OSMO: Ontology for Simulation, Modelling, and Optimization

M. Horsch,[1, 2, 3] D. Toti,[4, 5] S. Chiacchiera,[2] M. Seaton,[2] G. Goldbeck,[5] I. Todorov[2]

High Performance Computing Center Stuttgart,[1] UKRI STFC Daresbury Laboratory,[2] University of Central Lancashire,[3] Catholic University Brescia,[4] Goldbeck Consulting Ltd.[5]

Digitalization in materials modelling

European Materials Modelling Council (EMMC ASBL)

https://emmc.eu/

The non-profit association EMMC ASBL was created in 2019 to ensure the continuity, growth, and sustainability of community activities for modellers, materials data scientists, software owners, materials modelling translators, and manufacturers in Europe. The EMMC regards the **integration of materials modelling and digitalization** as critical for an advancement of industrial process and product design.

EMMC Focus Area Digitalization

In computational engineering, digitalization encompasses aspects of representing, managing, accessing, and utilizing digital information about products, components, materials, their behaviour, and their processing.

EMMC-guided metadata standardization

Community-governed development of metadata standards

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

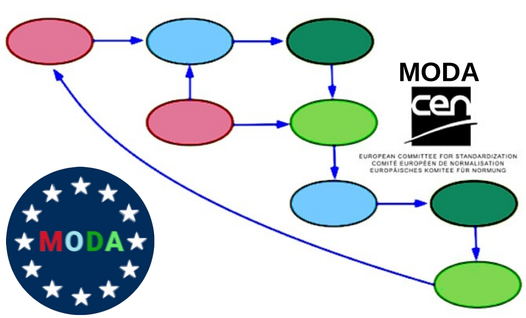
Review of Materials Modelling (compendium)

MODA (Model Data) tables & graphs

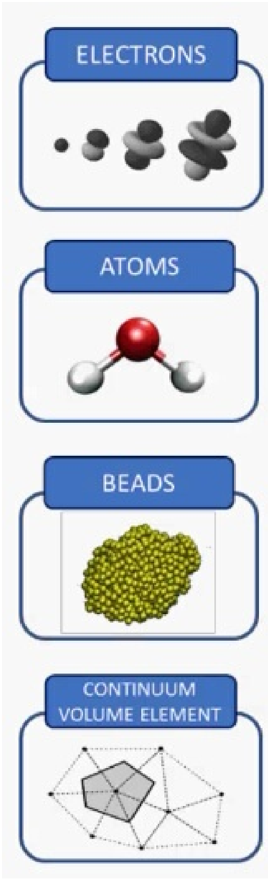
CEN workshop agreement

Domain ontologies

EMMO top-level ontology



OSMO



electronic

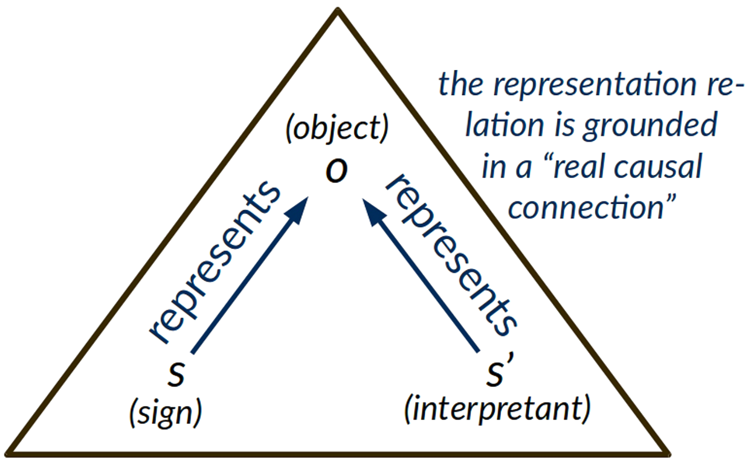
atomistic

mesoscopic

continuum

EMMC-guided ontology design: Foundational ontology

Peircean semiotics



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

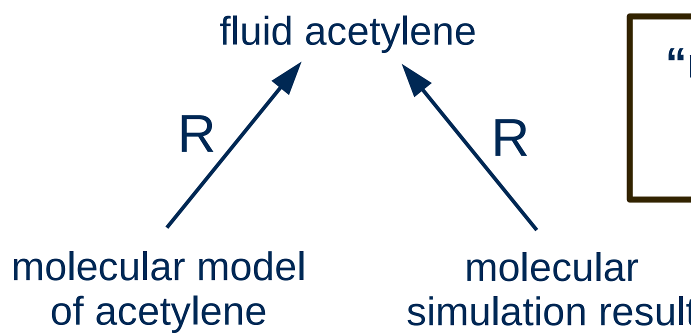
C. S. Peirce

Elementary Multiperspective Material Ontology[1, 2]

