethanol catalyst performance

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FAU

user story 16: water-gas shift reaction

user story 14: RDM for enzyme activity data

user story 15: modelling SILP catalysed reactions

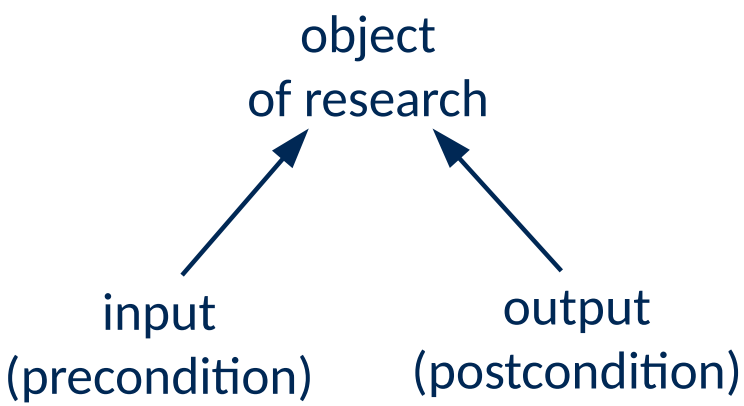
User stories: Representative research workflows

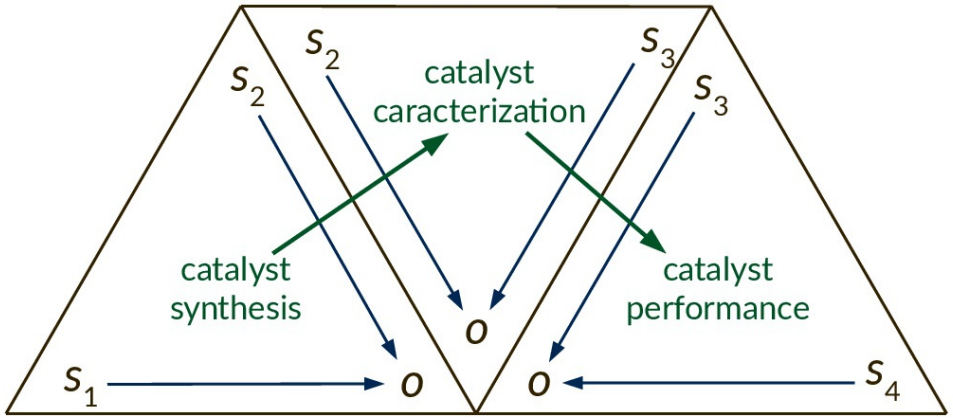
Interviews of 30 minutes each are conducted with internal prospective users.

For each research step, we jointly identify:

- **input**, *i.e.*, all that needs to be present in advance (incuding equipment)
- **output**, *i.e.*, that which is generated as an outcome of the research step

Pre- and postcondition are causally connected by participating in the same step of a research process, and they are applied to the same **object of research**.

