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# Marketplace Development for Modelling and Simulation of Materials – VIMMP Project



## VIMMP

VIRTUAL MATERIALS  
MARKETPLACE

NanoDome Conference

4th September 2018

Cambridge, UK

# Virtual Materials Marketplace: VIMMP (Horizon 2020)

## ■ H2020 Project

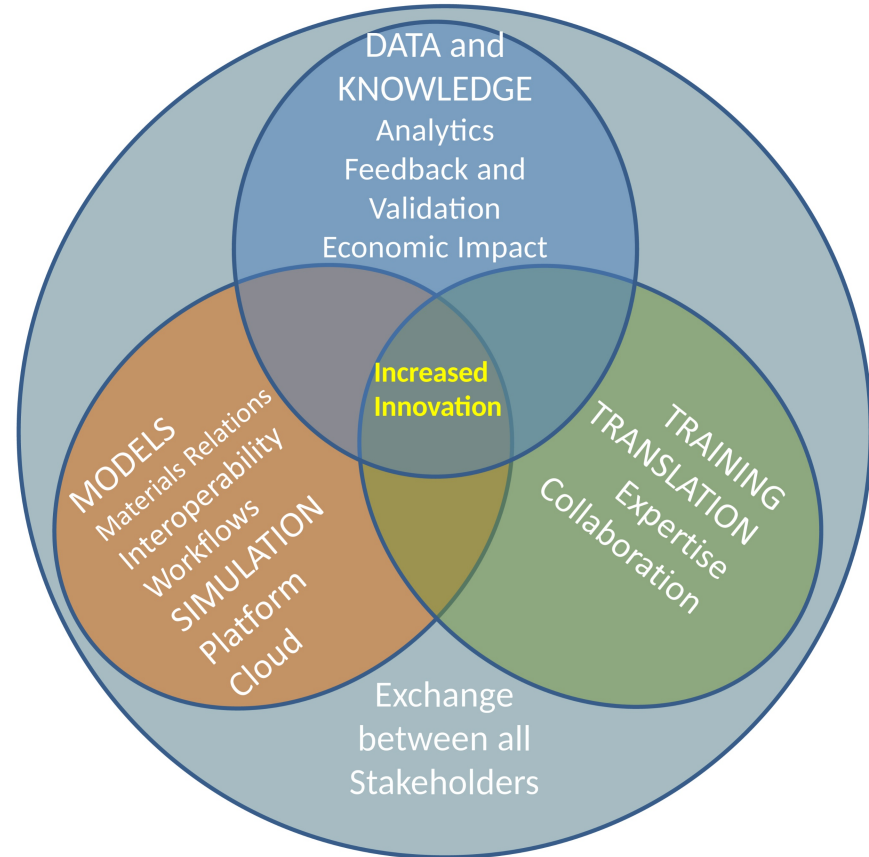
Virtual Materials Marketplace  
VIMMP (GA 760907)

H2020 (NMBP-25-2017)

- The **VIMMP Marketplace** will be a user-friendly hub that provides:

**Effective use of materials modelling** (by a wide spectrum of participants),  
facilitating an **accelerated speed of development** and market deployment for materials.

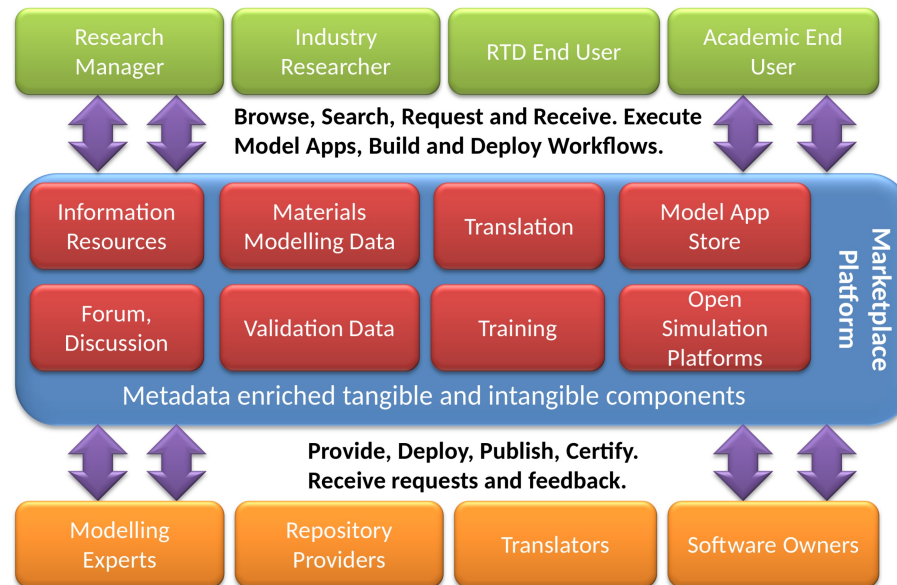
*This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 760907*





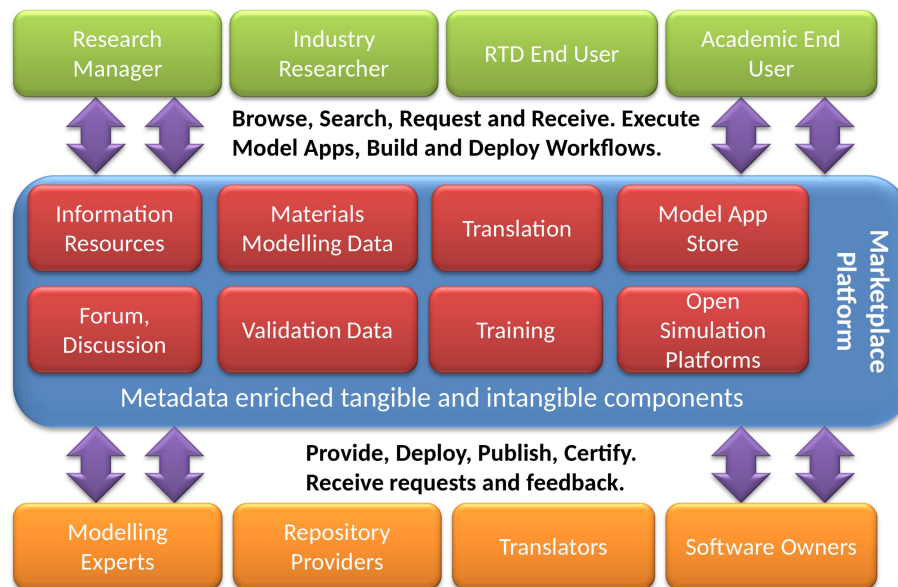
# Virtual Materials Marketplace: VIMMP (Horizon 2020)

**VIMMP Marketplace** concept: To serve its participants and facilitate exchange, e.g., between materials model providers, industrial & academic client end users, and translators.



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**VIMMP Marketplace** concept: To serve its participants and facilitate exchange, e.g., between materials **model providers**, industrial & academic **client** end users, and **translators**.



The **VIMMP Marketplace** will provide end-user interfaces to information resources, discussion forums, databases and repositories, translation and training services, validated models and modelling software, and the ability to utilise open simulation platforms to build and deploy workflows via cloud-based computing resources.