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

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

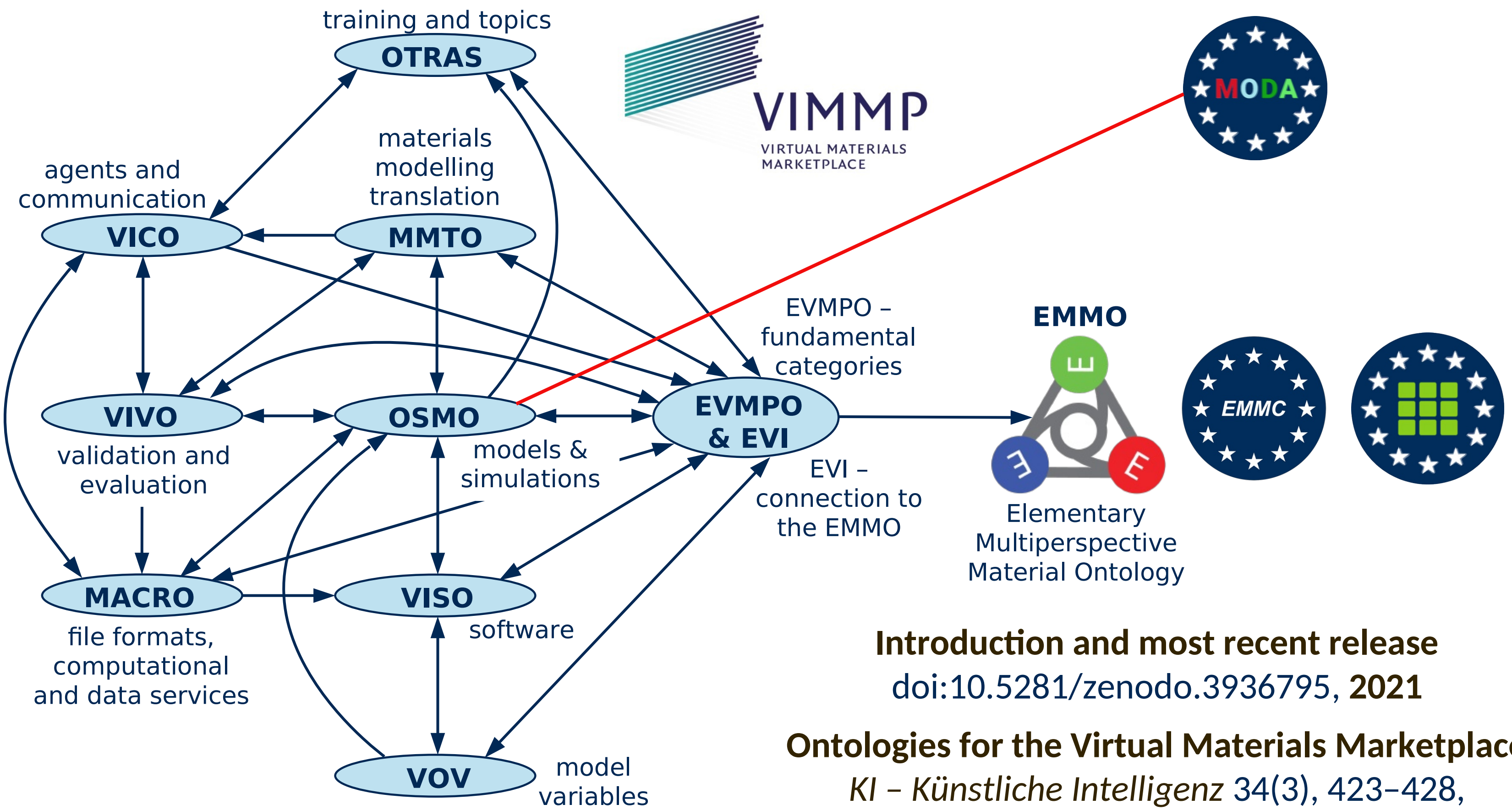
3) **Semiotics:**
   Representation of physical entities by signs



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

[1]J. F. Morgado, E. Ghedini, G. Goldbeck, *et al.*, *Proc. SeDiT 2020*, **2020**.
[2]H. Preisig, T. Hagelien, J. Friis, *et al.*, *Proc. WCCM-ECCOMAS 2020*, **2021**.

EMMC-guided ontology design for materials modelling



Introduction and most recent release
doi:10.5281/zenodo.3936795, **2021**

Ontologies for the Virtual Materials Marketplace
KI – Künstliche Intelligenz 34(3), 423–428,
doi:10.1007/s13218-020-00648-9, **2020**

