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UK Research and Innovation

Characterization of data provenance in computational engineering by an ontological representation of simulation workflows

VIMMP
VIRTUAL MATERIALS MARKETPLACE

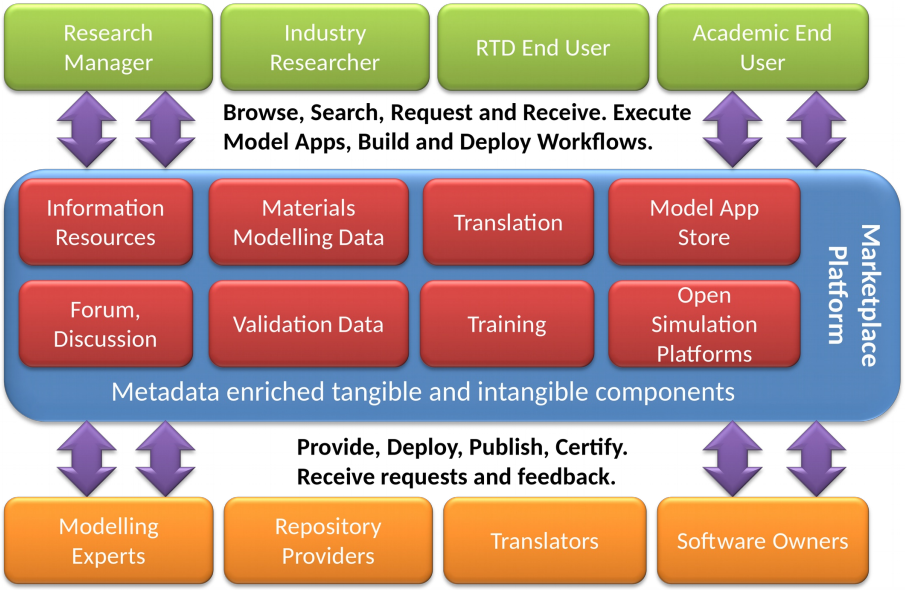
15th October 2019

DACOMSIN

Moscow

VIMMP: The Virtual Materials Marketplace

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



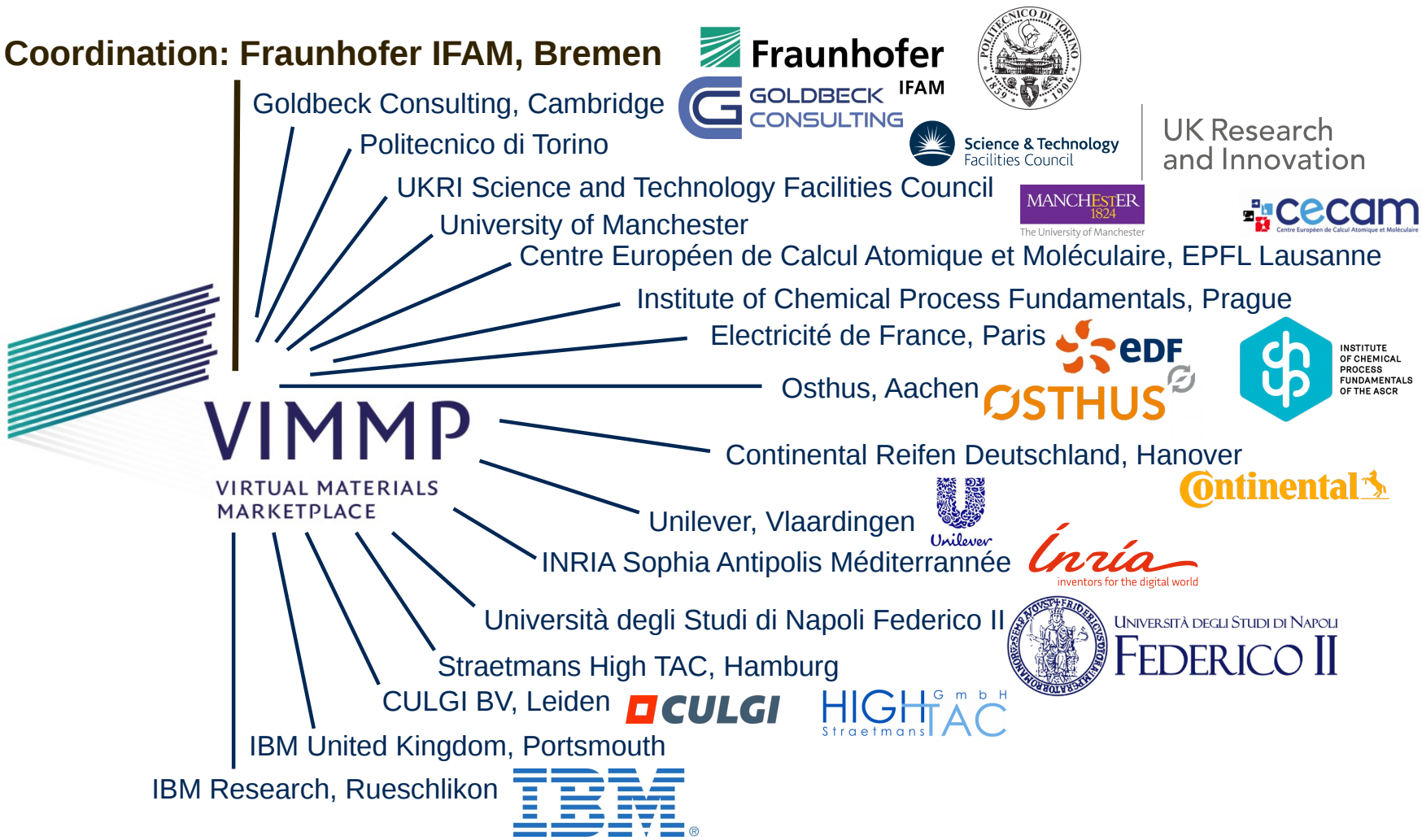
Coordination:

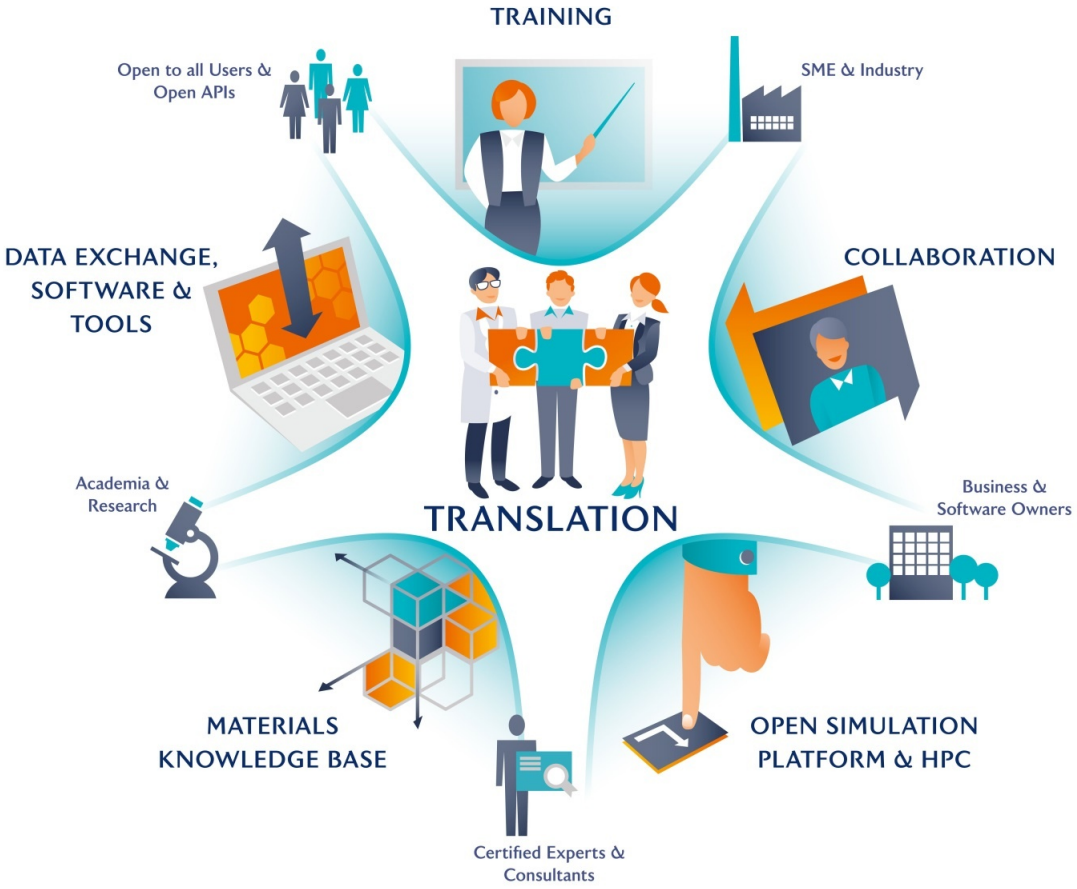
Fraunhofer IFAM

Funded by the Horizon 2020 Framework Programme of the European Union

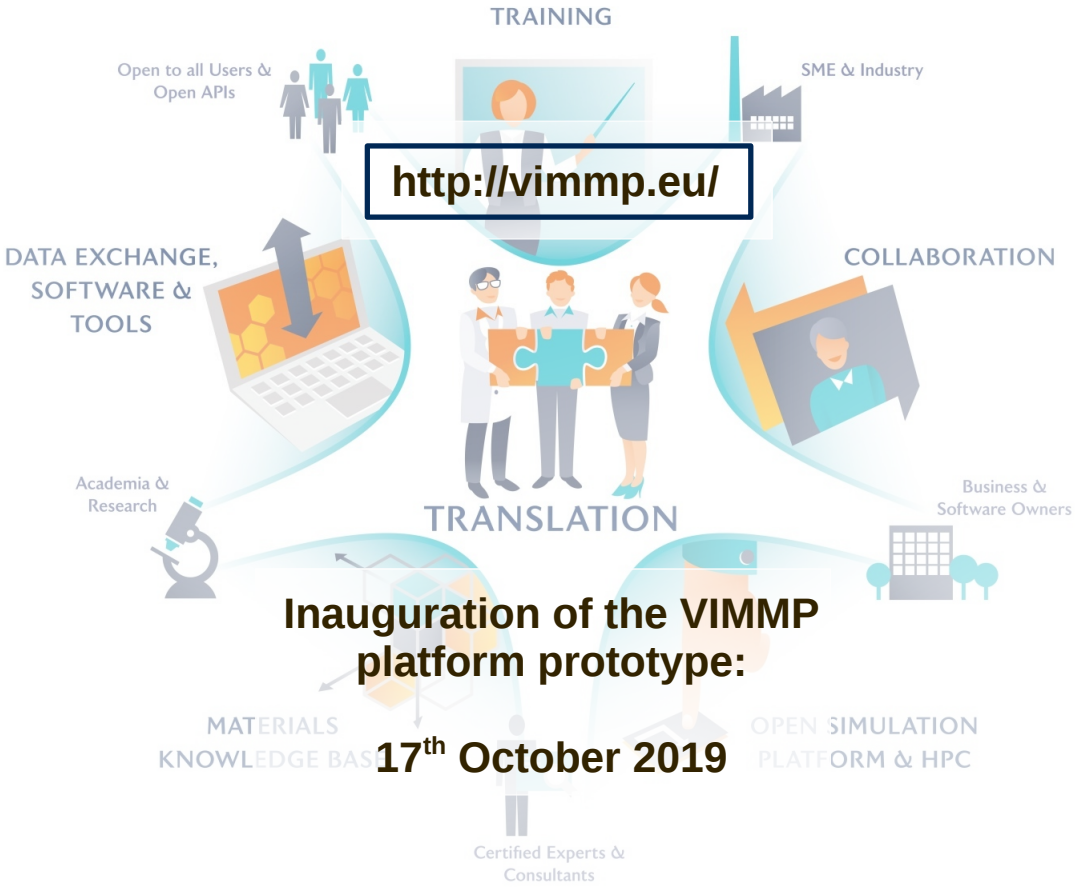
The **VIMMP Marketplace** will provide end-user interfaces to information resources, discussion forums, databases and repositories, translation and training services, validated models and modelling software, and the ability to utilise open simulation platforms to build and deploy workflows via cloud-based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

Virtual Materials Marketplace: Consortium





VIMMP will facilitate the **translation of industrial R&D challenges into materials modelling solutions**, and connect potential users and providers of modelling and simulation related services to each other, as an **open two-sided virtual marketplace**.