# Virtual Materials Marketplace: VIMMP (Horizon 2020)

Coordination: **Fraunhofer IFAM, Bremen**



Science & Technology  
Facilities Council

UK Research  
and Innovation



Goldbeck Consulting, Cambridge

Politecnico di Torino

UKRI Science and Technology Facilities Council

University of Manchester

Centre Européen de Calcul Atomique et Moléculaire, EPFL Lausanne

Institute of Chemical Process Fundamentals, Prague

Electricité de France, Paris



Osthus, Aachen



**VIMMP**

VIRTUAL MATERIALS  
MARKETPLACE

Continental Reifen Deutschland, Hanover

Unilever, Vlaardingen



INRIA Sophia Antipolis Méditerranée



Università degli Studi di Napoli Federico II



UNIVERSITÀ DEGLI STUDI DI NAPOLI  
**FEDERICO II**

Straetmans High TAC, Hamburg

CULGI BV, Leiden

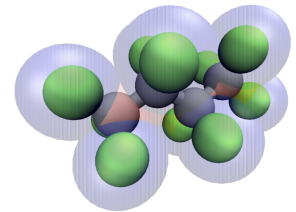
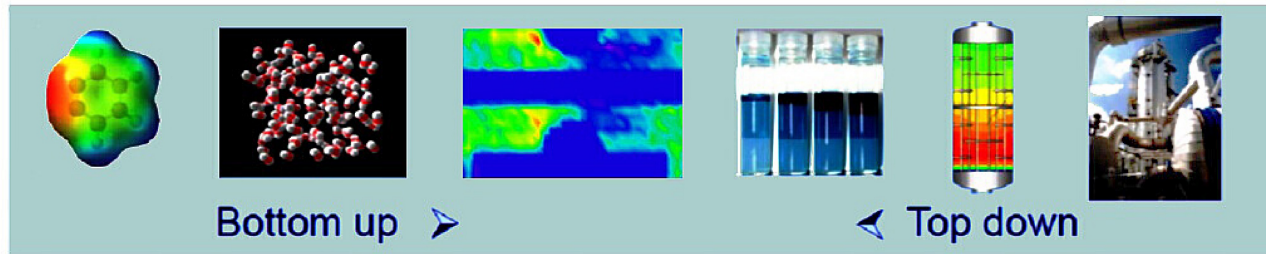


IBM United Kingdom, Portsmouth

IBM Research, Rueschlikon



# Physics-based and data-based modelling of materials



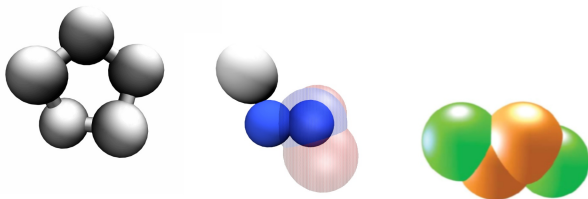
**physics-driven aspects  
(qualitative validity)**



**data-driven aspects  
(quantitative reliability)**

- Realistic representation of the underlying physical features

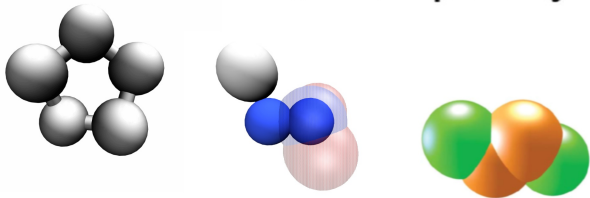
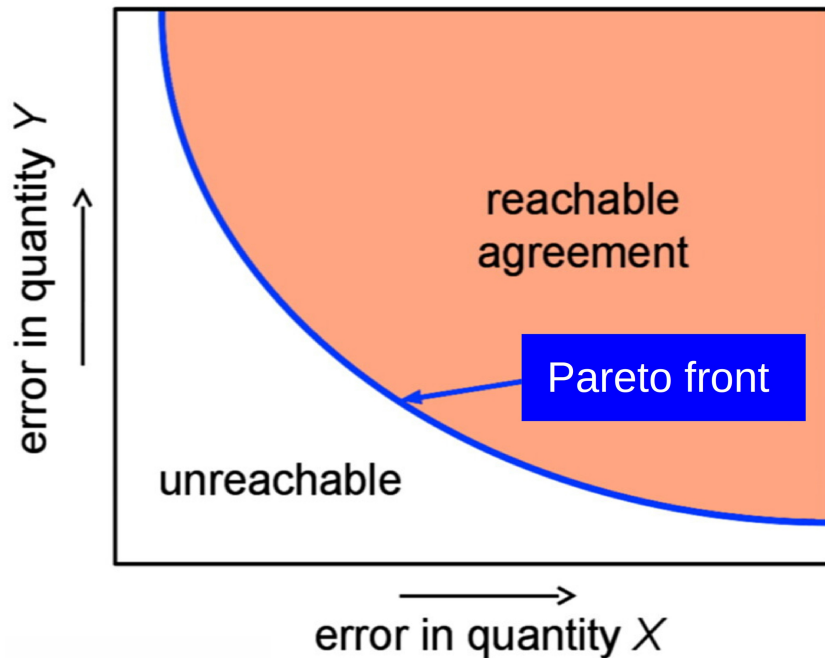
- Models with free parameters, which can be adjusted to experimental data
- Reliable interpolation, extrapolation and prediction of thermophysical properties



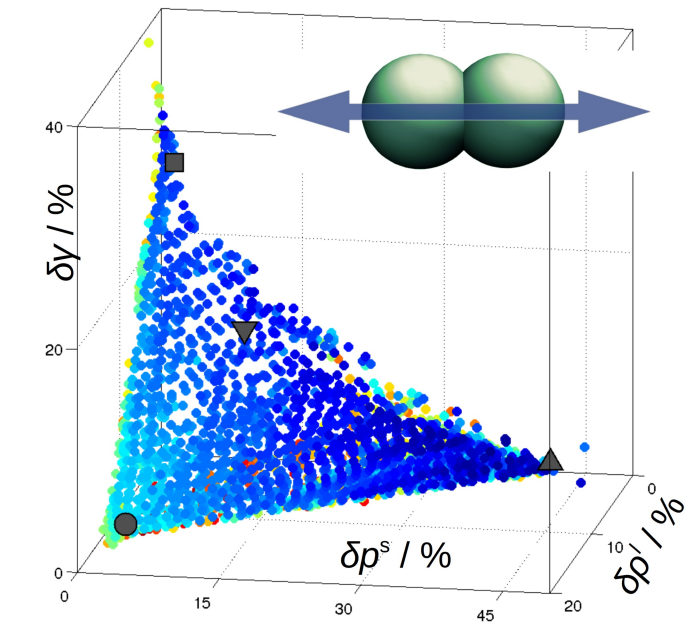


# Model optimization and uncertainty quantification

## Multidimensional objective space



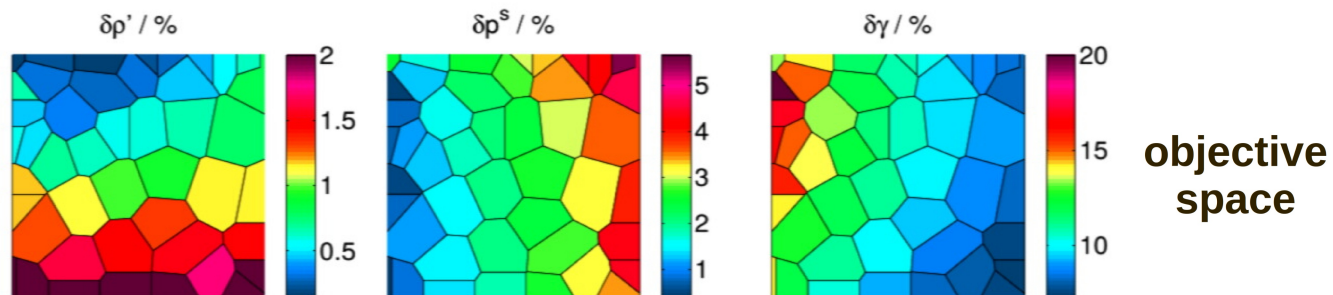
## Example: 2CLJQ molecular models of carbon dioxide



