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STFC Daresbury Laboratory
UK Research and Innovation

Ontologies and metadata in VIMMP

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Lausanne, 8 Nov 2018

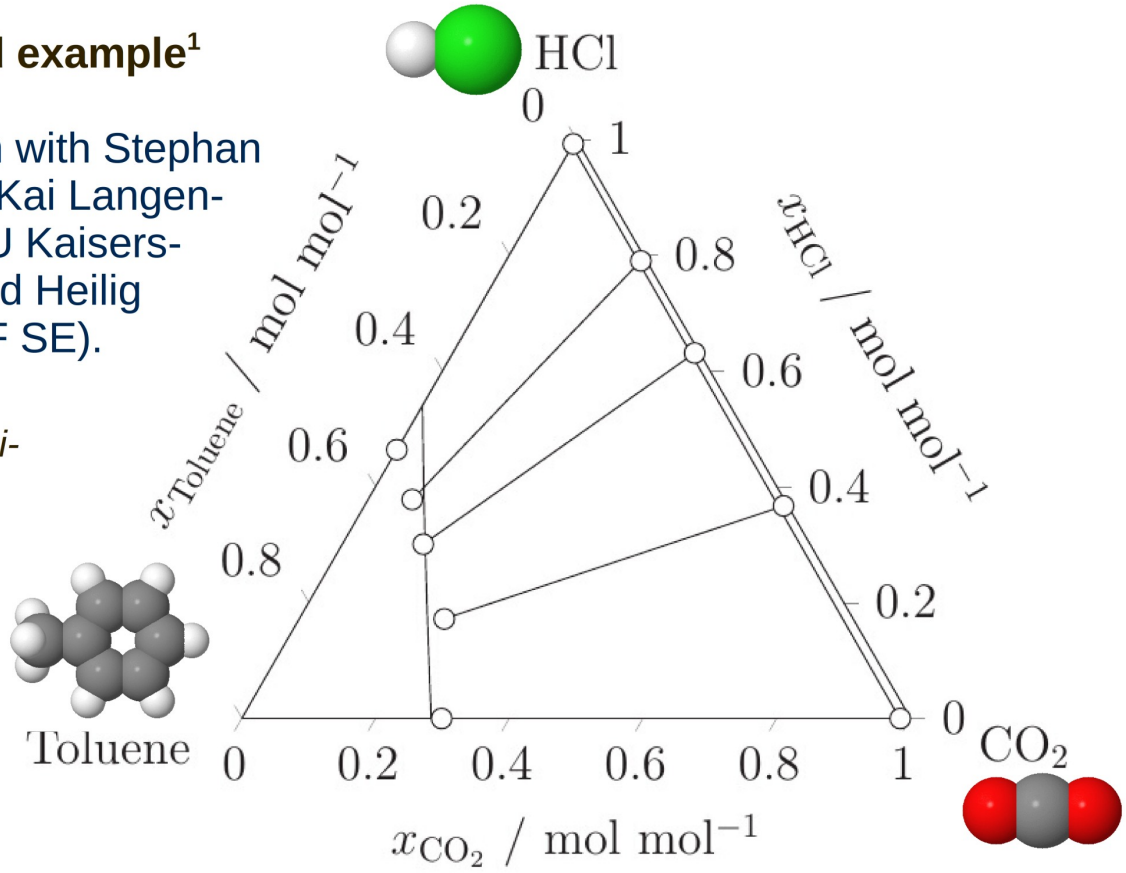
CECAM – EMMC Workshop on Coupling and Linking

“Science Highlight” (i.e., example): Case description

Context of the discussed example[1]

Work done in collaboration with Stephan Werth, Maximilian Kohns, Kai Langenbach, and Hans Hasse (TU Kaiserslautern), as well as Manfred Heilig and Gerd Haderlein (BASF SE).

[1]Werth *et al.*, *Fluid Phase Equilibria* 427, 219 – 230, **2016**.



(S. Werth *et al.*, *Fluid Phase Equilib.* 427, 219 – 230, **2016**.)

Figure 15: Vapor-liquid equilibrium compositions of the coexisting phases in the system toluene + CO_2 + HCl at $T = 353$ K and $p = 4.9$ MPa. Symbols are the present MD simulations results and lines are PC-SAFT results.

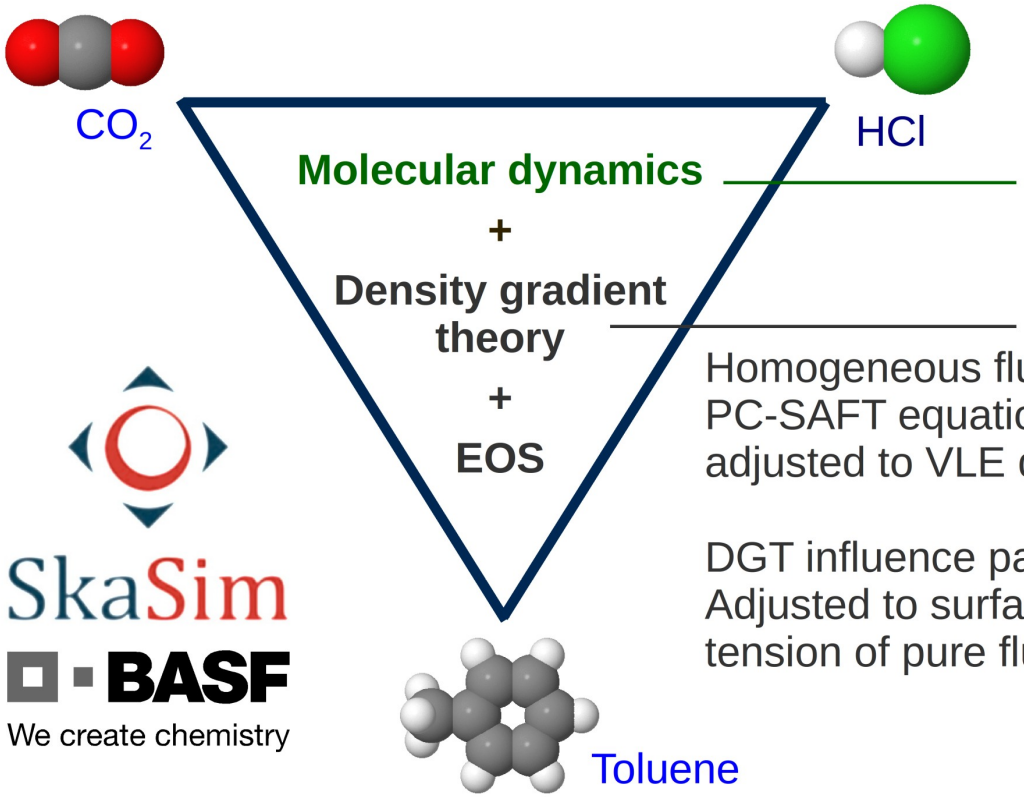
SkaSim

BASF
We create chemistry

“Science Highlight”: VLE and interfacial phenomena

Multiscale modelling and simulation of vapour-liquid interfaces of fluid mixtures

Modelling approach



pure fluid models and two binary subsystems from previous work

One binary system, i.e., toluene + CO2, from present work

Homogeneous fluid properties: PC-SAFT equation of state, adjusted to VLE data

DGT influence parameter: Adjusted to surface tension of pure fluids

Computational Molecular Engineering

SkaSim

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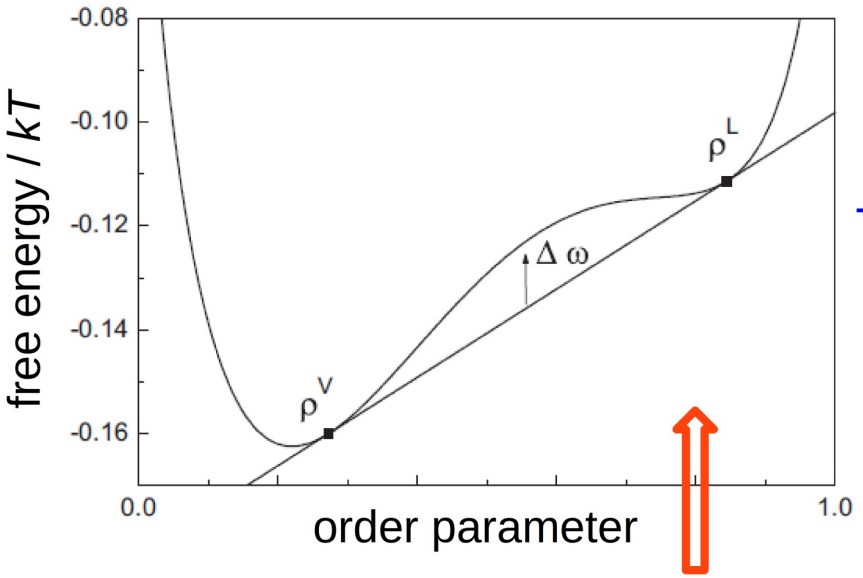
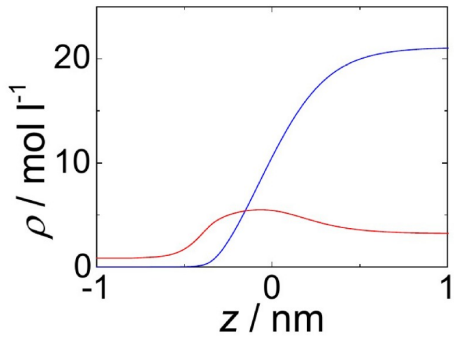
We create chemistry