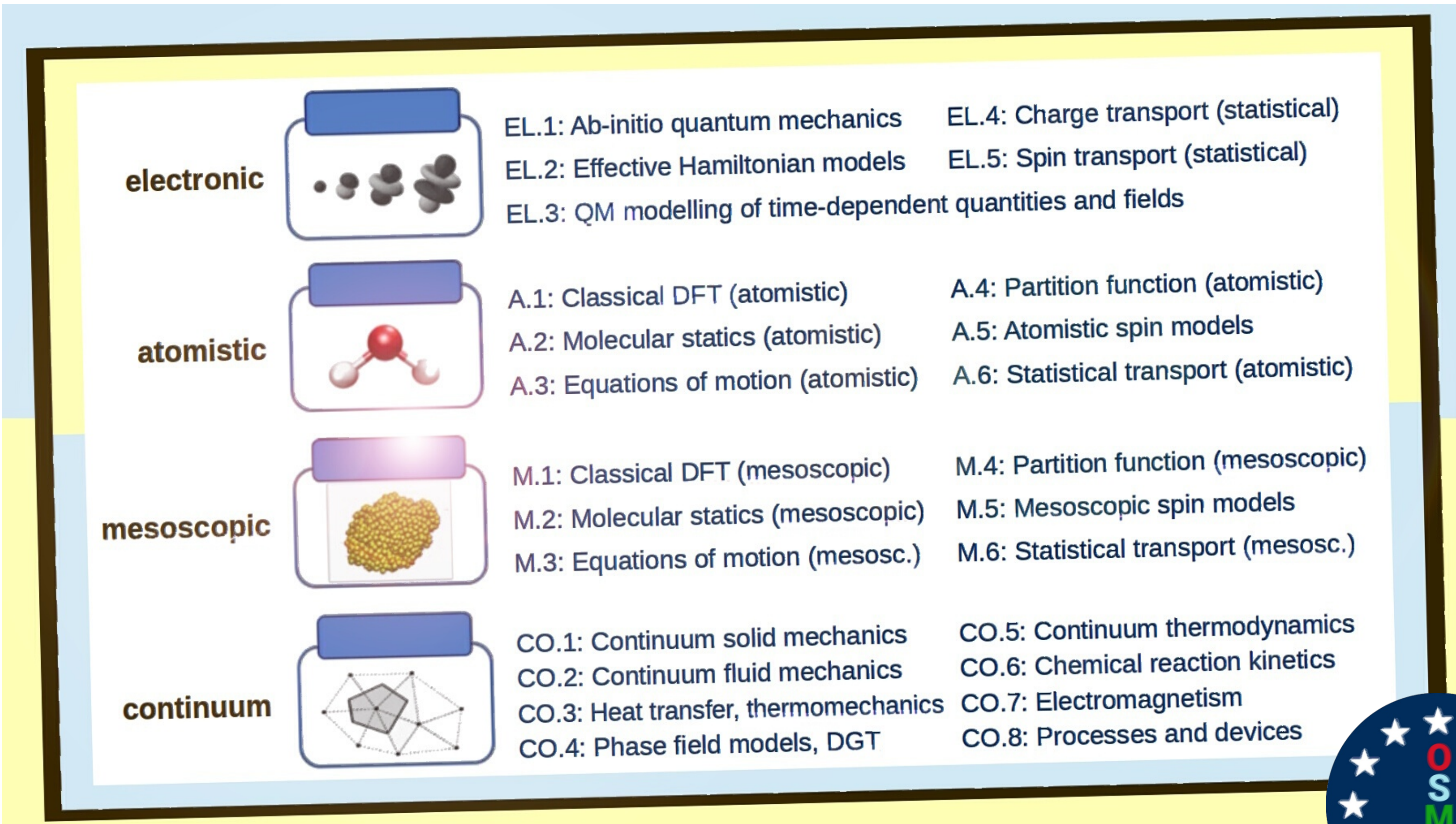
Science and Technology Facilities Council

VIMMP
VIRTUAL MATERIALS MARKETPLACE

Universität Stuttgart

HLRS

Simulation data provenance[1] on the basis of RoMM[2]

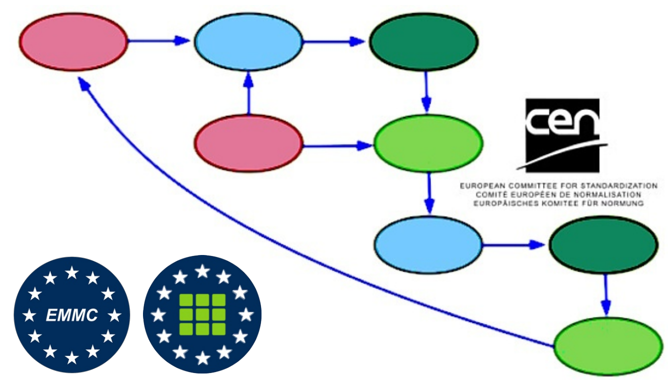


[1]*Journal of Chemical & Engineering Data* 65, 1313, doi:10.1021/acs.jced.9b00739, **2020**.
[2]A. F. de Baas (ed.), *What Makes a Material Function?*, ISBN 978-92-79-63185-6, **2017**.

