

Norges miljø- og biovitenskapelige universitet

# Knowledge representation for reliable materials modelling translation

M. T. Horsch,<sup>1, 2</sup> S. Chiacchiera,<sup>2</sup> C. Niethammer,<sup>3</sup> B. Schembera,<sup>4</sup> F. Diewald,<sup>5</sup> P. Klein,<sup>5</sup> S. Stephan,<sup>6</sup> H. A. Preisig,<sup>7</sup> N. A. Konchakova,<sup>8</sup> and W. L. Cavalcanti<sup>9</sup>

<sup>1</sup>Norweg. Univ. Life Sciences, <sup>2</sup>UKRI STFC Daresbury Laboratory, <sup>3</sup>High Performance Computing Center Stuttgart, <sup>4</sup>Univ. Stuttgart, <sup>5</sup>Fraunhofer ITWM, <sup>6</sup>TU Kaiserslautern, <sup>7</sup>Norweg. Univ. Science & Technology, <sup>8</sup>Helmholtz-Zentrum Hereon, <sup>9</sup>Fraunhofer IFAM

**ECCOMAS 2022** 

9<sup>th</sup> June 2022

Lillestrøm



## **Translation in materials modelling**





ECCOMAS 2022

## **Epistemic opacity**

**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 metadata:** Information that should be included in an adequate response to the queries "what **knowledge claims** have been formulated on the basis of the given data?" and "what exactly is the relation between the knowledge claims, their proponents, and the data?"

**European Al Act proposal:** "To address the **opacity** that may make certain Al systems **incomprehensible to or too complex for natural persons**, a certain degree of transparency should be required for high-risk Al systems.<sup>1</sup> Users should be able to interpret the system output and use it appropriately. High-risk Al systems should therefore be accompanied by **relevant documentation**".

<sup>1</sup>Systems with "high risk" include all "safety components" related to "water, gas, heating, and electricity."

## The aim: Epistemic FAIRness

Epistemic opacity and darkness of data can be countered by **epistemic FAIRness**, *i.e.*, FAIR provision of all the **relevant epistemic metadata** via digital infrastructures. Such infrastructures must permit reevaluating processes and results.



Q: 1. How were the data obtained - what is the **data provenance**?

- 2. What do the data say what **knowledge claims** do we base on the data?
- 3. Why should we accept them what is their **epistemic grounding**?

<sup>1</sup>K. Tulatz, *Epistemologie als Reflexion wissenschaftlicher Praxen*, **2018**. ECCOMAS 2022 9<sup>th</sup> June 2022 Norwegian University of Life Sciences



onto-

logization

## **Closed epistemic spaces: Example**

**MODA, the expired CWA** attempt at standardization,<sup>1, 2</sup> is a textbook example for a closed epistemic space, suitable for documenting **technical information** only – not the outcome from **scientific practice**.<sup>3</sup>



<sup>1</sup>A. F. de Baas (ed.), What Makes a Material Function?, ISBN 978-92-79-63185-6, 2017.
 <sup>2</sup>Journal of Chemical & Engineering Data 65, 1313, doi:10.1021/acs.jced.9b00739, 2020.
 <sup>3</sup>K. Tulatz, Epistemologie als Reflexion wissenschaftlicher Praxen, 2018.
 ECCOMAS 2022
 9<sup>th</sup> June 2022



### **BPMN** as a process model

BPMN is a powerful workflow notation, standardized<sup>1</sup> as ISO/IEC 19510:2013.



Example by A. Segatto, M. Milleri, C. Kavka, COMPOSELECTOR project deliverable 3.4, **2018**. <sup>1</sup>See also the specification at https://www.omg.org/spec/BPMN/2.0.2/PDF.

#### ECCOMAS 2022

## **VIMMP** system of ontologies



9<sup>th</sup> June 2022

Norwegian University of Life Sciences



Noregs miljø- og biovitskaplege universitet

## Mereosemiotics in knowledge representation

The novel platforms in materials digitalization all use ontologybased semantic technology. Some of them either plan or claim to be EMMO compliant.<sup>1</sup>

How can we work with the rather novel approach of the EMMO?