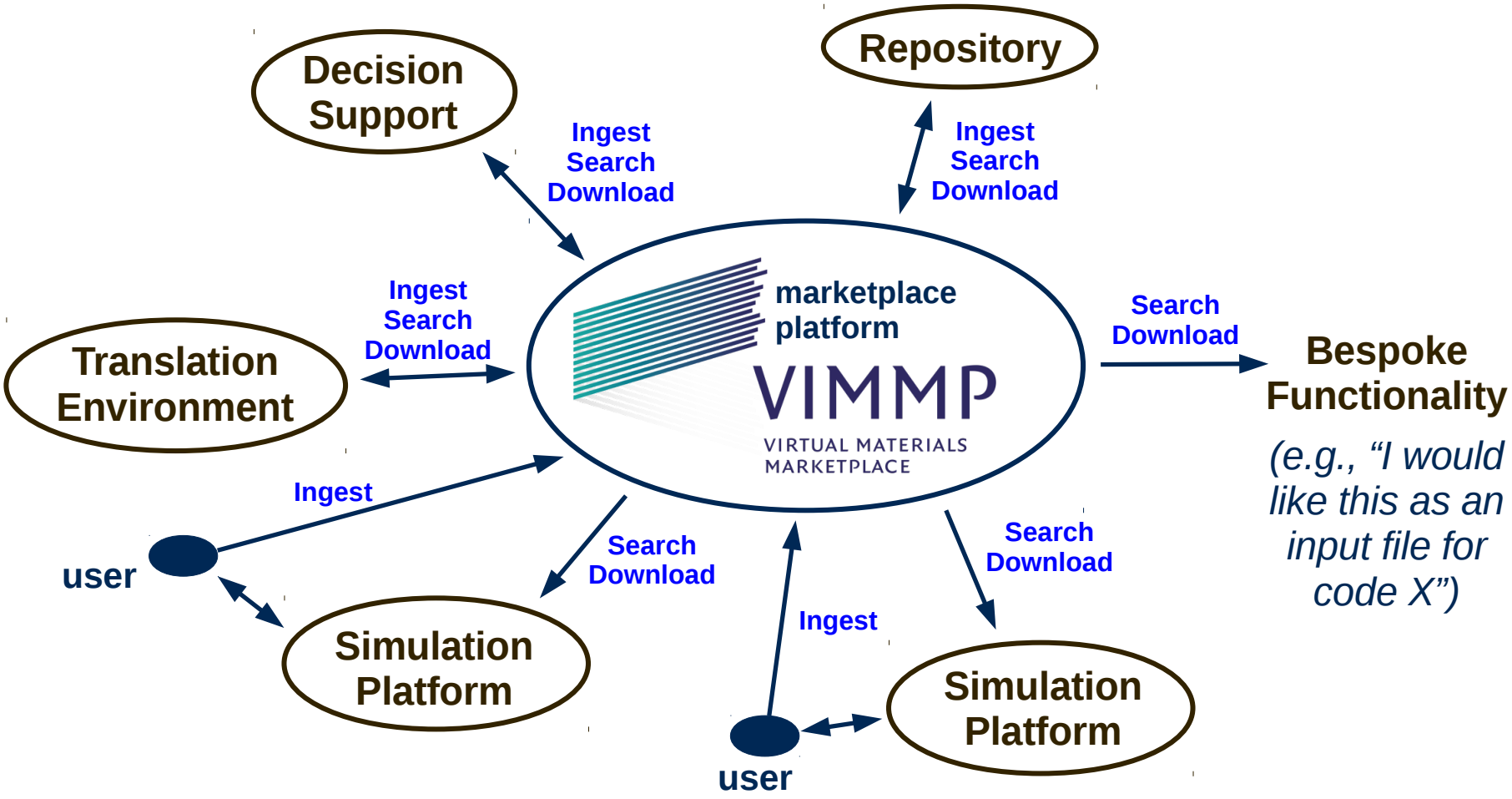


Inauguration of the VIMMP platform prototype:

17th October 2019

VIMMP will facilitate the **translation of industrial R&D challenges into materials modelling solutions**, and connect potential users and providers of modelling and simulation related services to each other, as an **open two-sided virtual marketplace**.

Interoperability in materials modelling



Interoperability in materials modelling

Time line of EMMC guided semantic-asset development

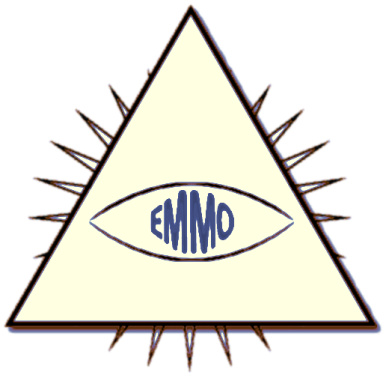
RoMM VI → **MODA** → **CWA 17284** → **Ontologies**

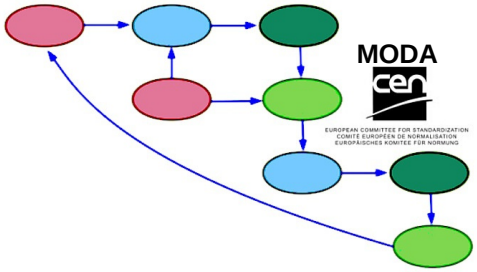
Semi-formalized terminology or vocabulary

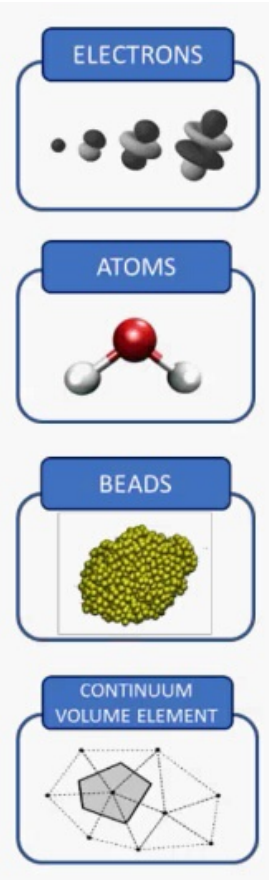
MODA workflow graph language

CEN European standard

EMMO, EVMPO, marketplace-level, and subdomain-specific ontologies







electronic

atomistic

mesoscopic

continuum

European Virtual Marketplace Ontology

The EVMPO provides a structure for the marketplace-level ontologies by formulating **fundamental paradigmatic categories** that correspond to irreducible terms which are seen as 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.