OSMO

Simulation data provenance using MODA

3	Solver and Computational translation of the specifications		
3.1	Numerical Solver		*Please give name andtype of the solver* *e.g. Monte Carlo, SPH, FE, ...iterative, multi-grid, adaptive,...*
3.2	Software tool		*Please give the name and if this is your own code, please specify if it can be shared with an evt link to website/publication.*
3.3	Time step		*If applicable, please give the time step used in the solving operations.* *This is the numerical time step and this is not the same as the time lapse of the case to be simulated (see 1.4)*
3.4	Computational Representation	Physics Equation, Material Relations, Material	*Computational representation of the physics equation, materials relation and material.* *There is no need to repeat user case info.* *"Computational" means that this only needs to be filled in when your computational solver represents the material, properties, equation variables, in a specific way.*
3.5	Computational boundary conditions		*If applicable.* *Please note hat these can be translations of the physical boundary conditions set in the user case or they can be pure computational. (e.g. a unit cell with mirror b.c. to simulate an infinite domain).*
3.6	Additional Solver Parameters		*Please specify pure internal numerical solver details (if applicable), like* • *Specific tolerances* • *Cut-offs, convergence criteria* • *Integrator options*



MODA cover — overview

MODA section 1 — use case

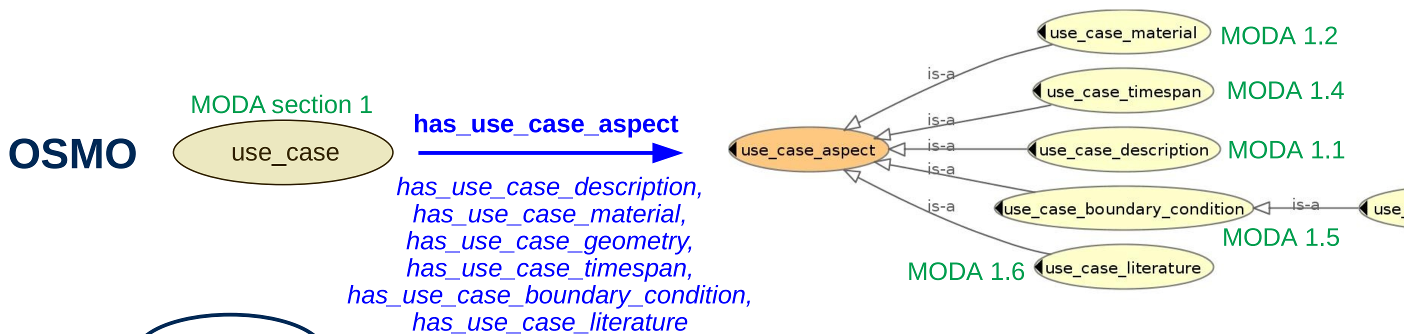
MODA section 2 — model

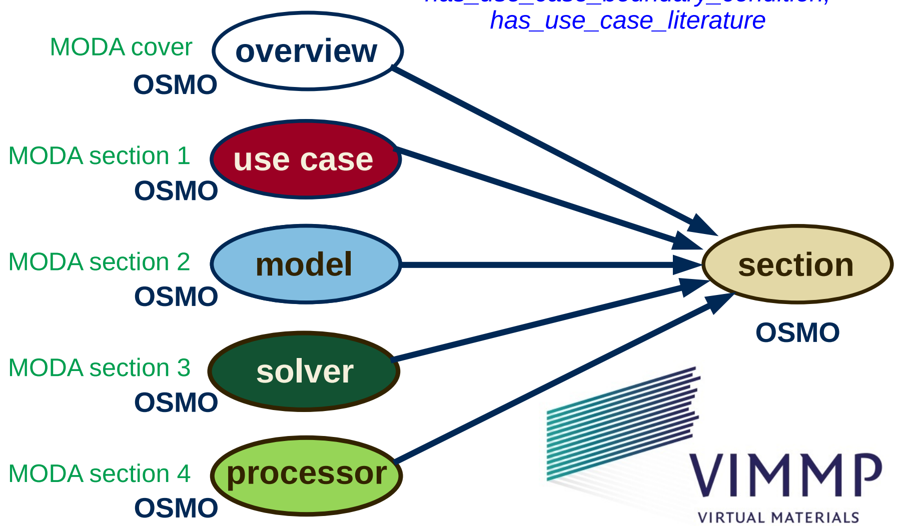
MODA section 3 — solver

MODA section 4 — processor

MODA

Simulation data provenance





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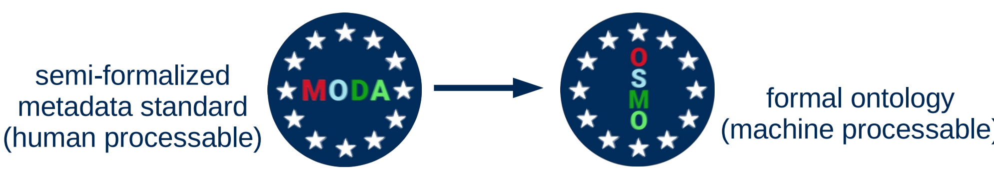
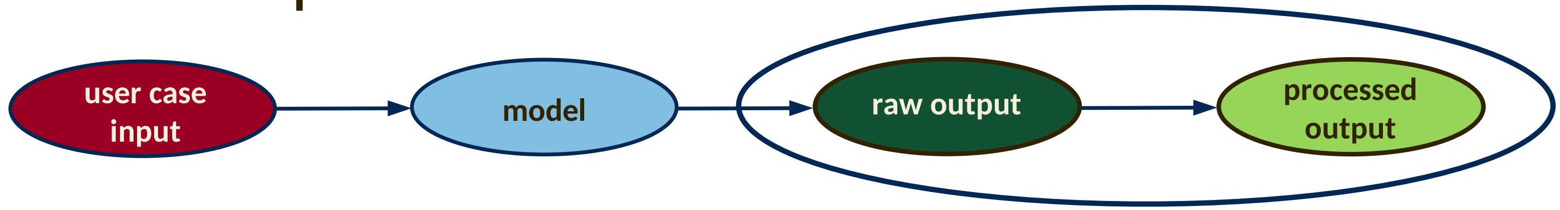