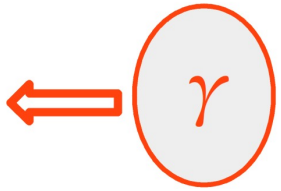
LABORATORY OF ENGINEERING THERMODYNAMICS
TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

“Science Highlight”: DGT coupled with PC-SAFT EOS



$+\kappa(\nabla\rho)^2$

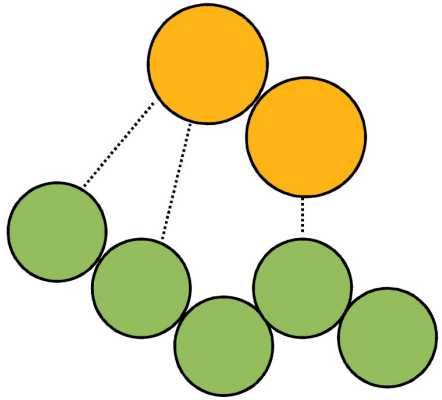




Perturbed-Chain Statistical Associating Fluid Theory

$$A = A^{\text{ideal}} + A^{\text{hard chain}} + A^{\text{dispersion}} + A^{\text{association}}$$

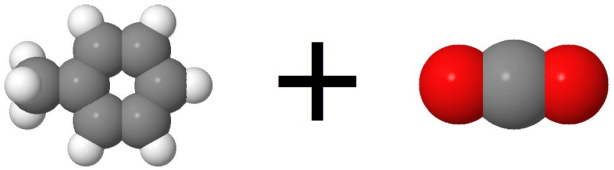
[1] L. D. Landau, E. M. Lifshitz, *Phys. Z. Sowjet.* 8, 153, **1935**;
[2] J. W. Cahn, J. E. Hilliard, *J. Chem. Phys.* 28, 258, **1958**;
[3] C. I. Poser, I. C. Sanchez, *Macromol.* 14, 361, **1981**;
[4] M. P. A. Fisher, M. Wortis, *Phys. Rev. B* 29, 6252, **1984**;
[5] H. Kahl, S. Enders, *Phys. Chem. Chem. Phys.* 4, 931, **2002**.

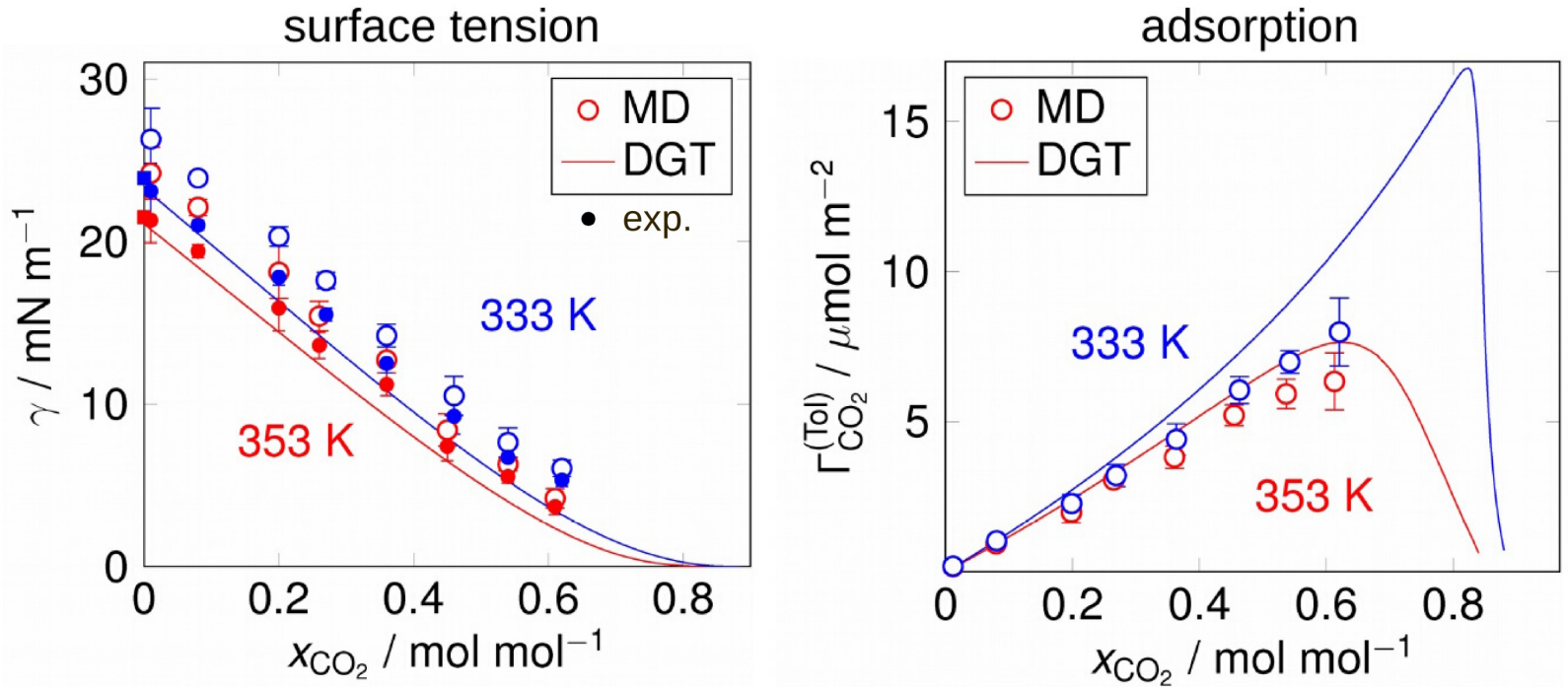


[6] J. Gross, G. Sadowski, *Ind. Eng. Chem. Res.* 40, 1244, **2001**;
[7] J. Gross, G. Sadowski, *Ind. Eng. Chem. Res.* 41, 5510, **2002**.

“Science Highlight”: Results from MD and DGT+EOS

Simulation and comparison between modelling and simulation approaches





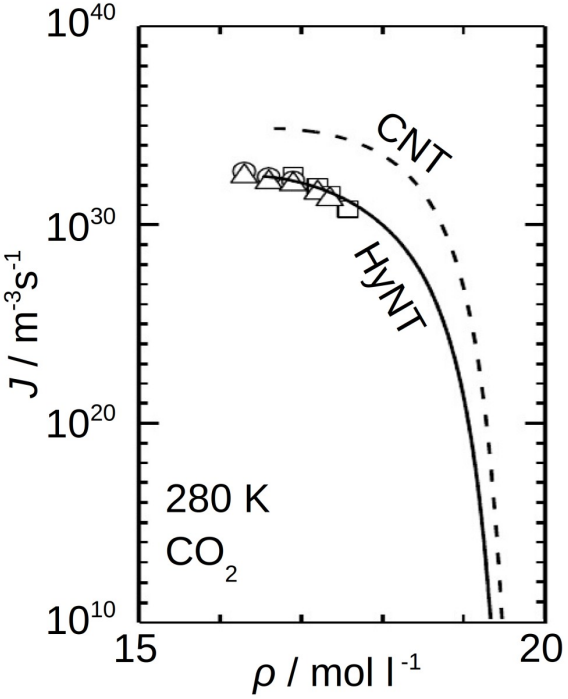
(S. Werth *et al.*, *Fluid Phase Equilib.* 427, 219 – 230, **2016**.)

“Science Highlight”: Hybrid nucleation theory (cavitation)