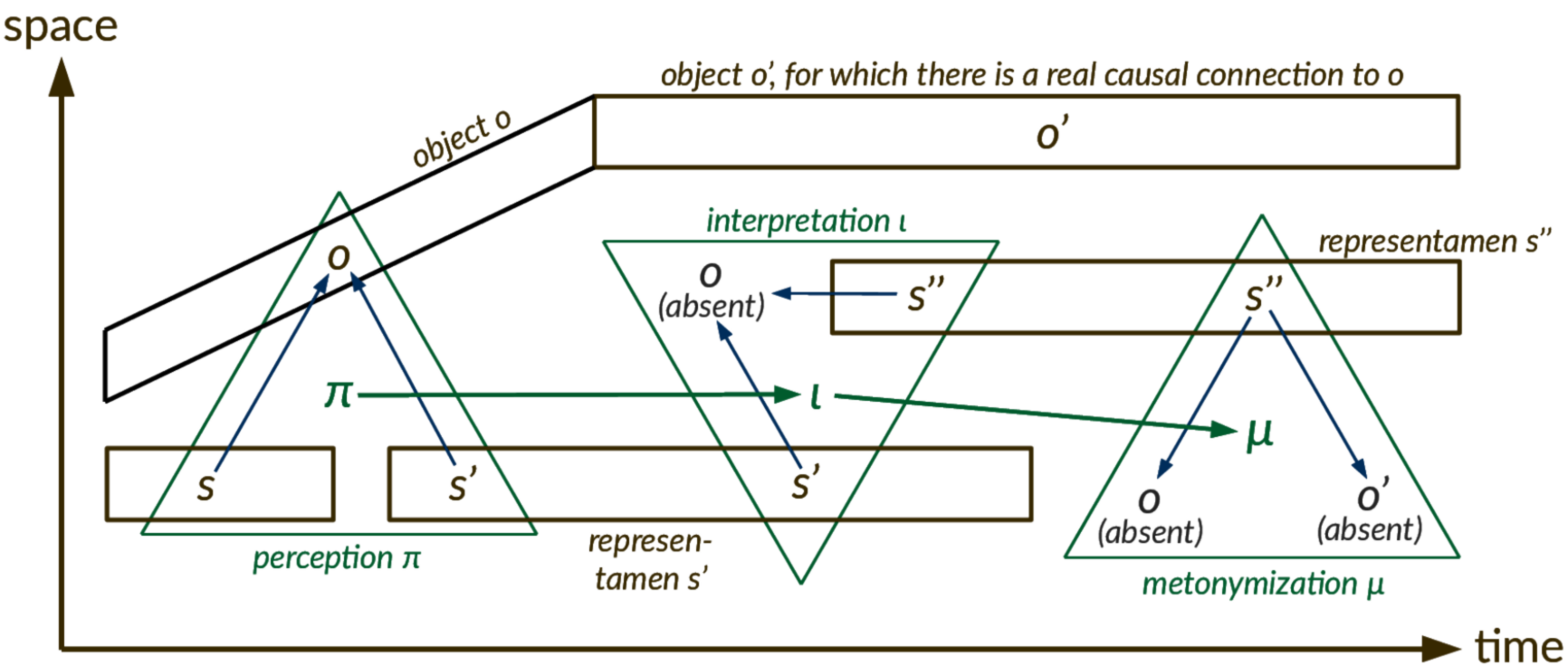




User story by A. Bordet, MPI CEC, Mülheim a. d. Ruhr

Cognitive processes following Peircean semiotics

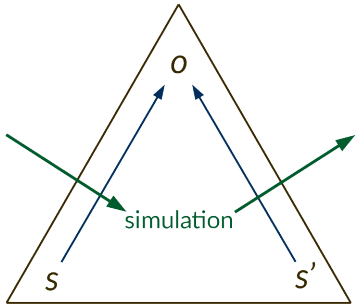
Mereosemiotics:[1] Combination of mereotopology and Peircean semiotics



[1]In *Proceedings of WCCM-ECCOMAS 2020*, doi:10.23967/wccm-eccomas.2020.297, **2021**.

Epistemic opacity: The challenge

Issue raised by Humphreys:[1] **Justification of *φ*** appears (to some) to be **opaque.**[1, 2]



alleged sources of opacity

validation becomes „holistic“

no explicit justification is computed

stochastic elements (Monte Carlo)

Lyapunov instability (molecular dynamics)

However, experiments are not usually viewed as opaque.

predetermination[3]

e.g., formal software verification[3]

usually inapplicable

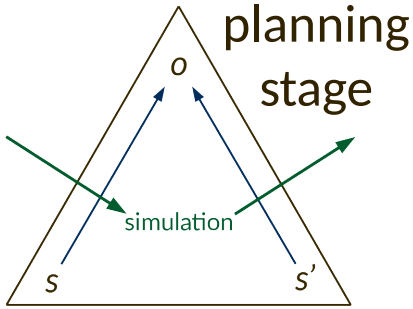
Underlying requirement: Provenance description delivering *scientia media* (system retains freedom).