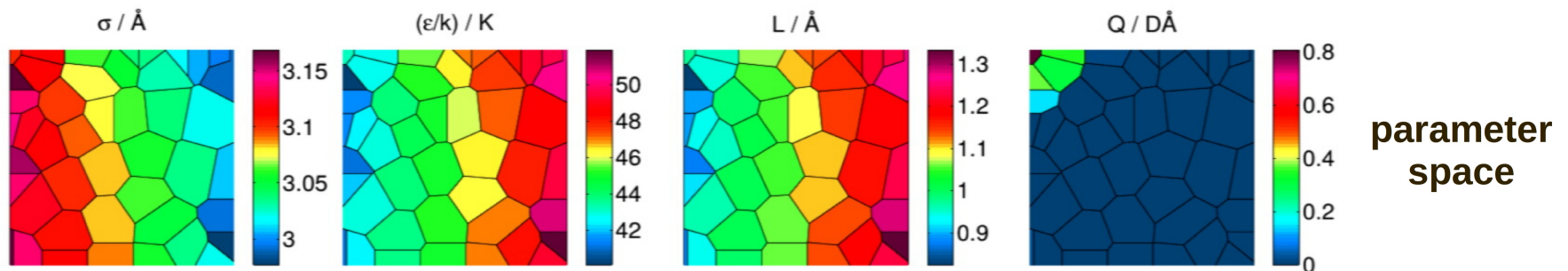


# Bespoke model parameterization for a user case

**Self-organized patch plots<sup>1</sup>** visualizing the Pareto front and the Pareto-optimal models:



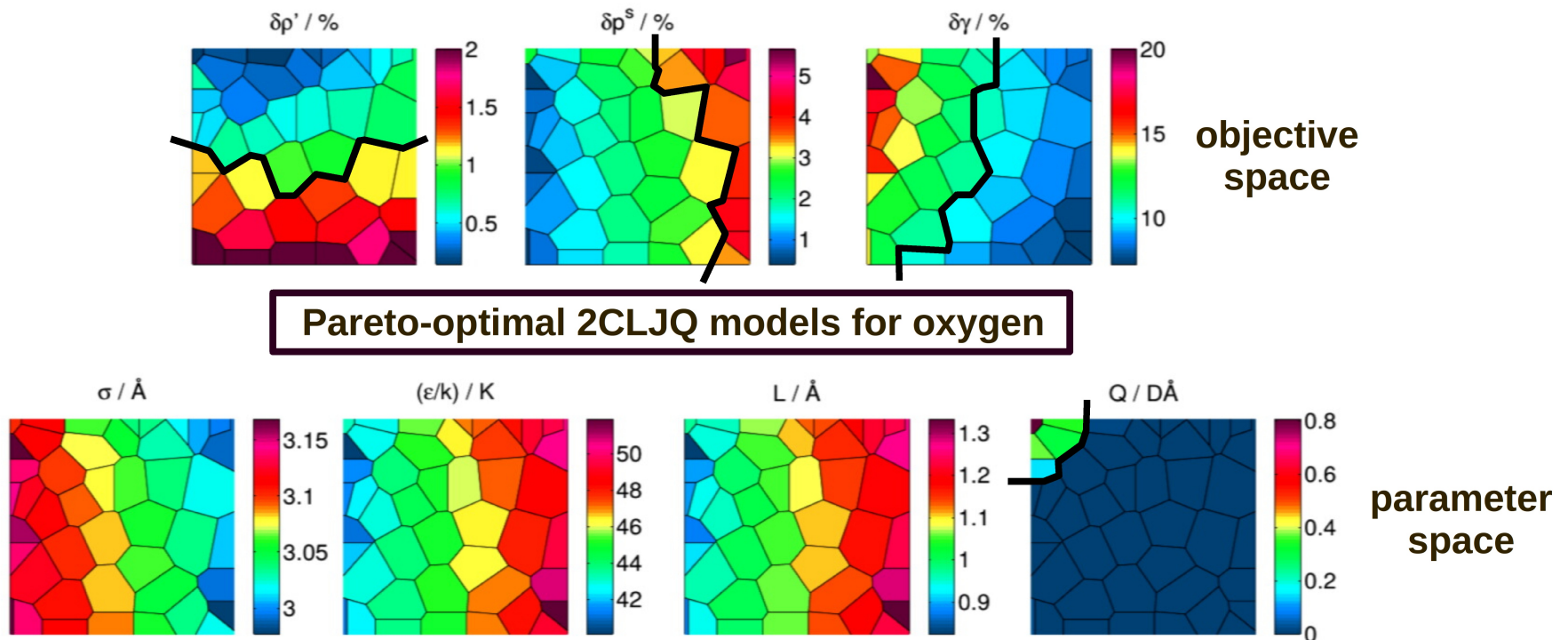
## Pareto-optimal 2CLJQ models for oxygen



<sup>1</sup>K. Stöbener *et al.*, *Fluid Phase Equilib.* 411, 33 – 42, 2016.

# Bespoke model parameterization for a user case

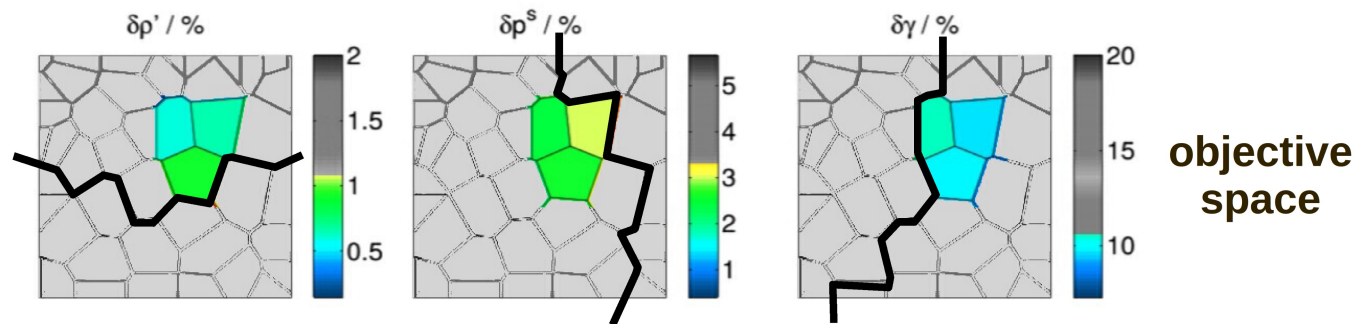
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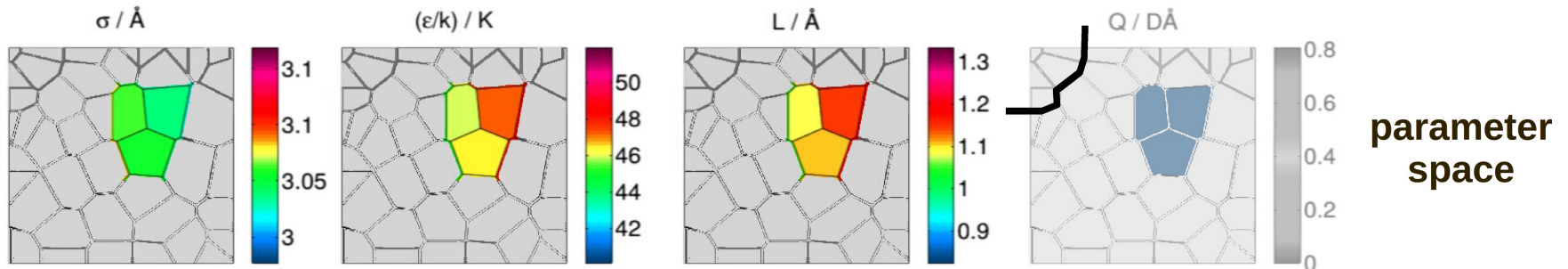
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# Bespoke model parameterization for a user case