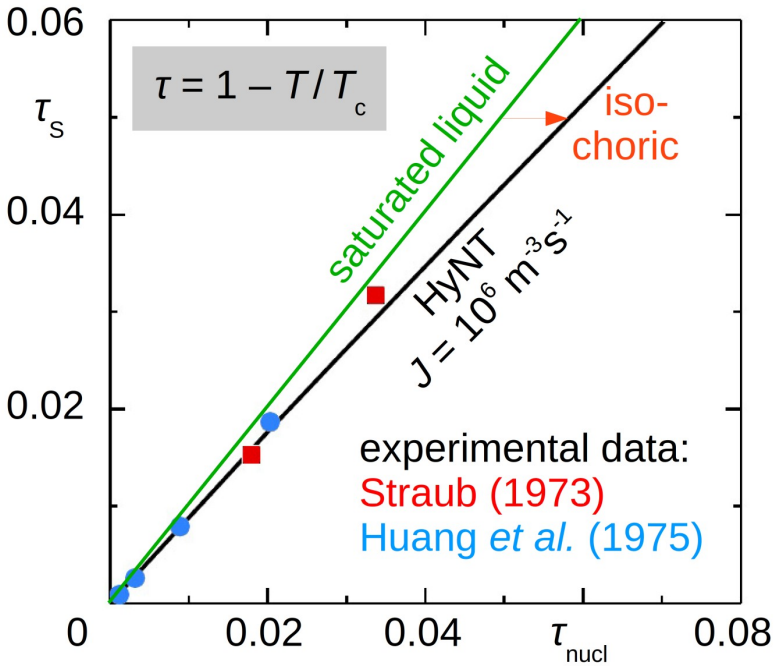
$$J = J_0 \exp\left(-\frac{\Delta A^*}{kT}\right)$$

thermodynamic factor from density gradient theory with the PC-SAFT EOS

kinetic factor from molecular dynamics



extrapolation by the hybrid nucleation theory

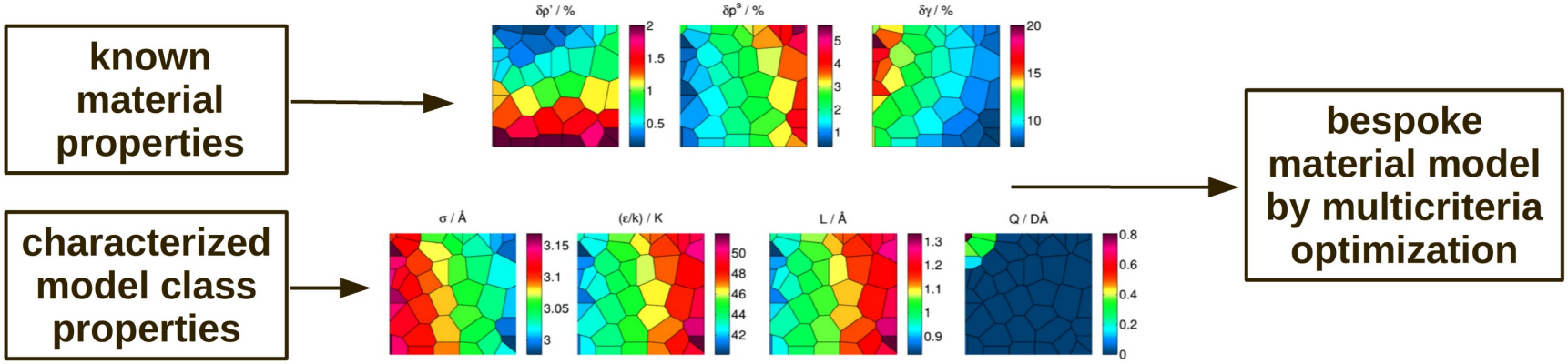


(K. Langenbach *et al.*, *J. Chem. Phys.* 148, 124702, **2018**.)

“Vision”: End-user controlled model design

“Design your own material model in five minutes”

- End-user controlled **multicriteria optimization**, e.g., model selection on patch plots.
- Can be put into practice for **well-characterized model classes** (2CLJQ, Mie-6, …).
- Expected to become a popular feature attracting a great number of users.



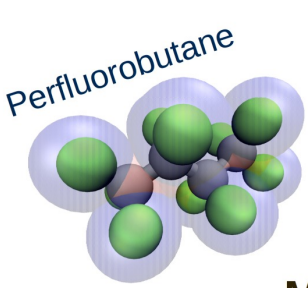
(Stöbener *et al.*, *Fluid Phase Equilib.* 411, 33 – 42, **2016**.)

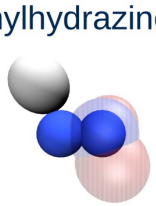
Preconditions for making this approach broadly applicable and interoperable:

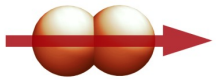
Agreement on semantic assets, e.g., ontology for simulation, modelling and opimization;

Workflow development, e.g., to capture the behaviour of a given class of material models.

“Vision”: Interoperability and shared semantic assets







Molecular Model Database

http://molmod.boltzmann-zuse.de/

Repository maintained by Simon Stephan *et al.* (Boltzmann-Zuse Society)

Computational Molecular Engineering

RDA Task Group
“Semantic Assets for Materials Science”

RESEARCH DATA ALLIANCE

http://schemas.nist.gov/

“SimScienceCenter”
High Performance Computing Center Stuttgart

H L R S

“Vision”: Modelling and simulation standardization

Time line of EMMC-governed standardization efforts

RoMM VI → **MODA** → **CWA 17284** → **Ontologies**

Semi-formalized terminology or vocabulary

Graph language & formalized terminology

CEN European standard

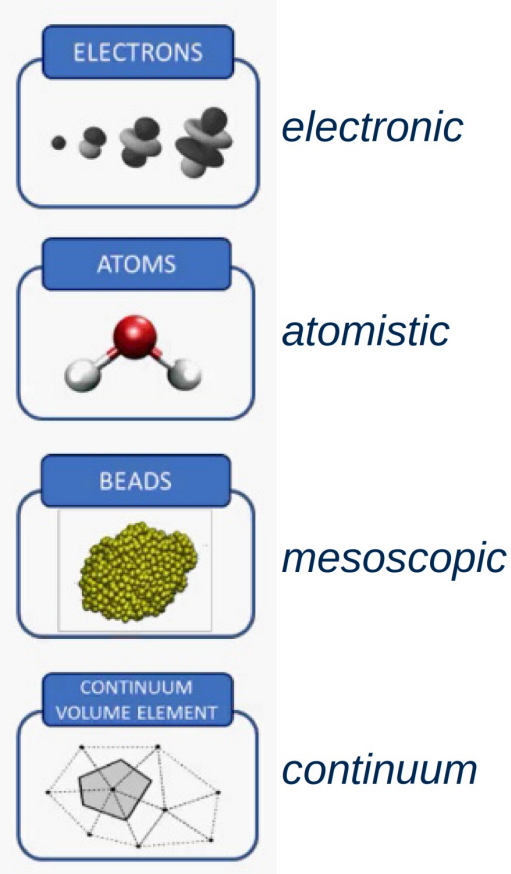
EMMO and EVMPO

(Ontology development is work in progress at present.)

EMMC

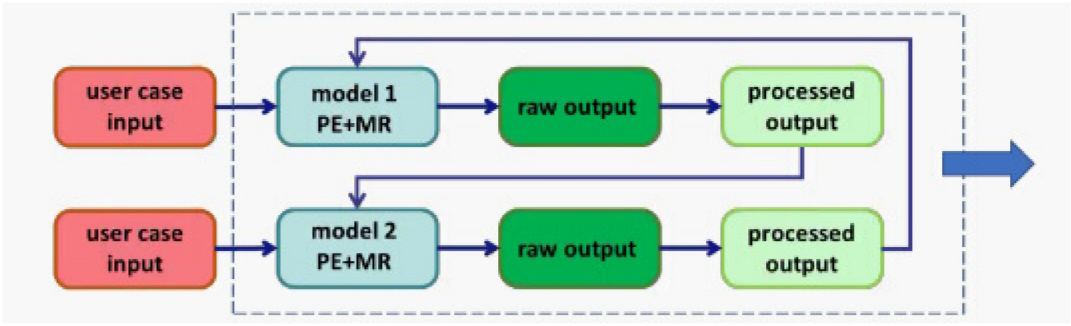
(1) User Case
(2) Model
(3) Solver
(4) Processing

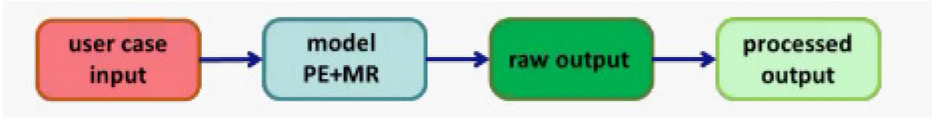
MODA
(graph language)

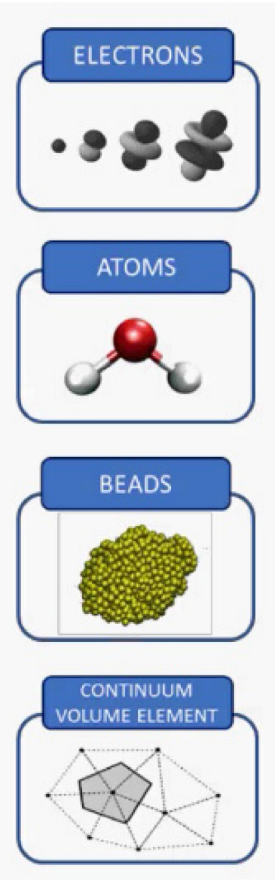


“Vision”: Modelling and simulation standardization

MODA – Modelling Workflow Graph Language (CEN standard by CWA 17284)