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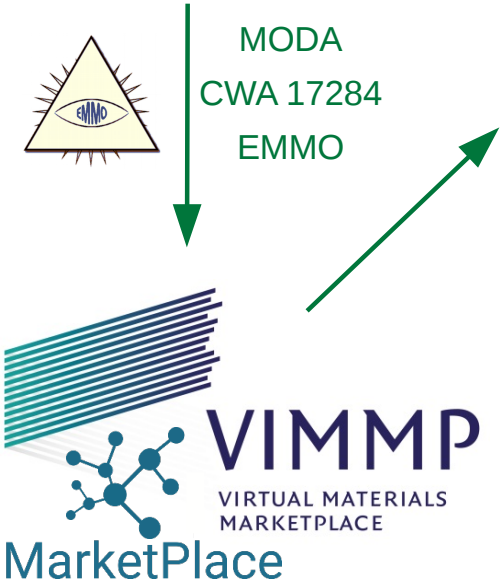
MarketPlace

Fundamental paradigmatic categories:

(1) **assessment**, i.e., proposition on accuracy, performance of an entity, or of an entity's trust in another entity
(2) **calendar_event**, i.e., meeting or activity that is scheduled or can be scheduled, equivalent to Vevent from ICALTZD
(3) **communication**, i.e., statement or sequence of statements that can be communicated at a virtual marketplace
(4) **information_content_entity** as defined in the Information Artifact Ontology (IAO)
(5) **infrastructure**, i.e., virtual-marketplace infrastructure (e.g., data access, hardware, and software)
(6) **material** as defined in the European Materials Modelling Ontology (EMMO)
(7) **model**, i.e., entity that can be described by the 2nd section of MODA, equivalent to "model" from the EMMO
(8) **process**, i.e., temporal evolution of one or multiple entities
(9) **product**, i.e., good or service that can be offered either at a virtual marketplace or off-site
(10) **property** as defined in the EMMO
(11) **role** as defined in the EMMO
(12) **simulation**, i.e., a simulation workflow (as in MODA)