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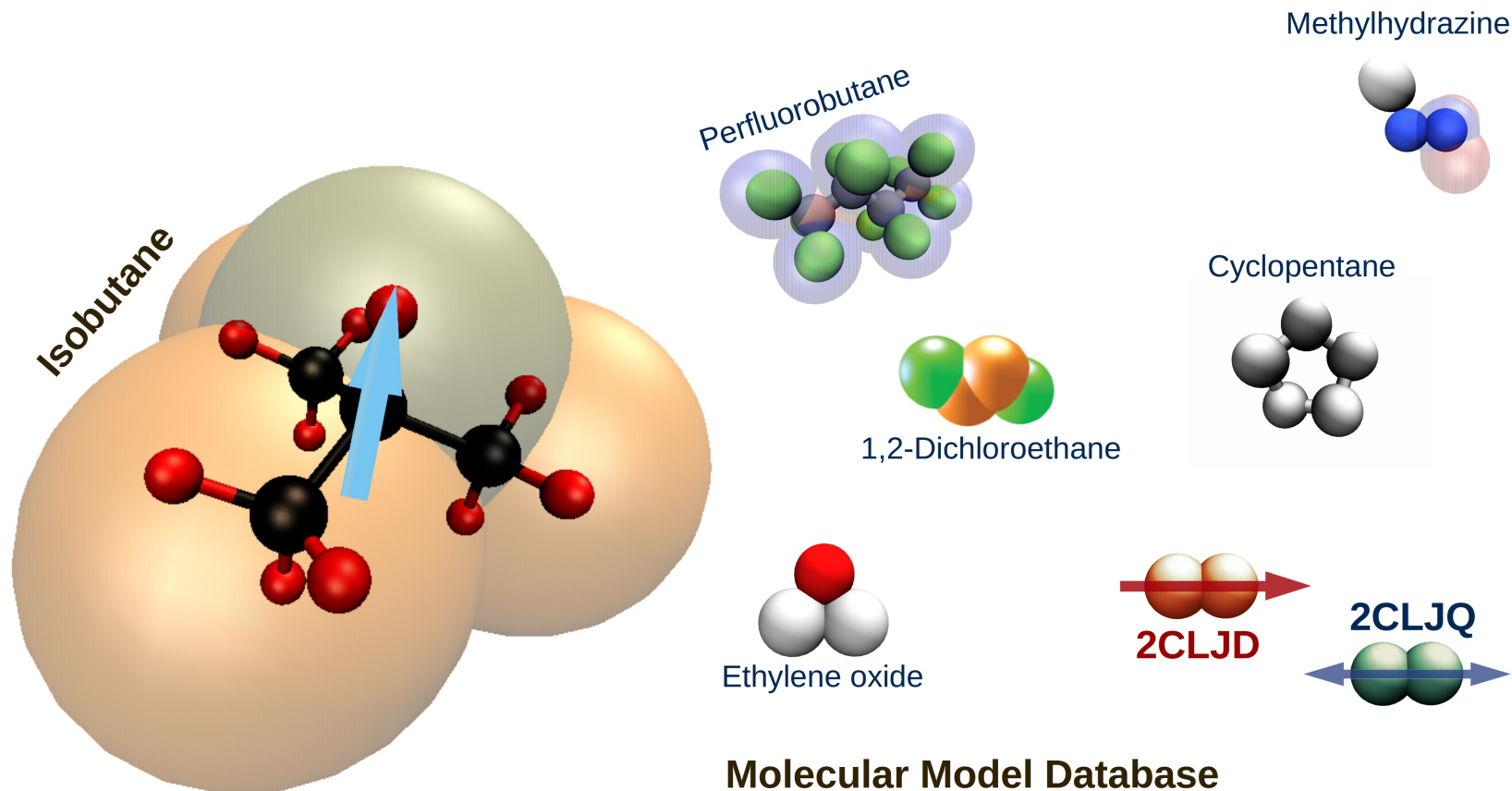


**Pareto-optimal 2CLJ models satisfying all constraints**



<sup>1</sup>K. Stöbener *et al.*, *Fluid Phase Equilib.* 411, 33 – 42, 2016.

# Model data and metadata repositories



**Molecular Model Database**

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

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

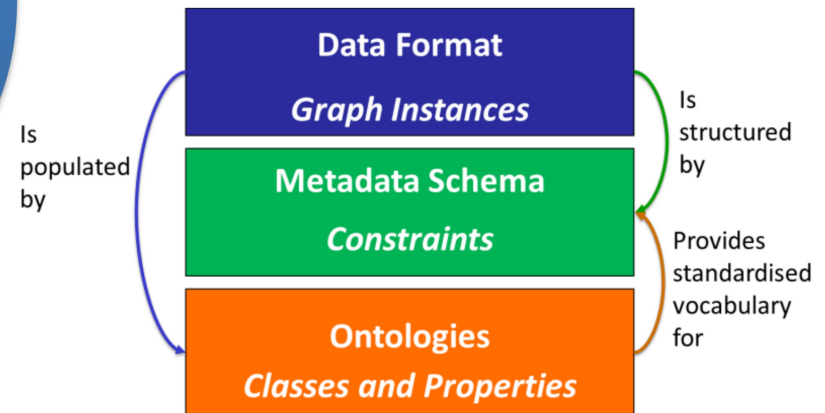


# Semantic interoperability of models and codes



## Marketplace platform

- Web-based portal, semantic platform
- Capabilities including training, translation, simulation software, materials data management, access, and data standards, are provided.





# Developments in materials modelling standardization

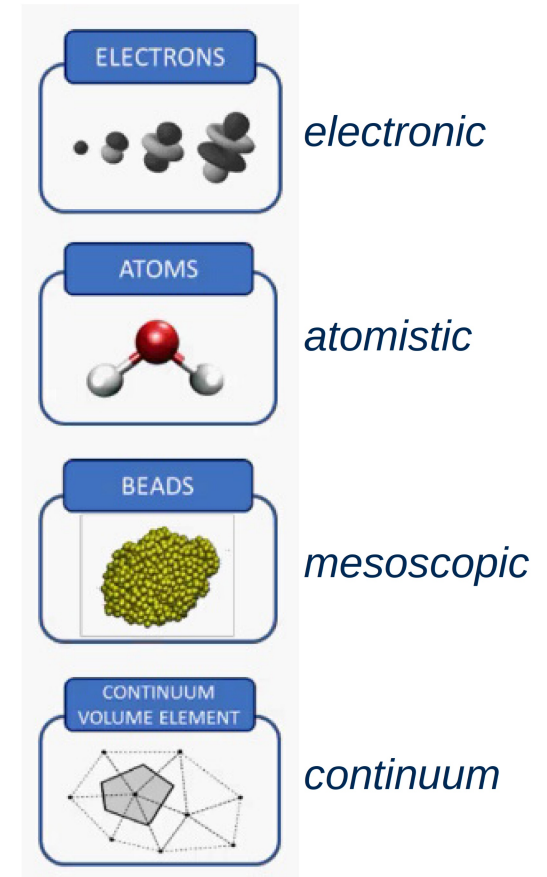
Review of Materials Modelling VI (edited by de Baas), 2017