electronic

atomistic

mesoscopic

continuum

EMMC

(1) User Case
(2) Model
(3) Solver
(4) Processing

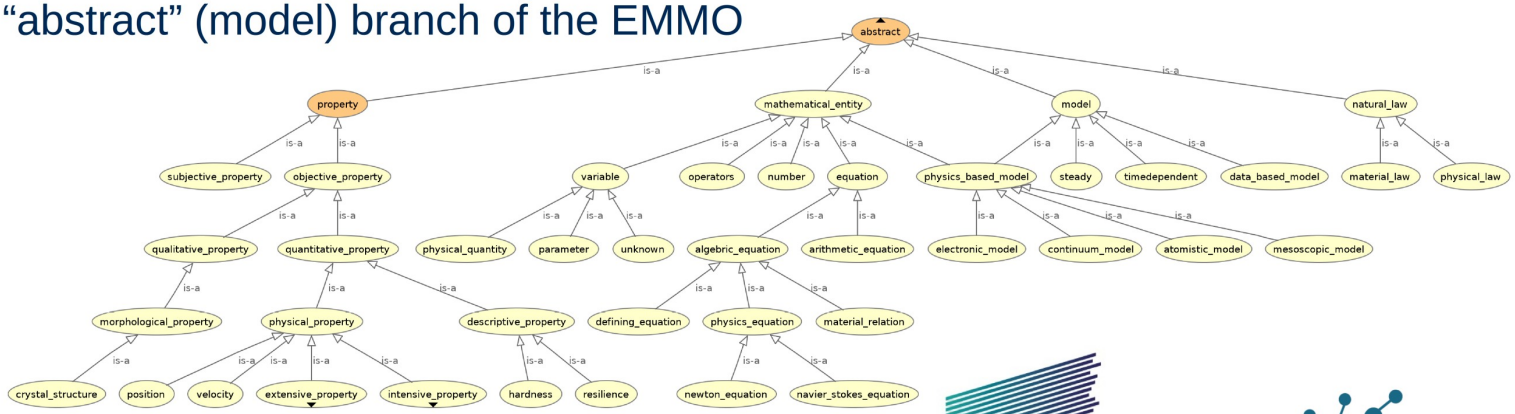
cen

EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

“Vision”: European Virtual Marketplace Framework

Disclaimer: The concrete realization is confidential to Ghedini *et al.* until published.

“abstract” (model) branch of the EMMO



Agreed point of departure: EMMO

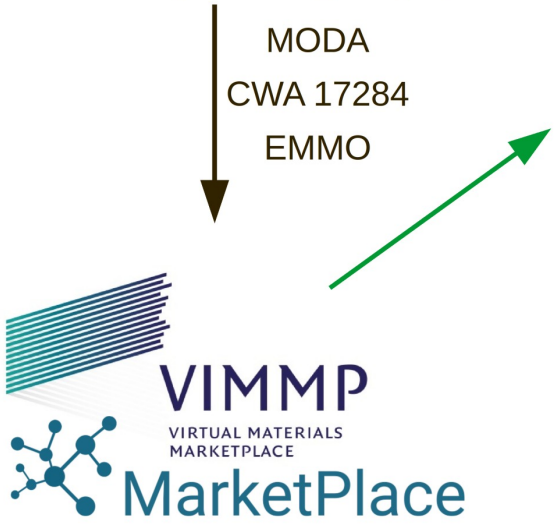
VIMMP VIRTUAL MATERIALS MARKETPLACE MarketPlace

The virtual-marketplace projects VIMMP and MARKETPLACE will continue this work with …

- … a **European Virtual Marketplace Ontology (EVMPO)** that extends EMMO;
- … **marketplace-level ontologies** based on MODA, EVMPO, EMMO, and others;
- … **subdomain-specific ontologies** based on MODA, e-CUDS, NOMAD, and others.

“Vision”: European Virtual Marketplace Framework

MODA Graph Language, CEN Workshop Agreement 17284, and EMMO (Ghedini *et al.*)



European Virtual Marketplace Ontology (EVMPO)

The upper level, defined by **EVMPO**, will prospectively be approved by the **VIMMP** and **MARKETPLACE** project consortia, by which a single coherent **European Virtual-Marketplace Framework** for modelling and simulation services will be established.

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- … a **European Virtual Marketplace Ontology (EVMPO)** that extends EMMO;
- … **marketplace-level ontologies** based on MODA, EVMPO, EMMO, and others;
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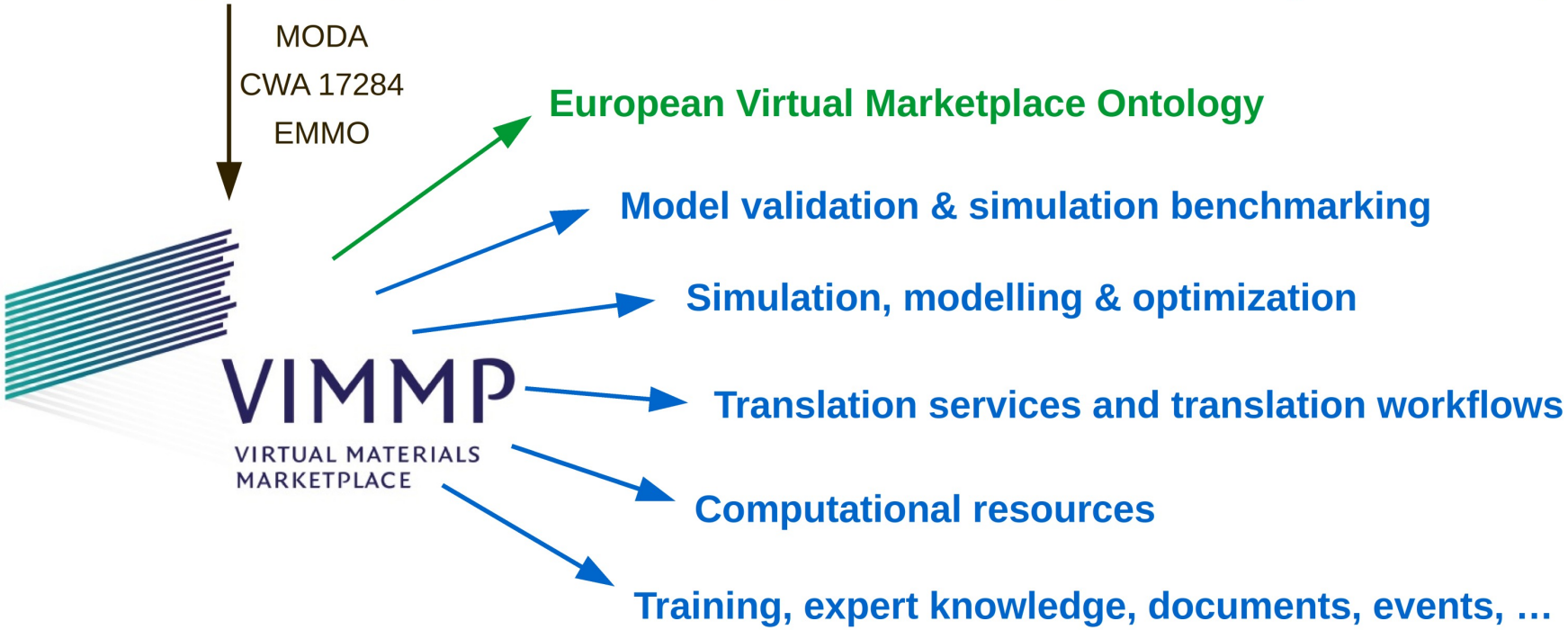
“Vision”: Development of marketplace-level ontologies

MODA Graph Language, CEN Workshop Agreement 17284, and EMMO (Ghedini *et al.*)



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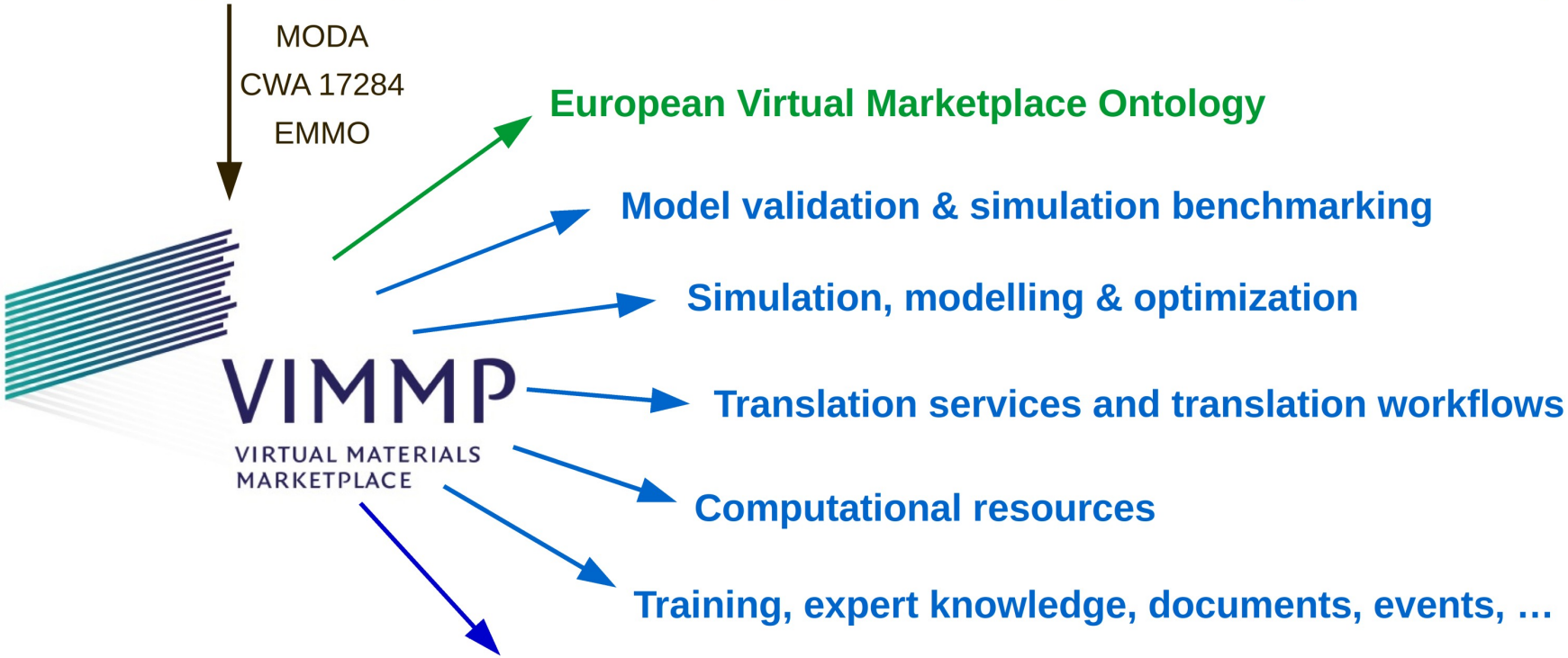
“Vision”: Development of subdomain-specific ontologies