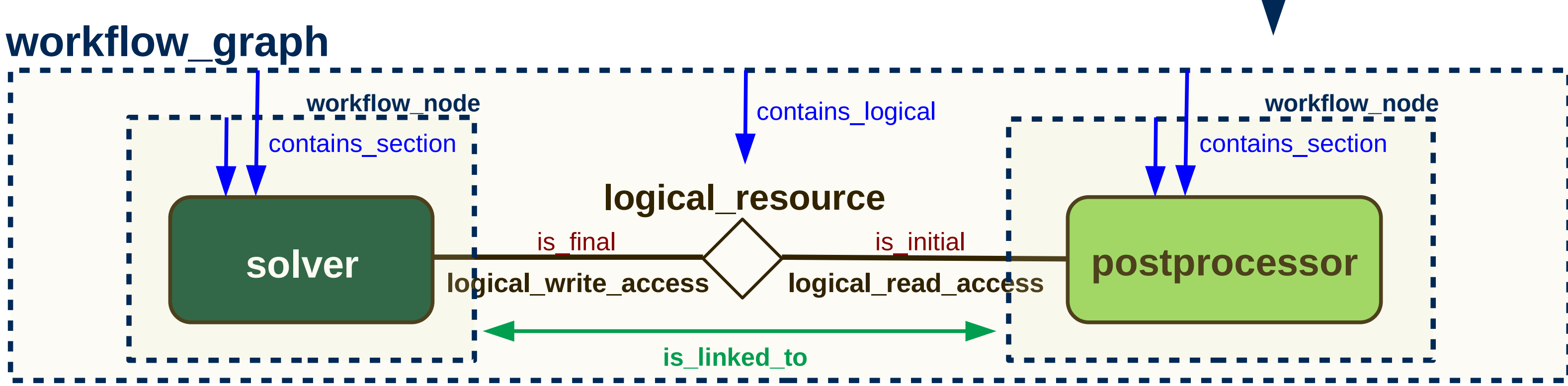
Simulation data provenance

MODA

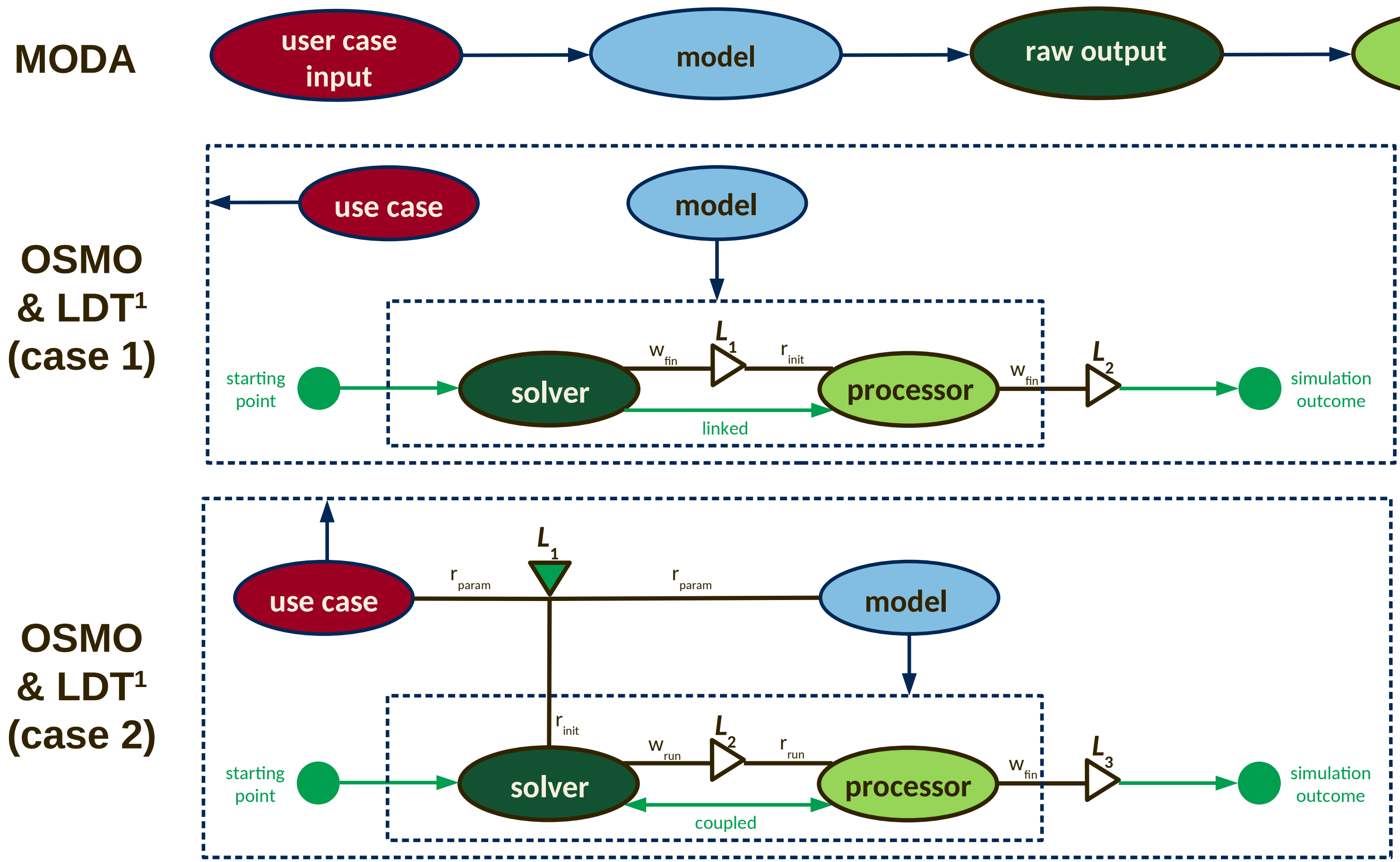


"What is the exact meaning of the blue arrows?"

OSMO: Characterization of workflow semantics by logical data transfer (LDT) graphs



Simulation data provenance using OSMO and LDT graphs



[1]*Journal of Chemical & Engineering Data* 65, 1313–1329, doi:10.1021/acs.jced.9b00739, **2020**.