Upper level ontology and connection to marketplaces

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



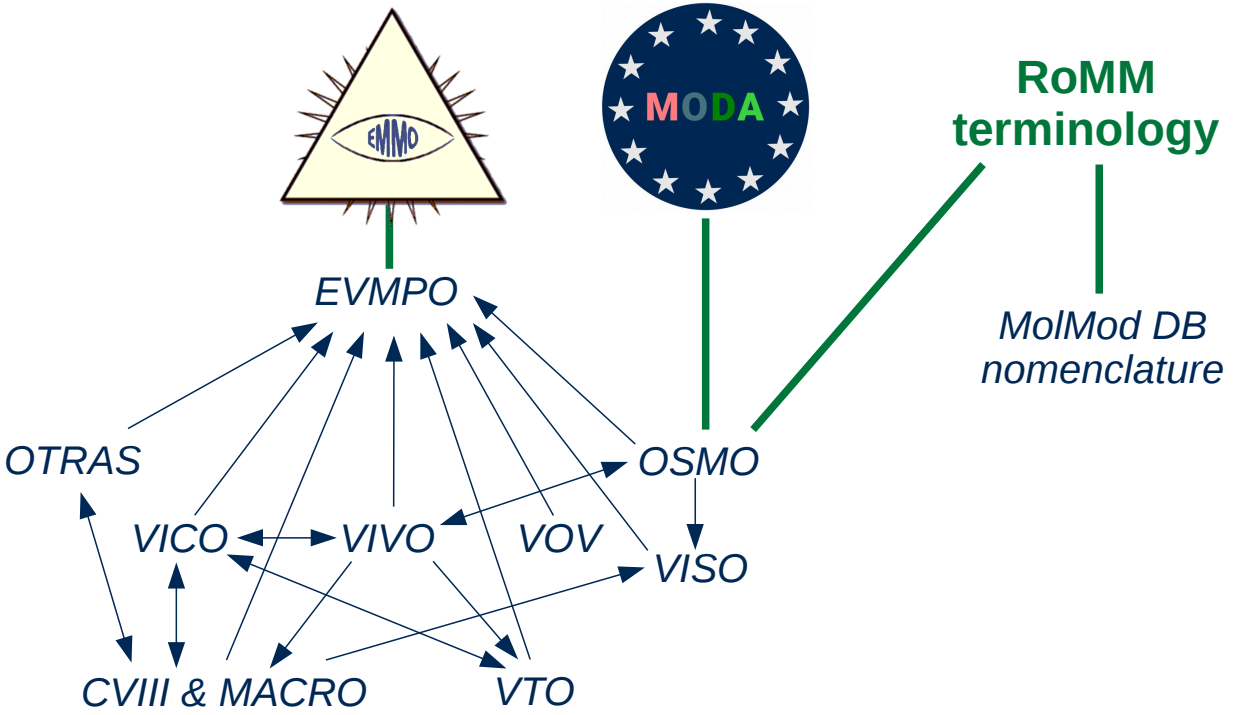
- **Upper level: EMMO extended by European Virtual Marketplace Ontology (EVMPO)**

VIMMP ontologies based on EMMO and EVMPO

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

- **Upper level: EMMO extended by European Virtual Marketplace Ontology (EVMPO)**
- **Marketplace-level ontologies: VIMMP in coordination with the MarketPlace project**
- **Subdomains: VOV, VISO branches (electronic, atomistic-mesoscopic, continuum)**