MODA Graph Language, CEN Workshop Agreement 17284, and EMMO (Ghedini *et al.*)



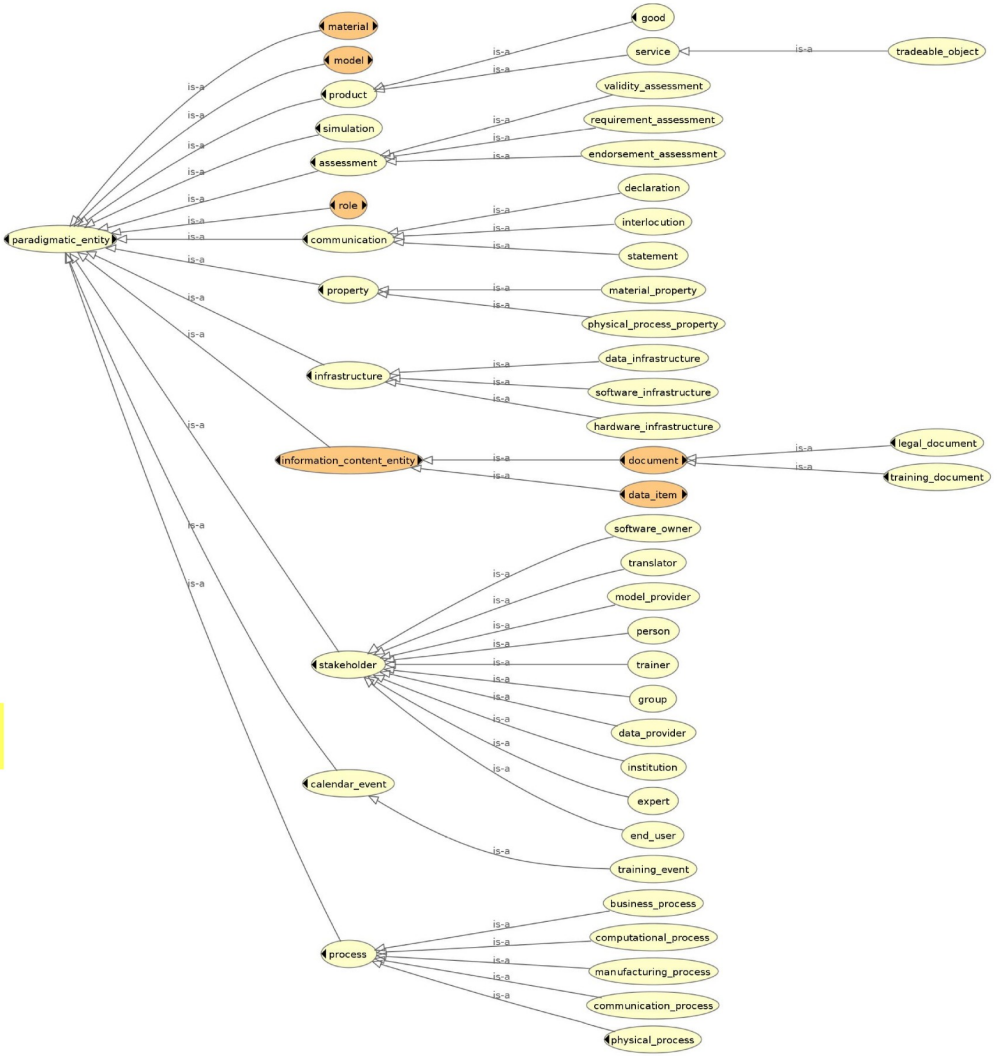
- … **subdomain-specific ontologies** based on MODA, e-CUDS, NOMAD, and others.

“Vision”: European Virtual Marketplace Ontology

The EVMPO will provide a structure for the marketplace-level ontologies by formulating **fundamental paradigmatic categories** which correspond to irreducible terms that are constitutive to the virtual-marketplace paradigm.

Recommendation: Any ontology at the marketplace level should follow the structure given by these categories as closely as possible.

preliminary work



VIMMP
VIRTUAL MATERIALS MARKETPLACE
MarketPlace

“Vision”: European Virtual Marketplace Ontology

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preliminary work

VIMMP
VIRTUAL MATERIALS MARKETPLACE
MarketPlace

Fundamental paradigmatic categories:

(1) **assessment**, i.e., proposition on accuracy, performance or trust in something/someone
(2) **calendar_event**, i.e., meeting or activity that is scheduled or can be scheduled
(3) **communication**, i.e., message or action that is communicated by a stakeholder
(4) **information_content_entity**, as defined in the Information Artifact Ontology (IAO)
(5) **infrastructure**, i.e., virtual-marketplace infrastructure such as DB, hardware, and software
(6) **material**, as defined in the European Materials Modelling Ontology (EMMO)
(7) **model**, as defined in the European Materials Modelling Ontology (EMMO)
(8) **process**, i.e., temporal evolution of one or multiple entities

…

“Vision”: European Virtual Marketplace Ontology

The EVMPO will provide a structure for the marketplace-level ontologies by formulating **fundamental paradigmatic categories** which correspond to irreducible terms that are constitutive to the virtual-marketplace paradigm.

Recommendation: Any ontology at the marketplace level should follow the structure given by these categories as closely as possible.

preliminary work

VIMMP
VIRTUAL MATERIALS MARKETPLACE
MarketPlace

Fundamental paradigmatic categories:

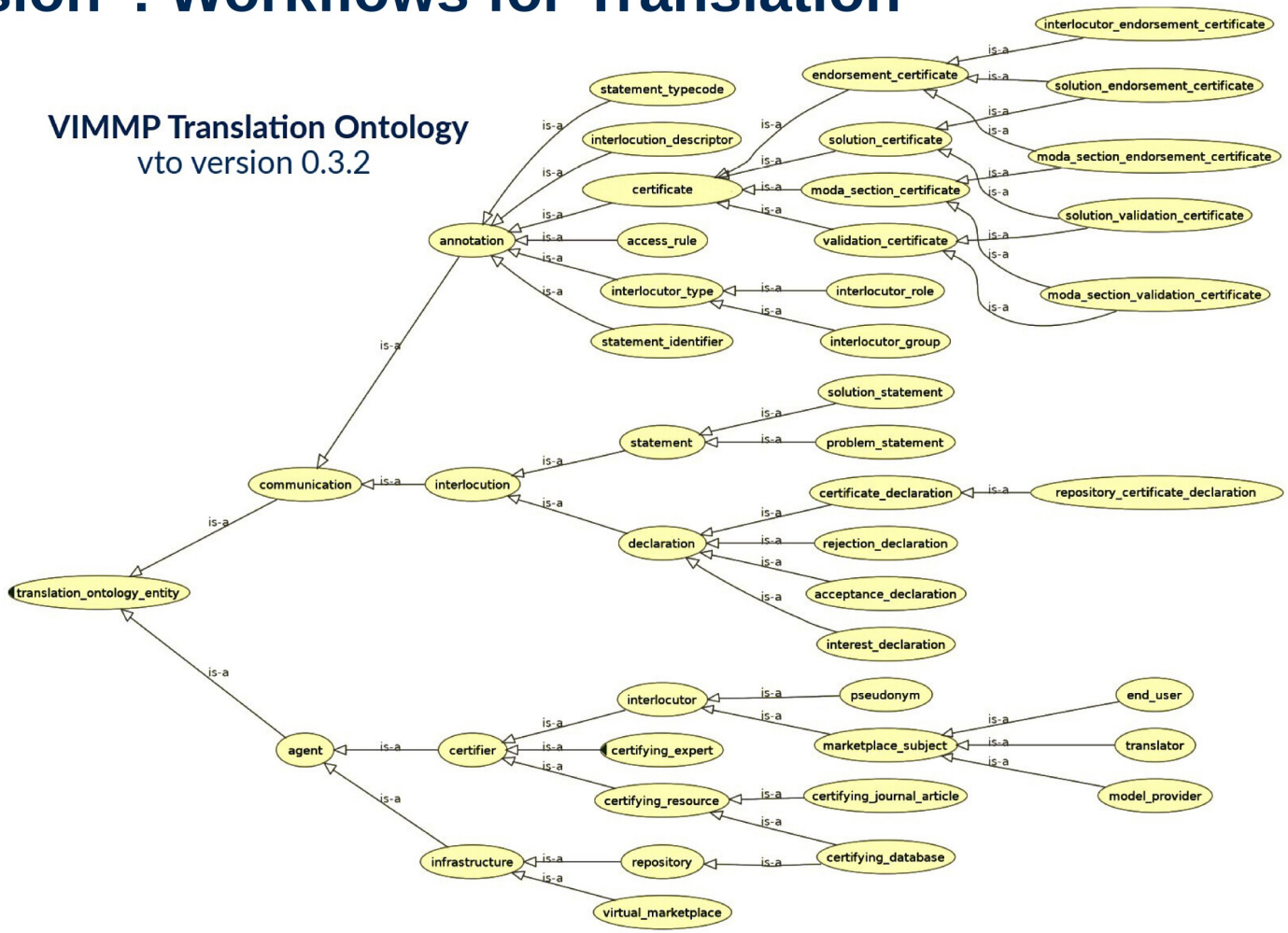
…

(8) **process**, i.e., temporal evolution of one or multiple entities
(9) **product**, i.e., good or service marketed off-site or on a virtual marketplace
(10) **property**, as defined in the European Materials Modelling Ontology (EMMO)
(11) **role**, as defined in the European Materials Modelling Ontology (EMMO)
(12) **simulation**, i.e., simulation workflow; including single simulations as elementary case
(13) **stakeholder**, i.e., individual, institution, or group related to a virtual marketplace

Fundamental non-paradigmatic category:

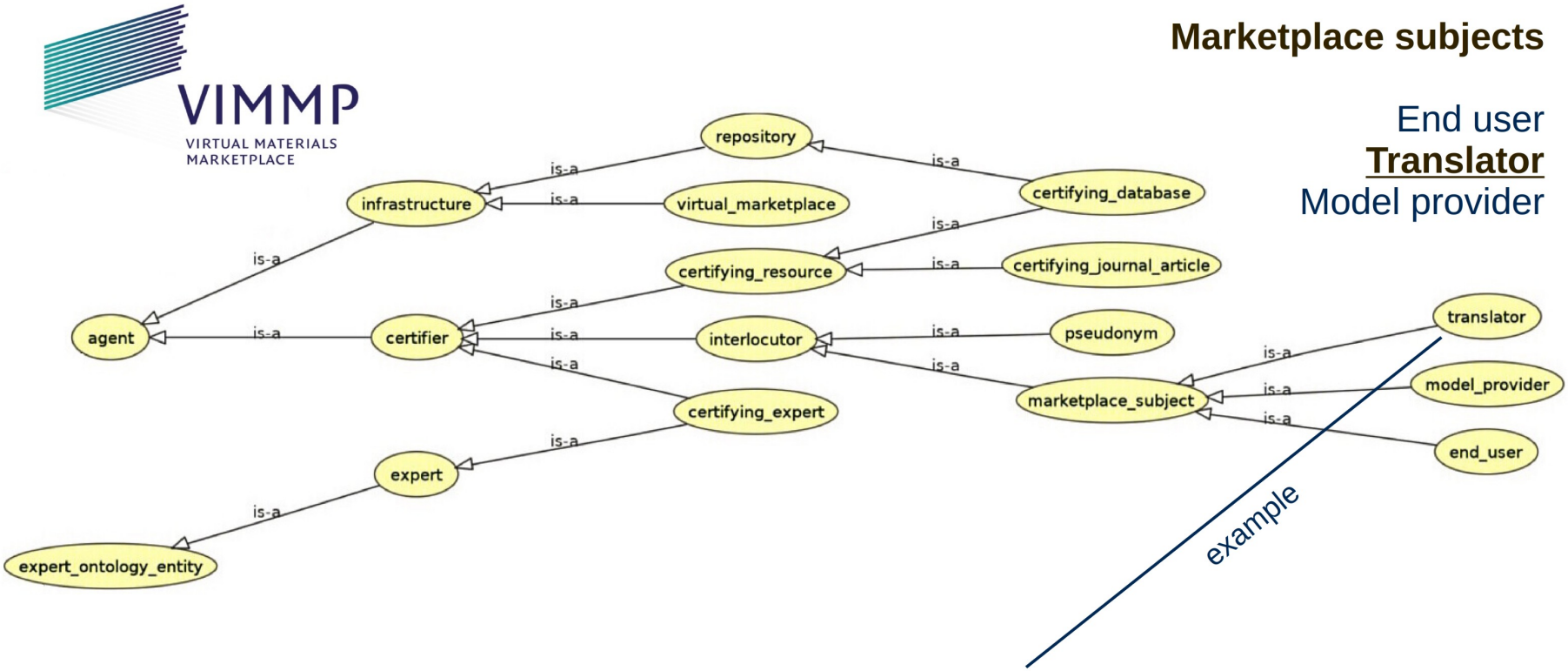
- **annotation**, i.e., non-paradigmatic aspect associated with an entity covered by EVMPO

“Vision”: Workflows for Translation

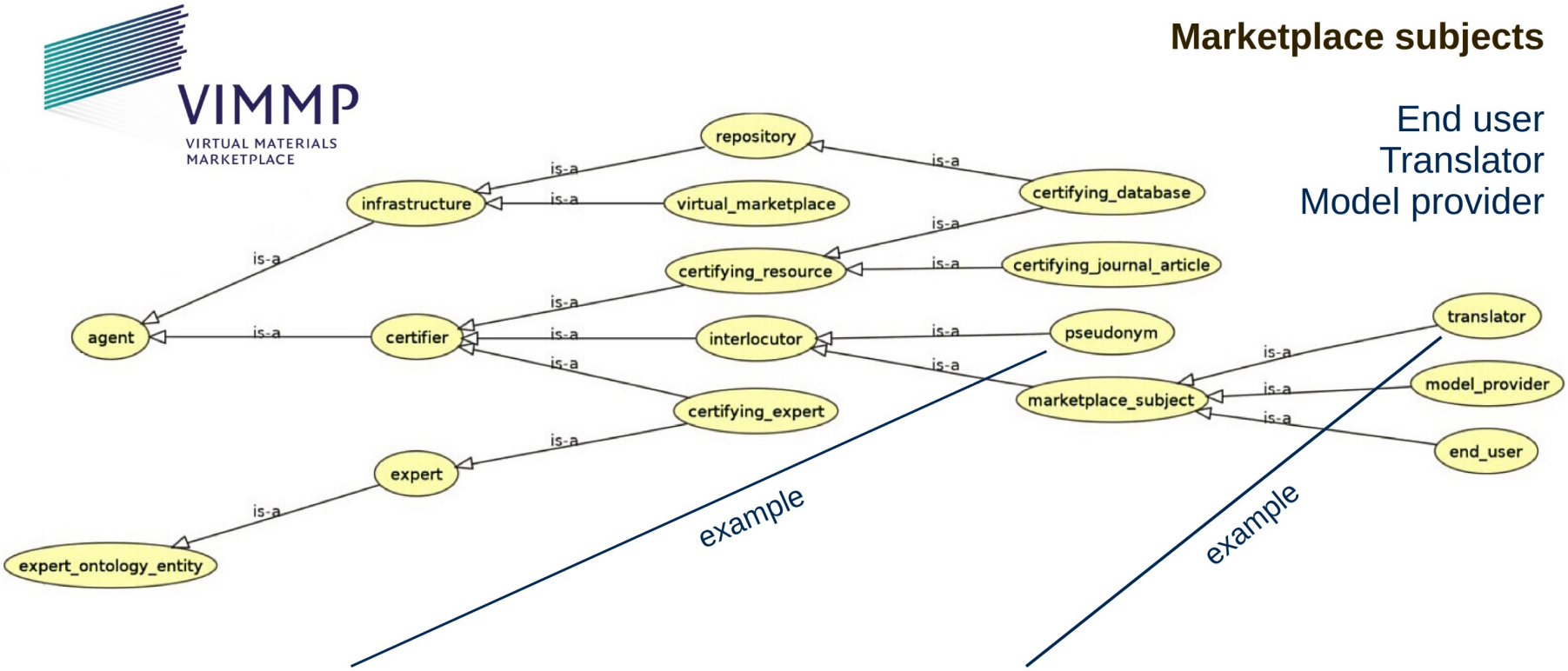


Disclaimer: Displayed ontology sketches represent an early stage of development.