RoMM VI

Semi-formalized terminology or vocabulary

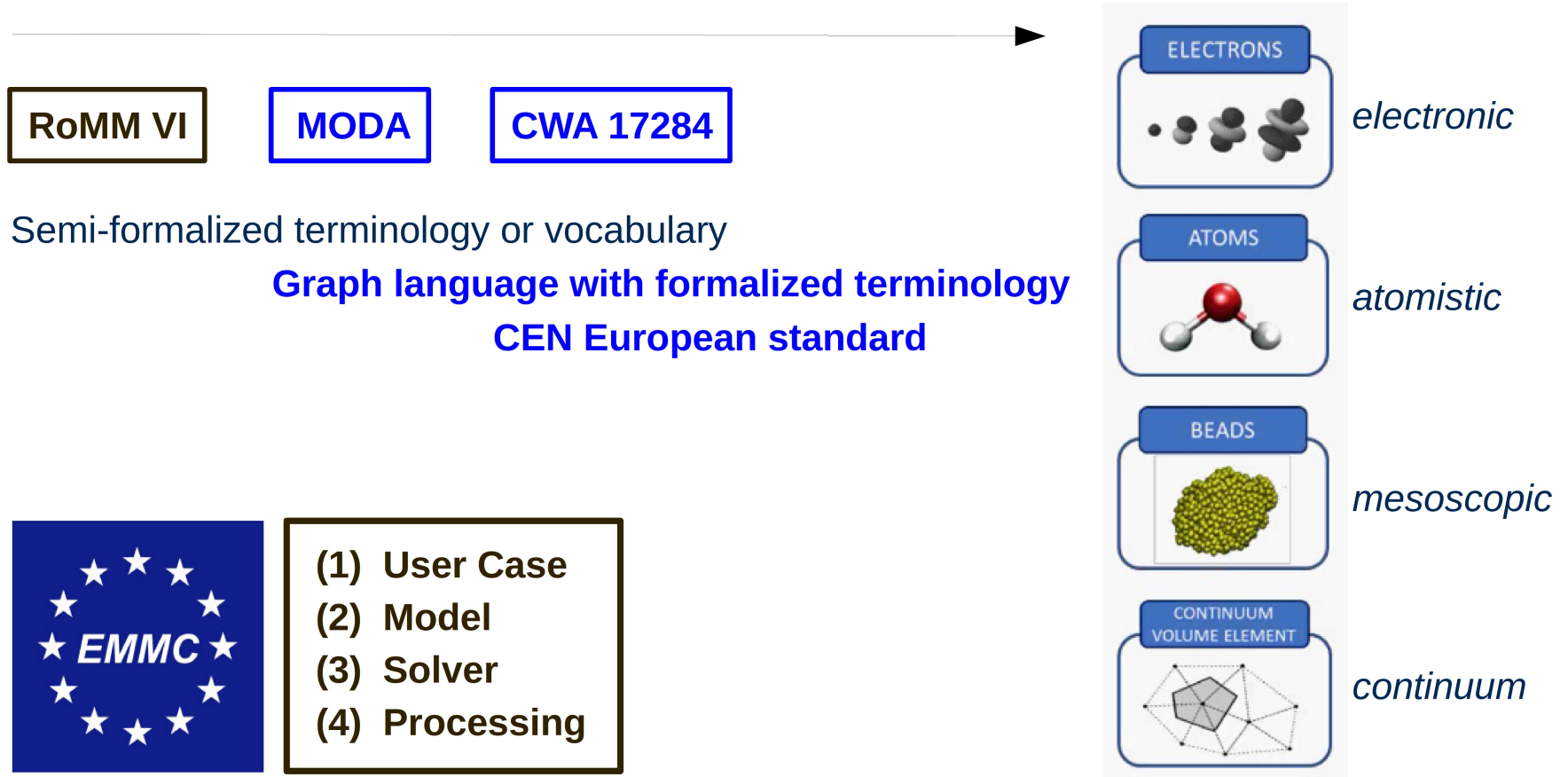
*“What makes a material function?”*

*Let me compute the ways ...”*



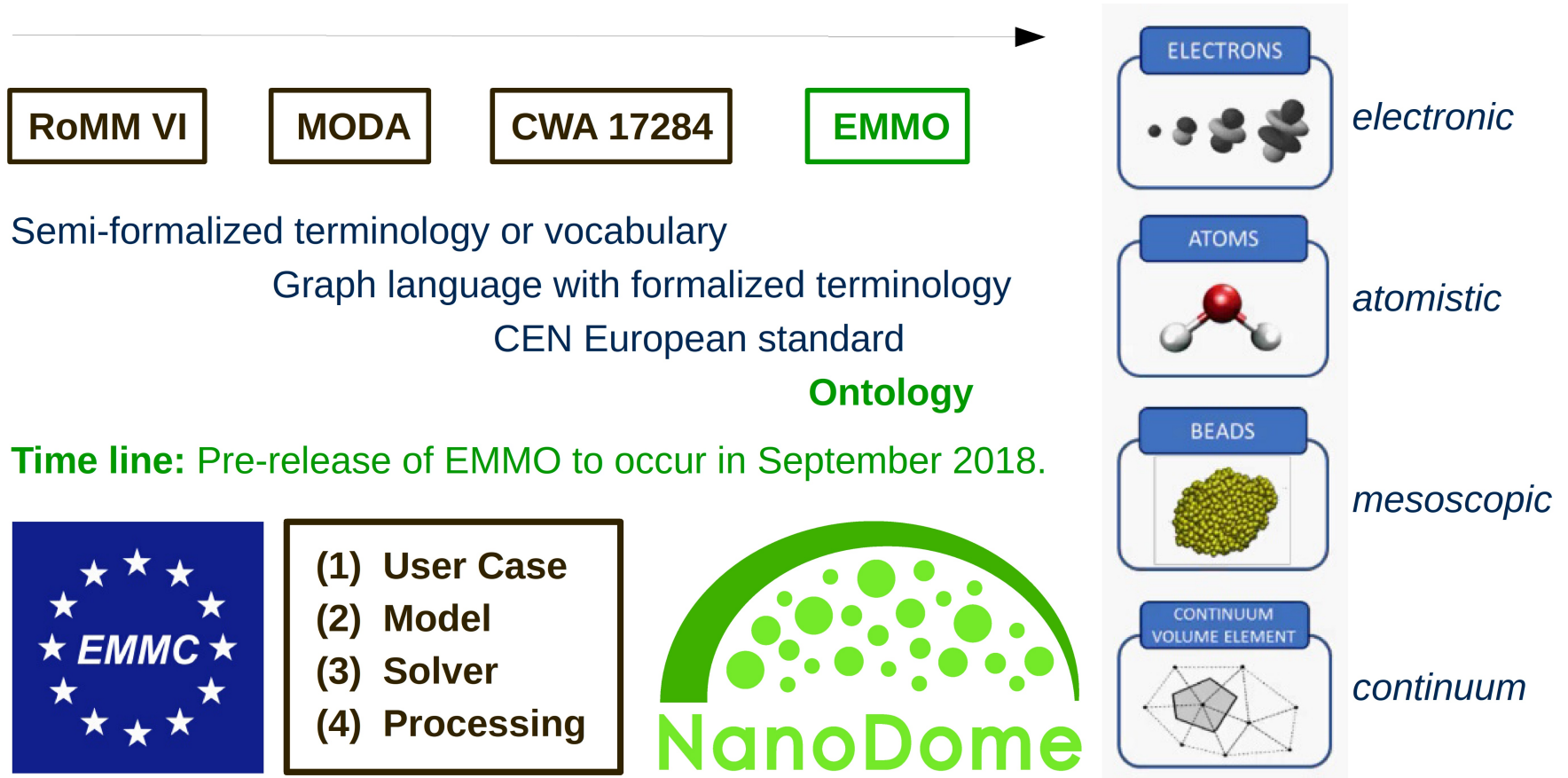
# Developments in materials modelling standardization

MODA: “Modelling Data” graph language & CEN Workshop Agreement 17284 (2018)



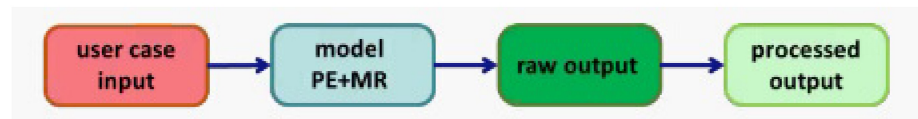
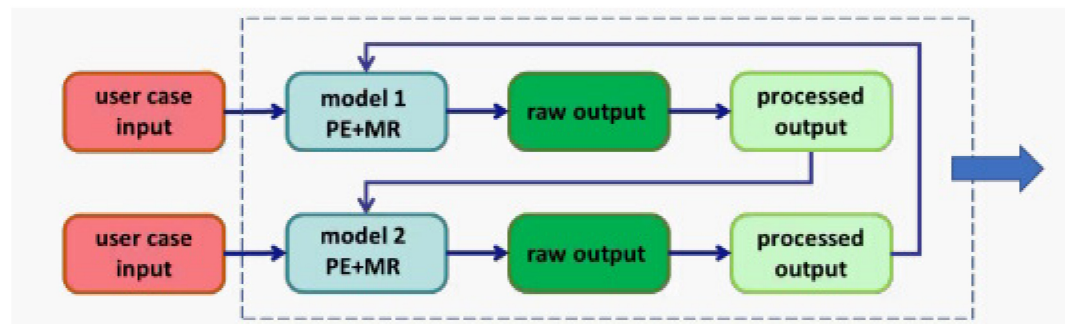
# Developments in materials modelling standardization