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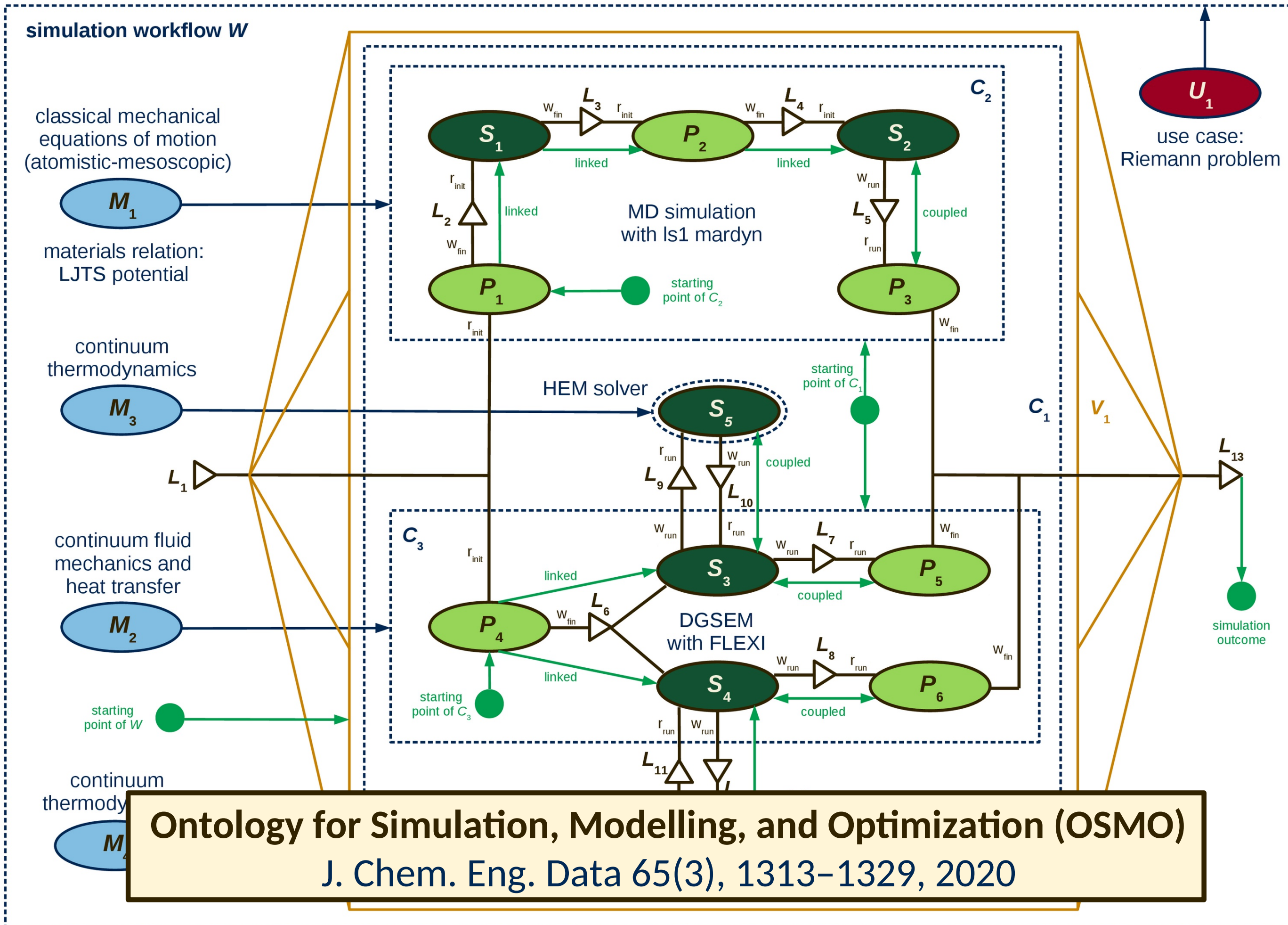
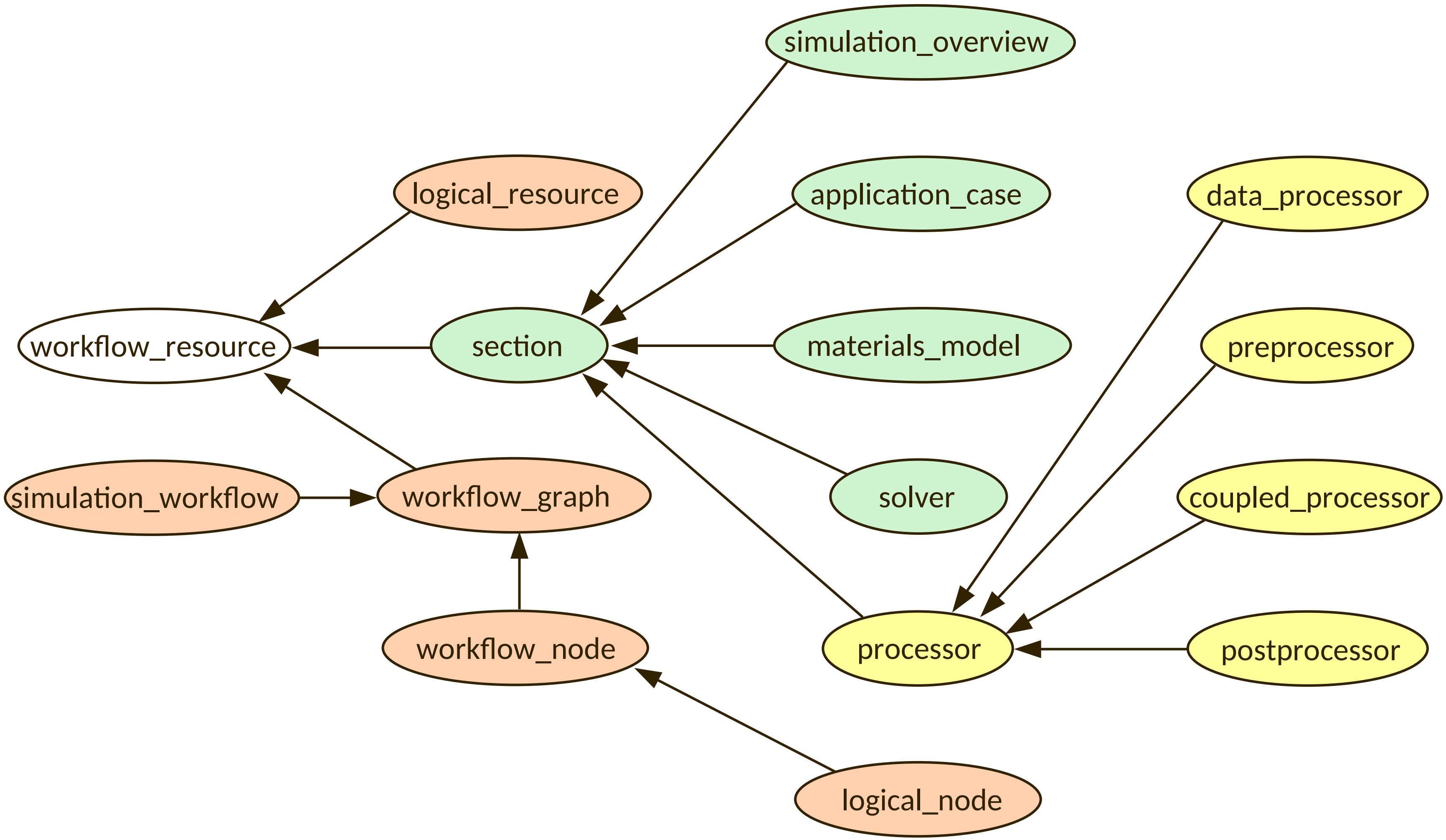


Ontology for Simulation, Modelling, and Optimization (OSMO)
J. Chem. Eng. Data 65(3), 1313–1329, 2020

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.