“Vision”: Work toward ontologies at marketplace level



“Vision”: Work toward ontologies at marketplace level




```
:CHASH a :pseudonym;
   :has_agentid 323;
   :has_hash_form "C1343A";
   :is_on_market :VIMMP_MARKETPLACE.
```

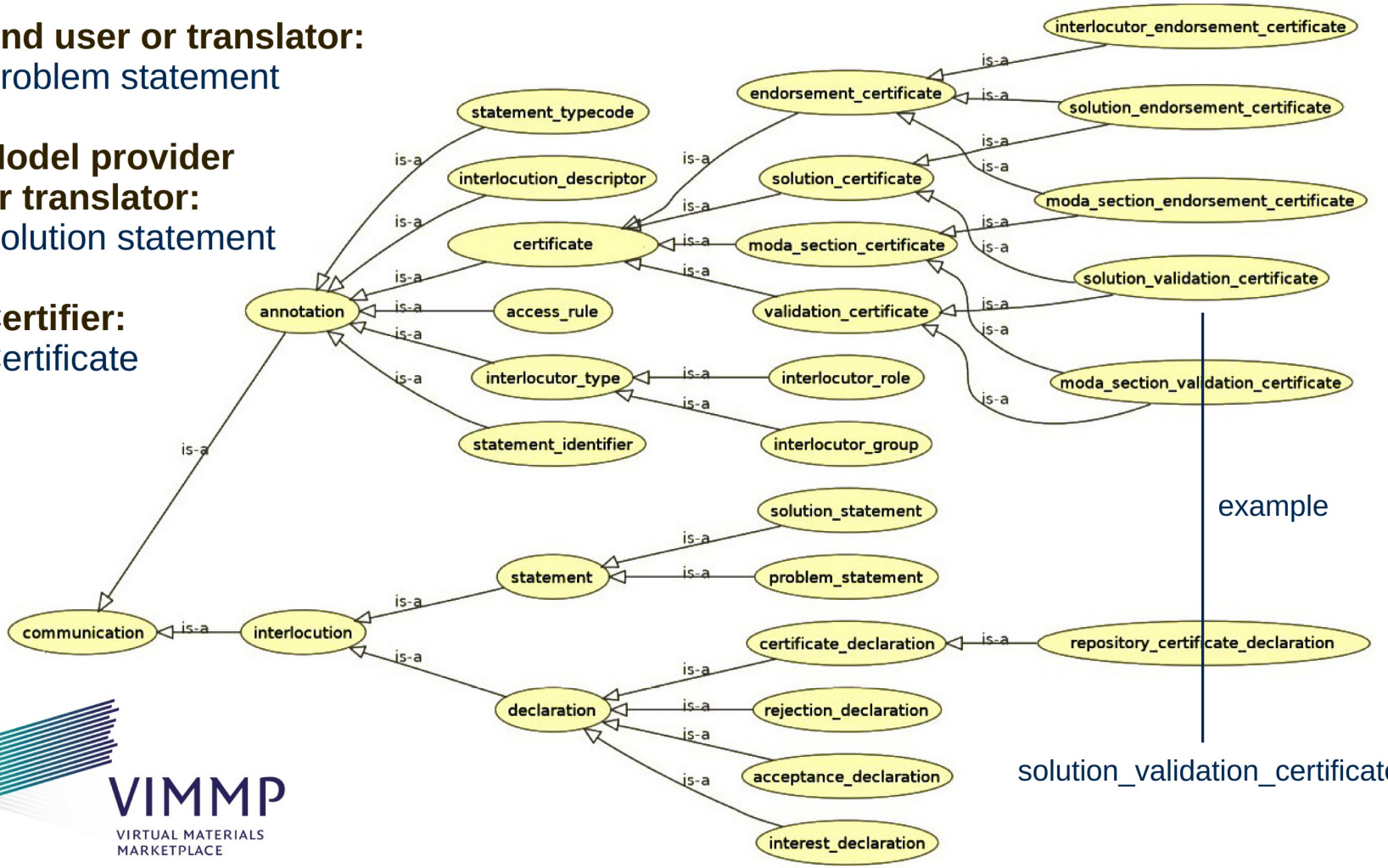
```
:BREMEN a :translator;
   :has_agentid 2;
   :has_name "VIMMP Coordination Group";
   :is_on_market :VIMMP_MARKETPLACE.
```

“Vision”: Work toward ontologies at marketplace level

End user or translator:
Problem statement

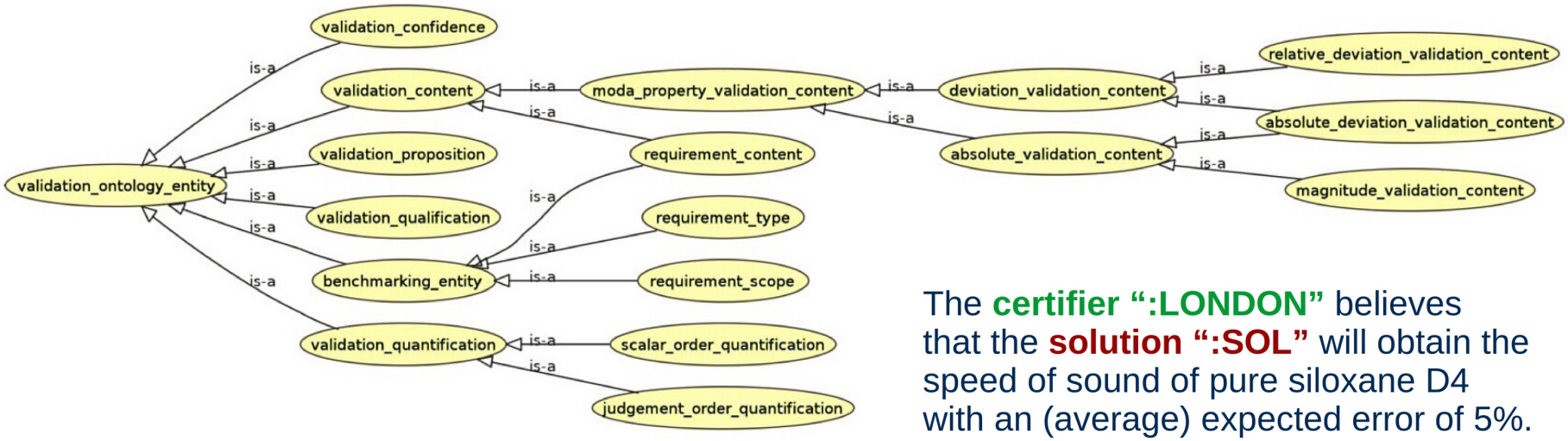
Model provider or translator:
Solution statement

Certifier:
Certificate



VIMMP
VIRTUAL MATERIALS MARKETPLACE

“Vision”: Validation ontology and epistemology

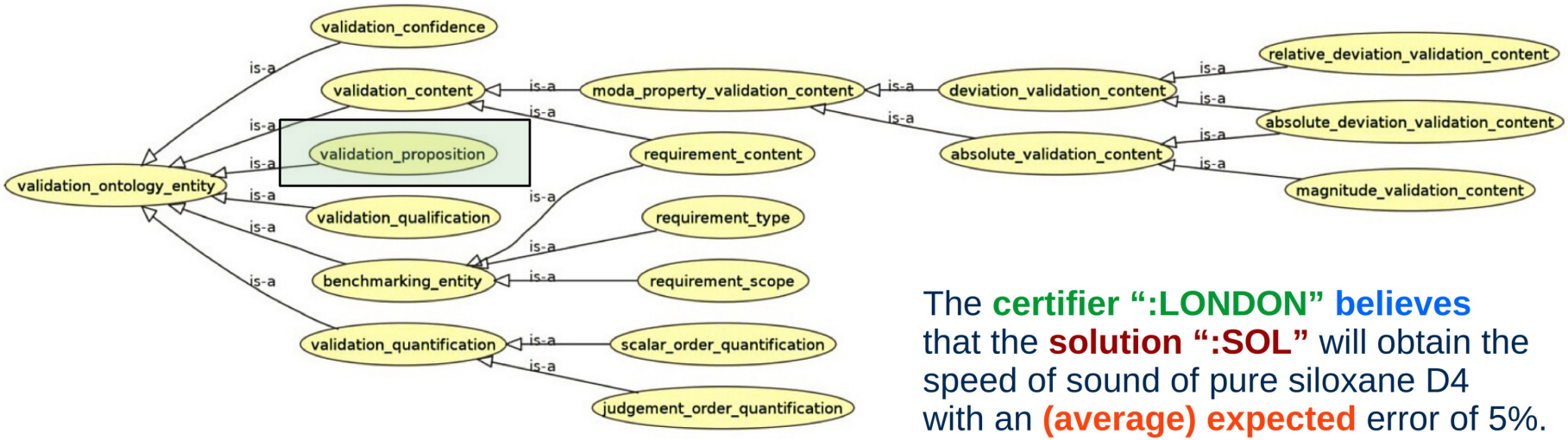


The **certifier “:LONDON”** believes that the **solution “:SOL”** will obtain the speed of sound of pure siloxane D4 with an (average) expected error of 5%.

:SOL_ACCURACY a :solution_validation_certificate;
:has_certifier :LONDON;
:refers_to_solution :SOL.