L. de Molina

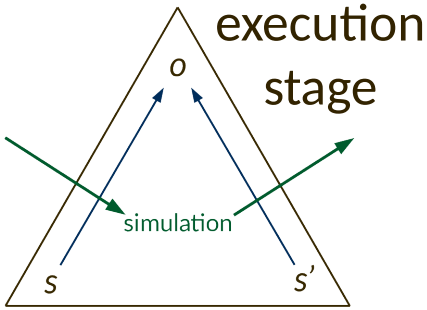
[1]Knowledge of *„all epistemically relevant elements“* cannot be attained (Humphreys, 2004, 2011).
[2]Durán and Formanek (2018): *„epistemically relevant elements“* = *„steps of the [...] justification“*.
[3]Required for non-opacity by Newman (2016), a requirement criticized by Durán & Formanek (2018).

Epistemic opacity as opposed to epistemic FAIRness

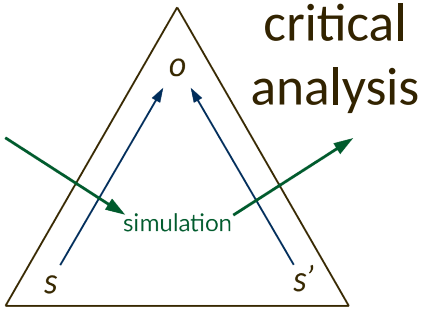
Three modes of justification by epistemic grounding:



ex ante
predetermination
(& model validation)



in actu
determination
„Reflexion im Vollzug“[1]



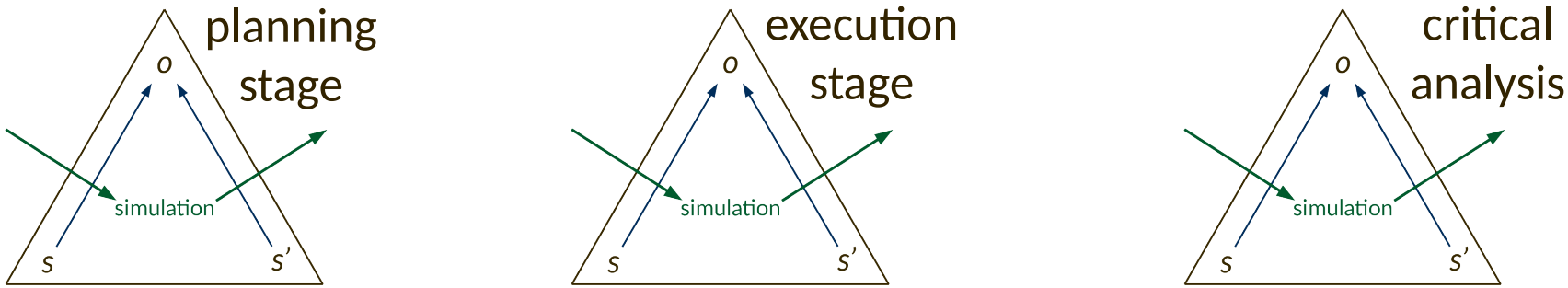
ex post
redetermination
„Reflexion des Vollzugs“[1]

Epistemic opacity is reduced by **epistemic FAIRness**, *i.e.*, the FAIR provision of a provenance description via a research data infrastructure that permits a reevaluation of the research workflow over an open epistemic space.

[1]Tulatz, *Epistemologie als Reflexion wissenschaftlicher Praxen*, **2018**.

Conclusion

To make scientific knowledge FAIR, research data infrastructures need to support the documentation, ingest, retrieval, and revision of data provenance.



Priorities ("DORIC principles") following doi:10.5281/zenodo.4571052

D	O	R	I	C
diversify technologies	**observe** practices	**realistic** objectives	**incentivize** open data	**co-design** data and workflows