EMMO: European Materials Modelling Ontology (Ghedini *et al.*), to appear

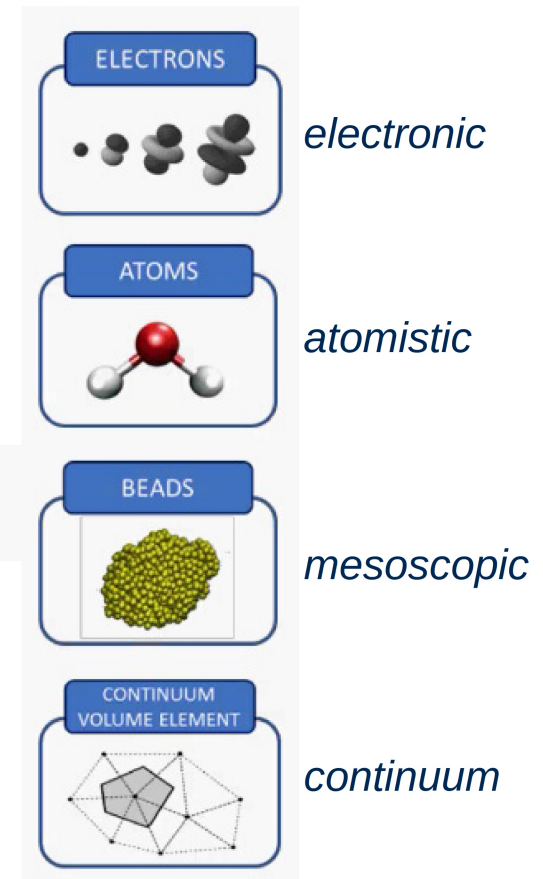


# Diagram representation of simulation workflows

## MODA: “Modelling Data” graph language

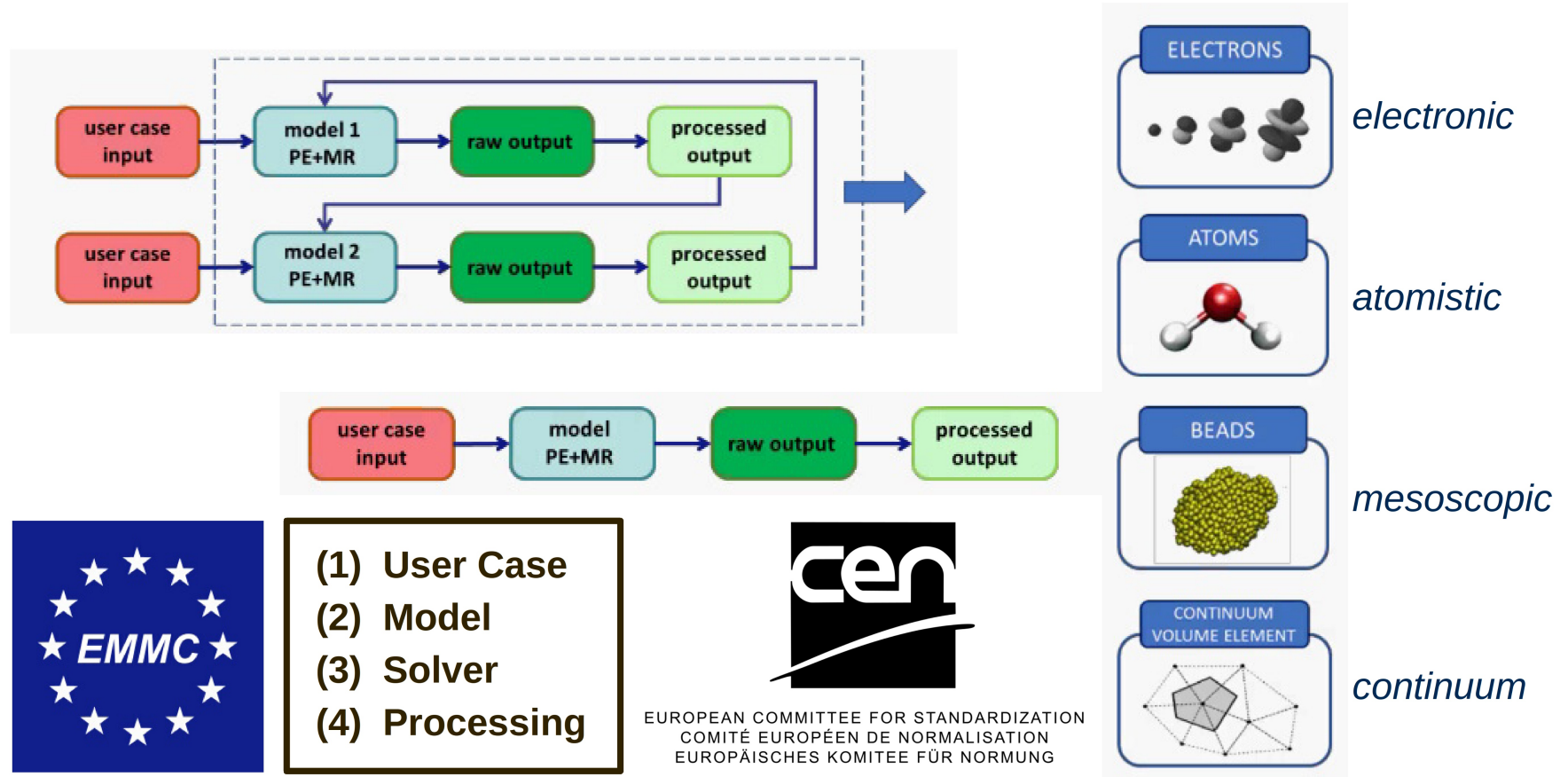


- (1) User Case
- (2) Model
- (3) Solver
- (4) Processing



# Diagram representation of simulation workflows

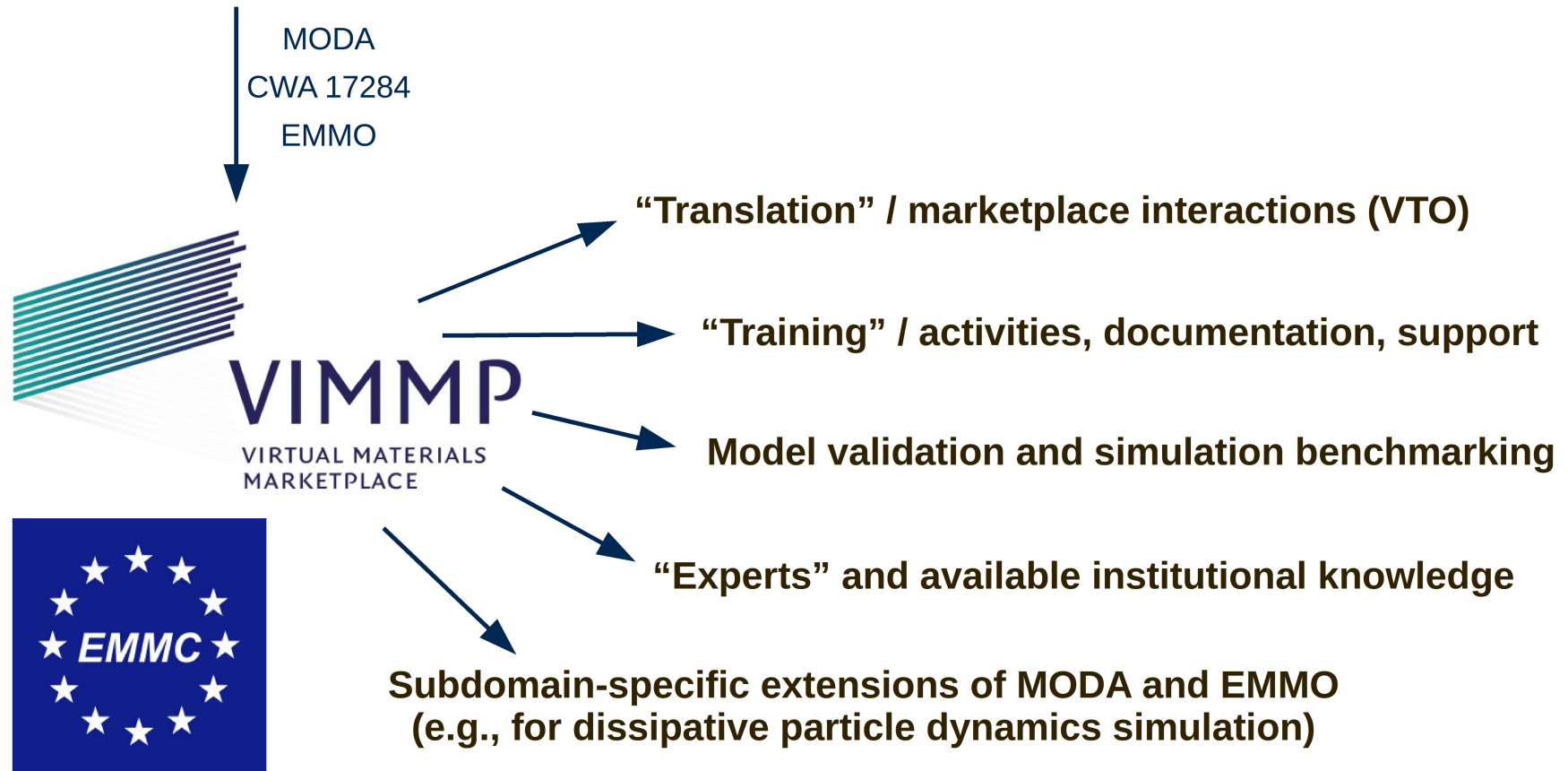
MODA: “Modelling Data” graph language & CEN Workshop Agreement 17824