VIRTUAL MATERIALS MARKETPLACE

H2020 GA no. 760907



H2020 GA no. 953163

ECCOMAS 2022



#### H2020 GA no. 952903



9<sup>th</sup> June 2022

<sup>1</sup>Since the EMMO stable release v1.0 has been delayed by over four years and has not occurred yet, this cannot go beyond an intention.

Lillestrøm

U

M +

### Molecular modelling knowledge graph<sup>N</sup>



<sup>1</sup>S. Stephan et al., Mol. Sim. 45, 806-814, **2019**. <sup>2</sup>M. Horsch et al., Proc. ISWC, **2020**.

ECCOMAS 2022

## Mereotopology and Peircean semiotics

#### **Peircean semiotics**



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





C. S. Peirce

Elementary Multiperspective Material Ontology<sup>1,2</sup>

#### 1) Taxonomy:

Conceptual hierarchy (subclass relation)

#### 2) Mereotopology:

Spatiotemporal parthood and connectivity

#### 3) Semiotics:

Representation of physical entities by signs



<sup>1</sup>H. A. Preisig *et al.*, doi:10.23967/wccm-eccomas.2020.262, no. 262 in *Proc. ECCOMAS 2020*, **2021**. <sup>2</sup>S. Clark *et al.*, *Adv. Energ. Mat.* 12(17), 2102702, doi:10.1002/aenm.202102702, **2022**.

#### ECCOMAS 2022

9<sup>th</sup> June 2022

Norwegian University of Life Sciences

#### 11

**Cognitive steps: Taxonomy** 

ECCOMAS 2022

PIMS-II is a mid-level ontology for scientific workflows as cognitive processes.<sup>1,2</sup>

perception requires participation (and overlap) of the perceived object







## **Cognitive steps in mereosemiotics**

PIMS-II is a mid-level ontology for scientific workflows as cognitive processes.<sup>2, 3</sup> Mereosemiotics:<sup>1-3</sup> Combination of mereotopology and Peircean semiotics

Norwegian University of Life Sciences



 <sup>1</sup>M. T. Horsch, S. Chiacchiera, B. Schembera, M. A. Seaton, I. T. Todorov, in *Proc. ECCOMAS 2020*, **2021**.

 <sup>2</sup>M. T. Horsch, no. 3 in *Proc. JOWO 2021*, **2021**.

 <sup>3</sup>P. Klein *et al.*, no. 26 in *Proc. JOWO 2021*, **2021**.

 ECCOMAS 2022
 9<sup>th</sup> June 2022

 12



<sup>1</sup>P. Klein *et al.*, no. 26 in *Proc. JOWO 2021*, **2021**.

ECCOMAS 2022



Noregs miljø- og biovitskaplege universitet

## Conclusion



H2020 GA no. 760907



H2020 GA no. 953163

**ECCOMAS 2022** 



#### H2020 GA no. 952903



In research data provenance and workflow documentation, a new standardization effort is needed. The MODA CWA has expired.

We need a shift toward making the knowledge claims machineactionable, not mainly workflows.

> There, standardization must permit both semantic and epistemic heterogeneity.





Norges miljø- og biovitenskapelige universitet

# Knowledge representation for reliable materials modelling translation

M. T. Horsch,<sup>1, 2</sup> S. Chiacchiera,<sup>2</sup> C. Niethammer,<sup>3</sup> B. Schembera,<sup>4</sup> F. Diewald,<sup>5</sup> P. Klein,<sup>5</sup> S. Stephan,<sup>6</sup> H. A. Preisig,<sup>7</sup> N. A. Konchakova,<sup>8</sup> and W. L. Cavalcanti<sup>9</sup>

<sup>1</sup>Norweg. Univ. Life Sciences, <sup>2</sup>UKRI STFC Daresbury Laboratory, <sup>3</sup>High Performance Computing Center Stuttgart, <sup>4</sup>Univ. Stuttgart, <sup>5</sup>Fraunhofer ITWM, <sup>6</sup>TU Kaiserslautern, <sup>7</sup>Norweg. Univ. Science & Technology, <sup>8</sup>Helmholtz-Zentrum Hereon, <sup>9</sup>Fraunhofer IFAM

**ECCOMAS 2022** 

9<sup>th</sup> June 2022

Lillestrøm