VIMMP ontologies and pre-existing semantic assets

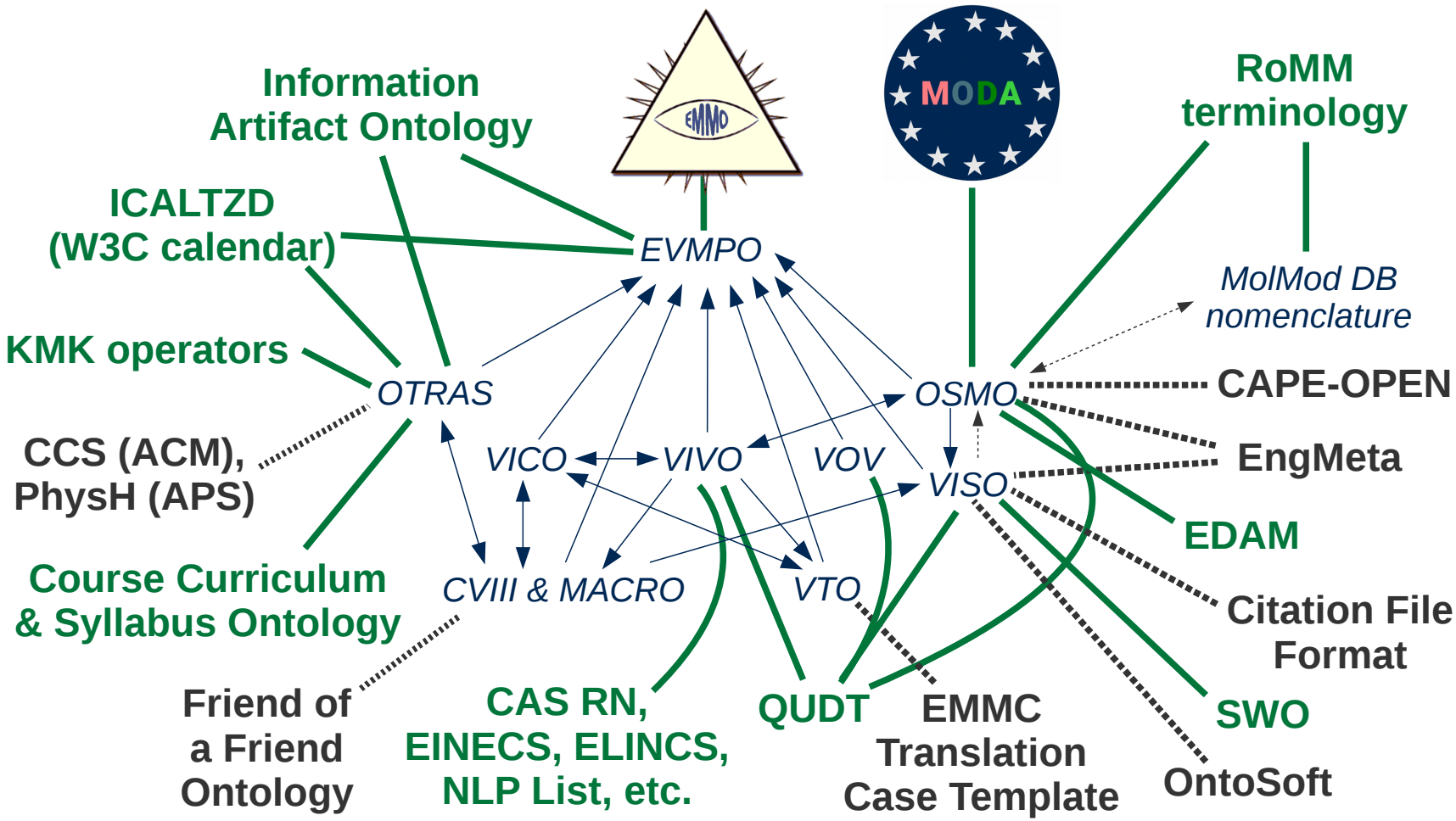


EMMC line of semantic asset development:

1) **Review of Materials Modelling (RoMM)**
2) **CWA 17284 – Model Data (MODA)**
3) **European Materials & Modelling Ontology (EMMO)**

Blue: Semantic assets co-developed by the Virtual Materials Marketplace (VIMMP) project

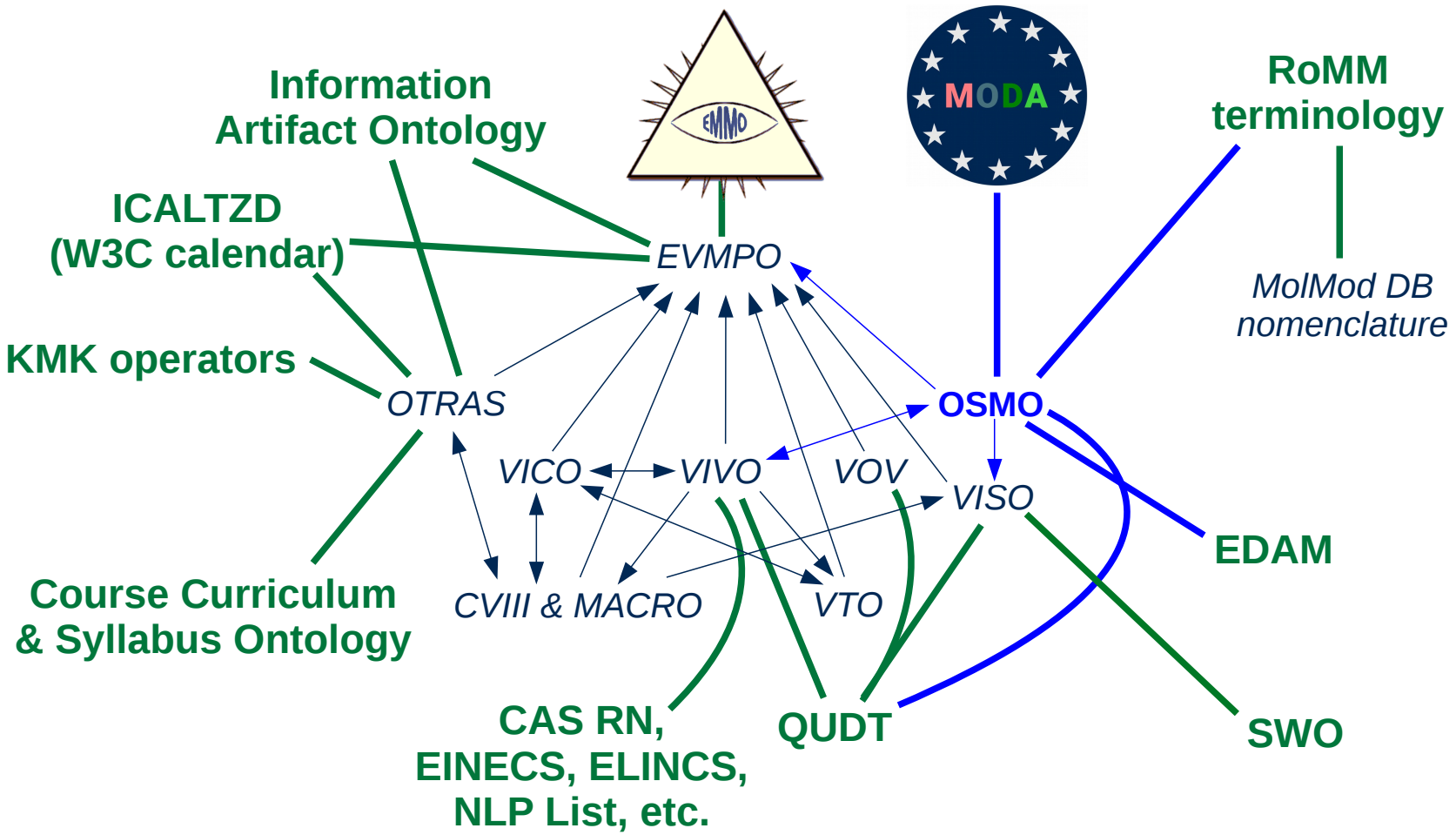
VIMMP ontologies and pre-existing semantic assets