VIMMP
VIRTUAL MATERIALS MARKETPLACE

“Vision”: Validation ontology and epistemology



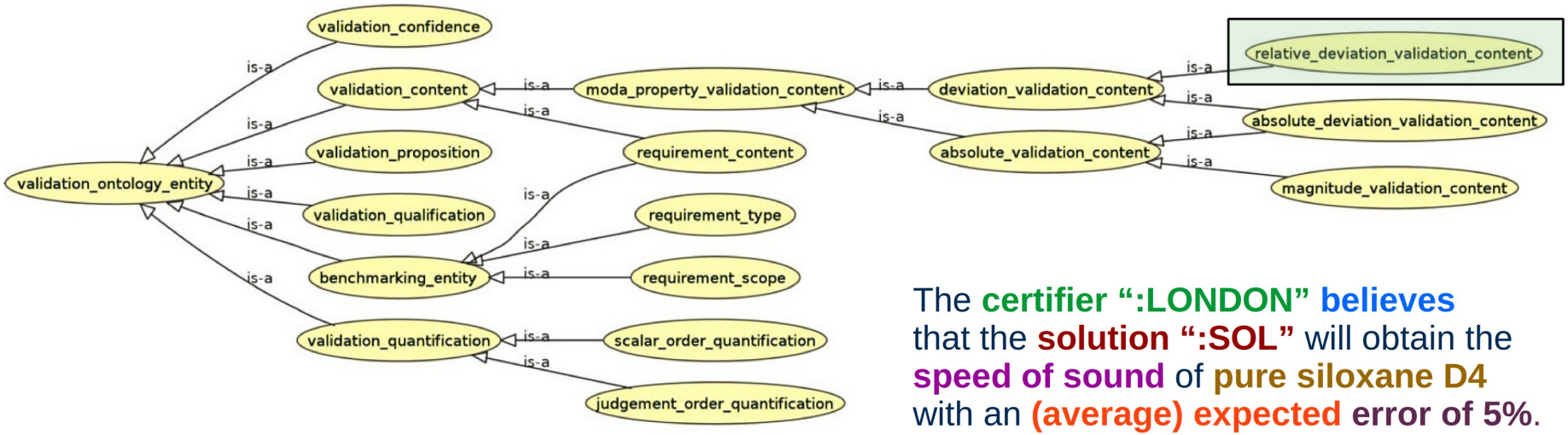
The **certifier “:LONDON”** **believes** that the **solution “:SOL”** will obtain the speed of sound of pure siloxane D4 with an **(average) expected** error of 5%.

:SOL_ACCURACY a :solution_validation_certificate;
:has_certifier :LONDON;
:refers_to_solution :SOL;
:states **:SOL_ACCURACY_PROP.**

:SOL_ACCURACY_PROP a :validation_proposition;
:has_confidence :STATEMENT_OF_BELIEF;
:has_qualification :EXPECTATION.

VIMMP
VIRTUAL MATERIALS MARKETPLACE

“Vision”: Validation ontology and epistemology



The **certifier “:LONDON”** **believes** that the **solution “:SOL”** will obtain the **speed of sound** of **pure siloxane D4** with an **(average) expected** **error of 5%**.

:SOL_ACCURACY a :solution_validation_certificate;
:has_certifier :LONDON;
:refers_to_solution :SOL;
:states **:SOL_ACCURACY_PROP.**

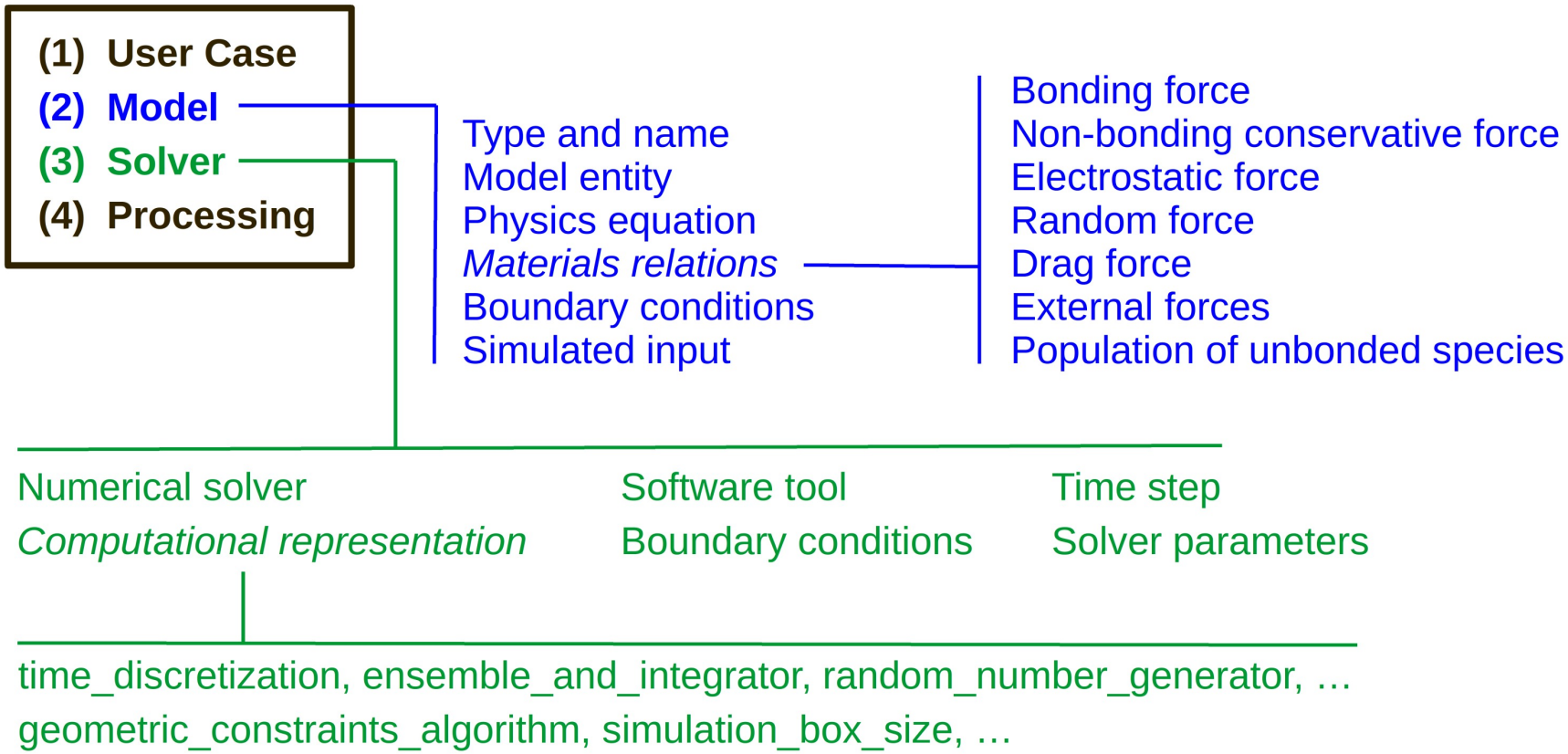
:SOL_ACCURACY_PROP a :validation_proposition;
:has_confidence :STATEMENT_OF_BELIEF;
:has_qualification :EXPECTATION;
:has_content **:SOL_ACCURACY_CONT.**

:SOL_ACCURACY_CONT a :relative_deviation_validation_content;
:asserts_magnitude 0.05;
:refers_to_material :D4_PURE;
:refers_to_property :SPEED_OF_SOUND.

VIMMP
VIRTUAL MATERIALS MARKETPLACE

“Vision”: Standardized subdomain-specific metadata

Example: Data and metadata for molecular dynamics and dissipative particle dynamics



“Policy”: Semantic assets for molecular methods (1/2)

To interoperate with thermodynamic property databases, end-user accessible frontends, and numerical solvers that use thermodynamic data (in particular, process simulation), major efforts need to be directed toward **automatization of bespoke model design**. Thereby, an application engineer first trains a multicriteria optimization engine, which can then choose model parameters autonomously, e.g., based on the rough-set method.

Applications to be built on this basis include an end-user accessible frontend (“app” style) providing estimates for thermodynamic properties of fluids from molecular modelling. The user does not need any concrete knowledge of the molecular models.

The suitable molecular and mesoscopic model classes are **data-informed physics-based models**, or physics-informed data-based models. Models which are only data-based (correlations) or only physics-based (ab initio) cannot **extrapolate and predict data reliably**, which is typically the main requirement. The distinction between data-based and physics-based models, up to now quite rigid in EMMC/RoMM terminology, will need some nuance.

“Policy”: Semantic assets for molecular methods (2/2)

To interoperate with thermodynamic property databases, end-user accessible frontends, and numerical solvers that use thermodynamic data (in particular, process simulation), major efforts need to be directed toward **automatization of bespoke model design**.

The European Materials Modelling Ontology needs to be supplemented to capture all aspects of modelling and simulation. The **MODA Workflow Graph Language** is an excellent point of departure; it permits the description of complex simulation workflows. So far, MODA has not attained the required level of formalization – it needs to be developed into an Ontology for Simulation, Modelling and Optimization.

Beyond the ontological level of reasoning, a **quantitative epistemological calculus**, defined over modelling and simulation workflows, needs to be developed for model validation and uncertainty quantification.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907.

UK Research
and Innovation

Science & Technology
Facilities Council

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