Workflow resource branches of OSMO



Knowledge representation in molecular modelling

Geometry

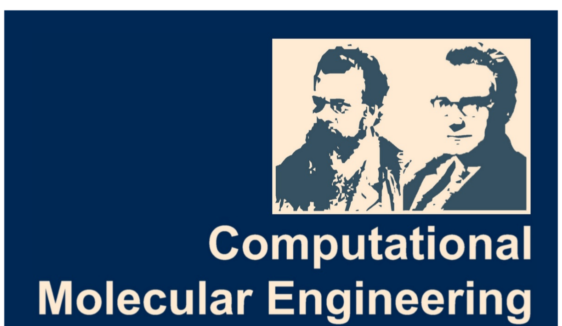
Types and positions of interaction sites

Dispersion and repulsion

Lennard-Jones or Mie potential:
Size and energy parameters

Electrostatics

Point charge or multipole (point dipole or quadrupole):
Magnitude and orientation



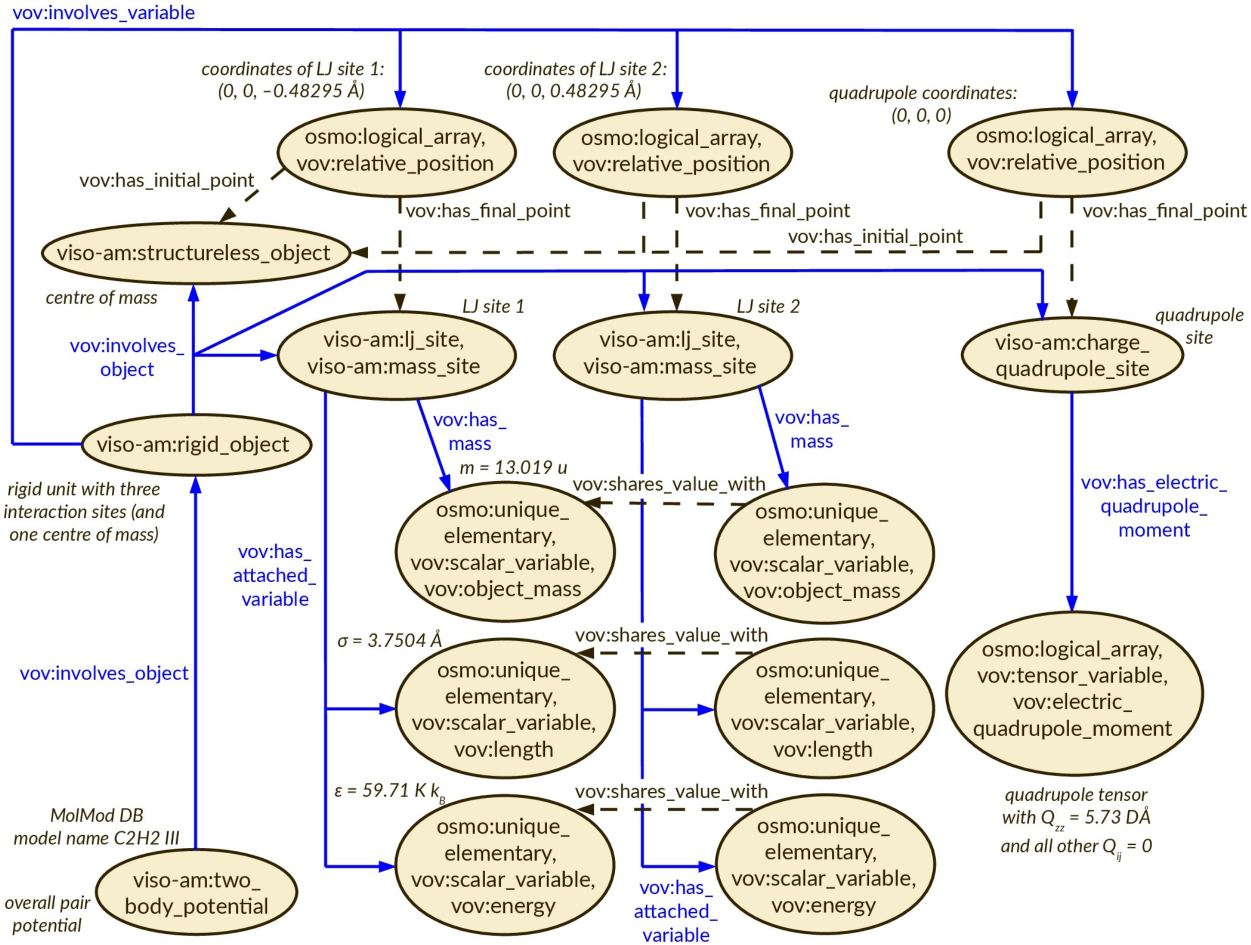
Molecular model database (MolMod DB[1])

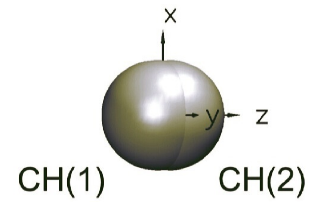
http://molmod.boltzmann-zuse.de/

Pair potentials for over 150 molecular fluids

[1]S. Stephan, M. Horsch, J. Vrabec, H. Hasse, *Mol. Sim.* 45, 806–814, **2019**.

Knowledge representation in molecular modelling[1, 2]





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