Blue: Semantic assets co-developed by the Virtual Materials Marketplace (VIMMP) project

Green: Connected external semantic assets **(Grey: Related, but not connected)**

VIMMP ontologies and pre-existing semantic assets



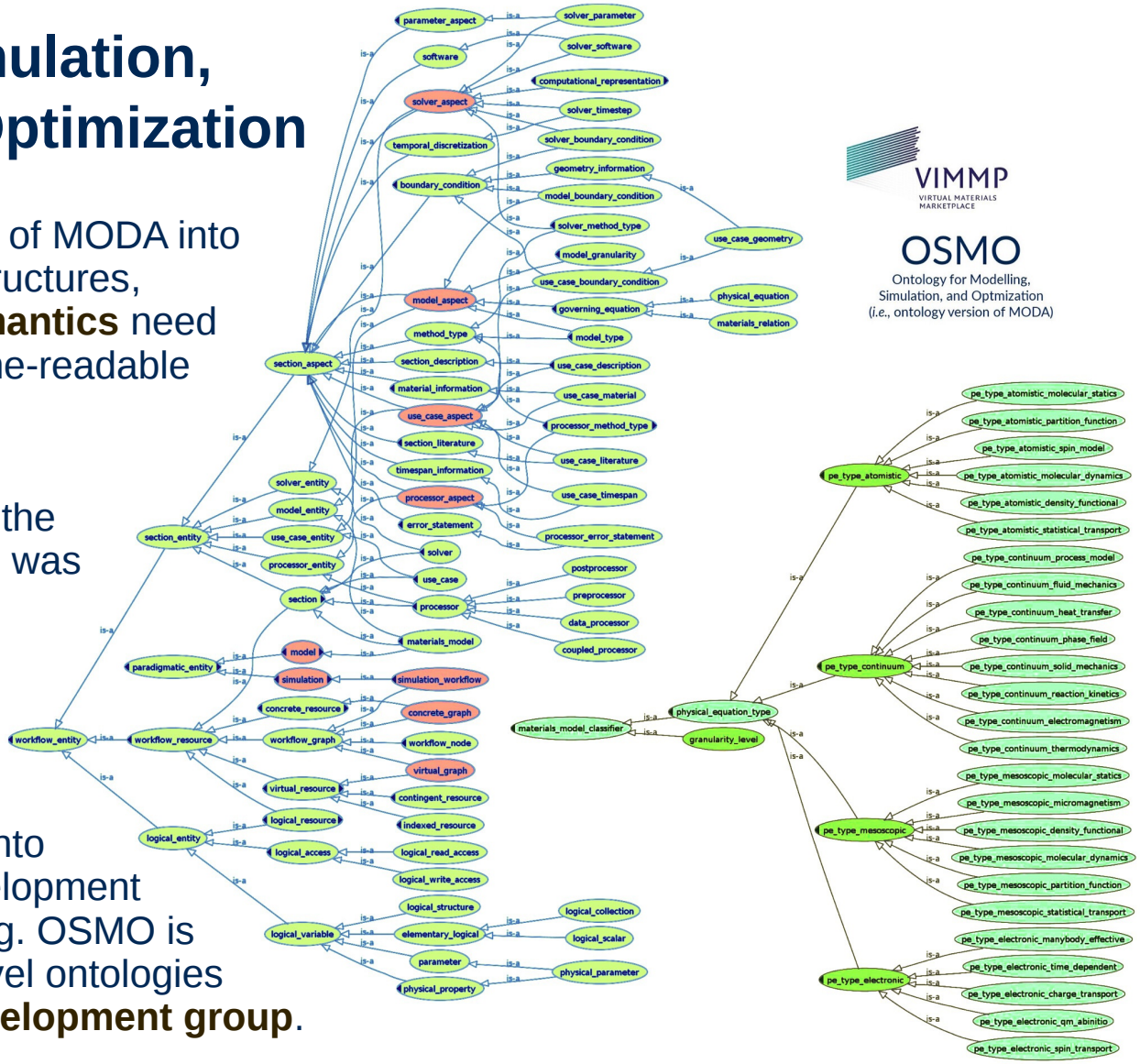
OSMO: Ontology for Simulation, Modelling, and Optimization