# Development of ontologies on the basis of MODA

Modelling and simulation of materials (EMMO), developed by Ghedini *et al.*



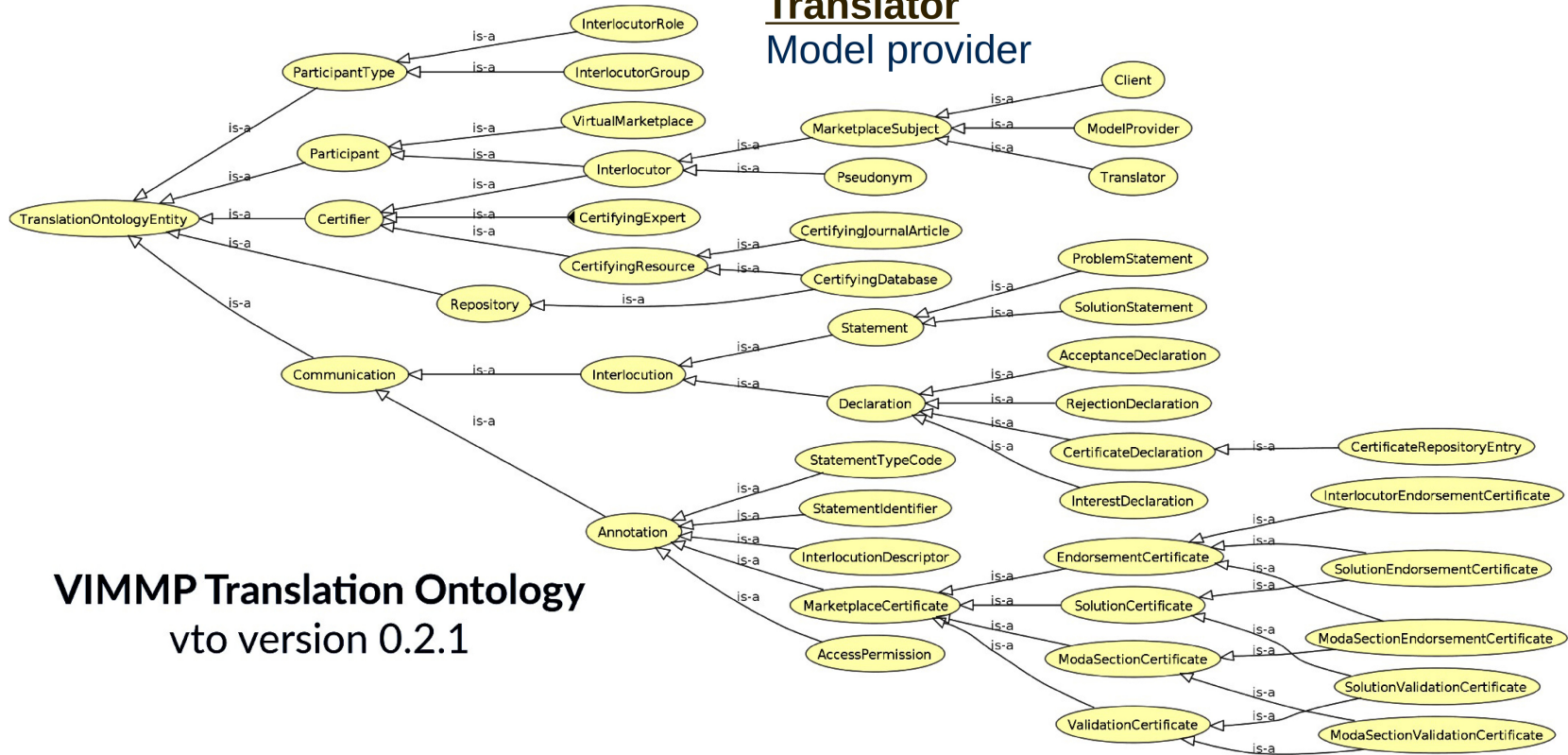
# Development of ontologies on the basis of MODA

**Client:** Problem statement

**Marketplace participants**

**Model provider:** Solution statement

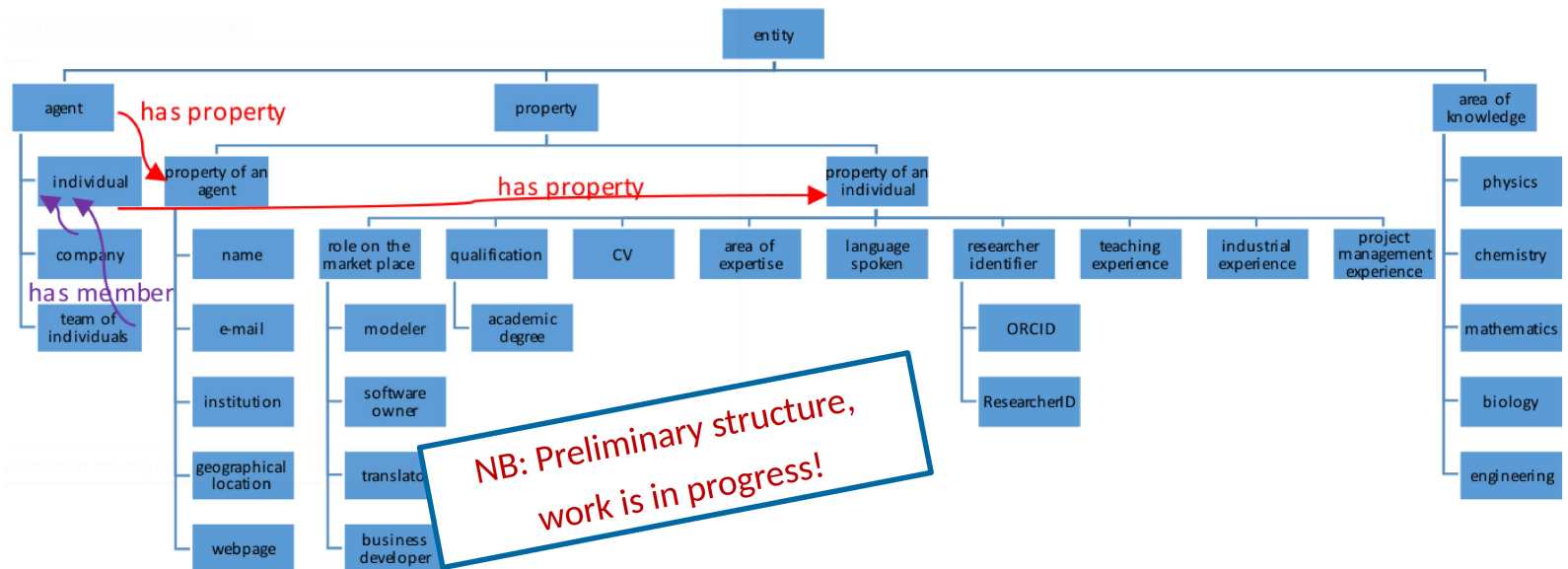
**Client**  
**Translator**  
**Model provider**



**VIMMP Translation Ontology**  
vto version 0.2.1

# Development of ontologies on the basis of MODA

## VIMMP Expert Knowledge Ontology

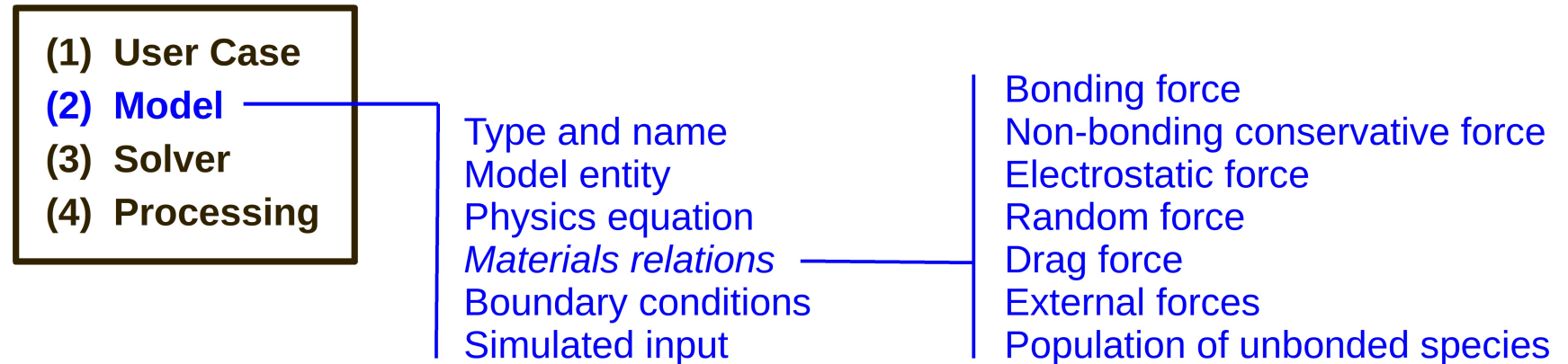


Above: a taxonomy, separating the agents acting on the marketplace from their properties.

We are currently reviewing existing relevant ontologies for branches such as: areas of knowledge, classification of materials and chemical entities, workflows.

# Development of ontologies on the basis of MODA

Modelling and simulation data and metadata for dissipative particle dynamics



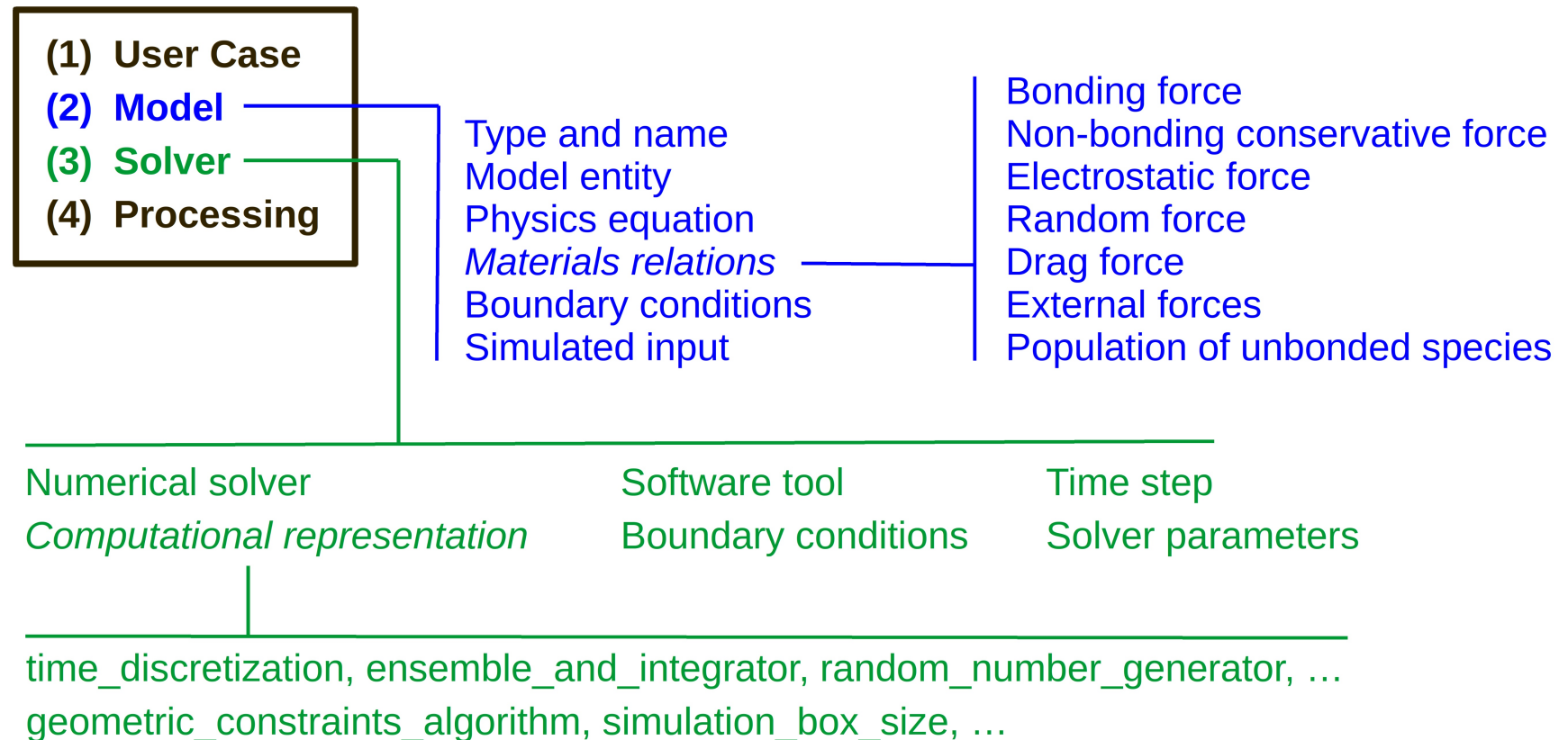
DPD simulation code DL\_MESO

[https://www.scd.stfc.ac.uk/Pages/DL\\_MESO.aspx](https://www.scd.stfc.ac.uk/Pages/DL_MESO.aspx)

Developed by Michael Seaton *et al.* (STFC Daresbury Laboratory)

# Development of ontologies on the basis of MODA

## Modelling and simulation data and metadata for dissipative particle dynamics





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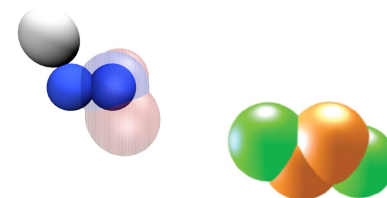
# Verification, validation, and benchmarking

- **Verification of software codes:**
  - Fundamental tests: time integration accuracy, electrostatics, ...
  - Comparisons with exact results (when possible)
  - Comparisons with independent numerical results (same method or others)
  - Existence of a repository, Continuous Integration (CI) of changes
  - Test suite (number of tests, code coverage)
- **Benchmarking of software codes:**
  - Performance, scaling (weak and strong)
  - Ranges of usage (max number of particles, ...)
- **Validation of model parameters:** parameter provider, model, target property, experimental value, reference publication

Note: For some categories we may provide **workflows** in the market place

**Caveat:** With numerical methods, often difficult to disentangle the aspects tested (method, model and code)

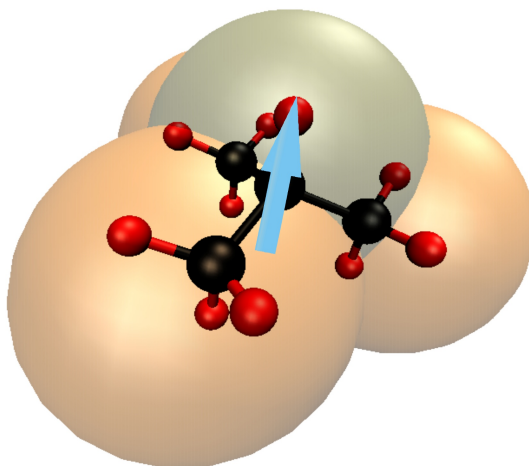
# Paradigm shift in modelling and simulation



## Modelling of materials as an art practised by academic experts

- A very limited community of people is qualified to design materials models;
- for each substance, an expert develops a model, to be looked up from literature;
- it is usually not disclosed how the model was designed and optimized.

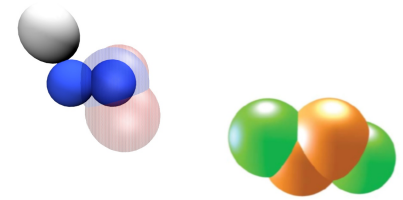
**Users** need a background (e.g., in molecular thermodynamics and statistical mechanics), to assess the model quality, and they **cannot actively contribute** to adjusting the model without repeating the expert work.



Molecular Model Database

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

# Paradigm shift in modelling and simulation



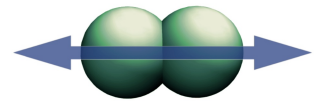
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## Modelling of materials as a technology accessible to all industrial engineers

- Models are flexibly adjustable, e.g., by multicriteria optimization, based on a preceding characterization of the model class;
- bespoke models for specific user cases can be obtained with little effort; or automatically, interoperating with other platforms (e.g., process simulation)
- reliable statements on the model uncertainty are available to the user.



**Users** who may not possess a background in materials modelling and simulation are enabled to **actively guide** modelling and simulation practice – supported by “**translators**”.

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