Ontology for Simulation, Modelling, and Optimization

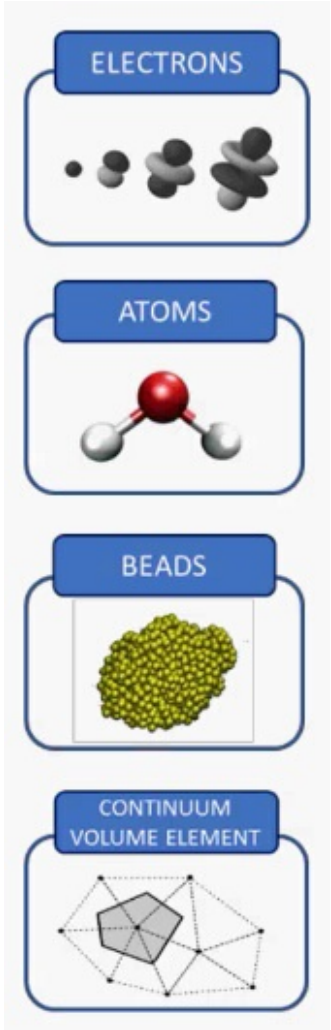
To facilitate the integration of MODA into virtual marketplace infrastructures, **simulation workflow semantics** need to be provided at a machine-readable level of formalization.

Following the approach of the EMMC community, OSMO was developed: **The ontology version of MODA.**

By OSMO, simulation workflow semantics from MODA can be integrated into the ongoing ontology development work in materials modelling. OSMO is one of the marketplace-level ontologies shared in the **EVMPO development group**.



Model classes from EMMC Review of Materials Modelling



electronic

EL.1: Ab-initio quantum mechanics
EL.2: Effective Hamiltonian models
EL.3: QM modelling of time-dependent quantities and fields
EL.4: Charge transport (statistical)
EL.5: Spin transport (statistical)

atomistic

A.1: Classical DFT (atomistic)
A.2: Molecular statics (atomistic)
A.3: Equations of motion (atomistic)
A.4: Partition function (atomistic)
A.5: Atomistic spin models
A.6: Statistical transport (atomistic)

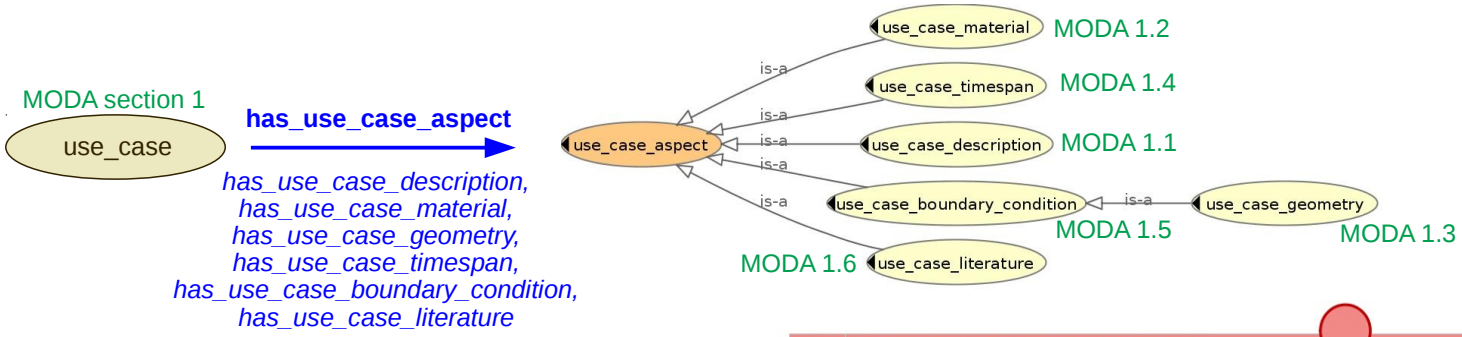
mesoscopic

M.1: Classical DFT (mesoscopic)
M.2: Molecular statics (mesoscopic)
M.3: Equations of motion (mesosc.)
M.4: Partition function (mesoscopic)
M.5: Mesoscopic spin models
M.6: Statistical transport (mesosc.)

continuum

CO.1: Continuum solid mechanics
CO.2: Continuum fluid mechanics
CO.3: Heat transfer, thermomechanics
CO.4: Phase field models, DGT
CO.5: Continuum thermodynamics
CO.6: Chemical reaction kinetics
CO.7: Electromagnetism
CO.8: Processes and devices

Sections and aspects of a simulation from MODA



MODA section 1 **use case**

MODA section 2 **model**

MODA section 3 **solver**

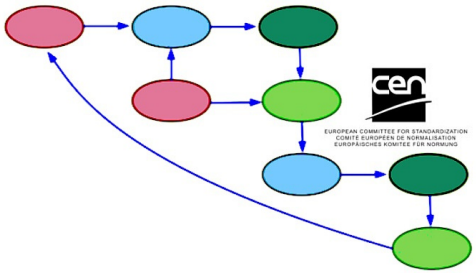
MODA section 4 **processor**

"sections"

"aspects"

OSMO

"graphs"



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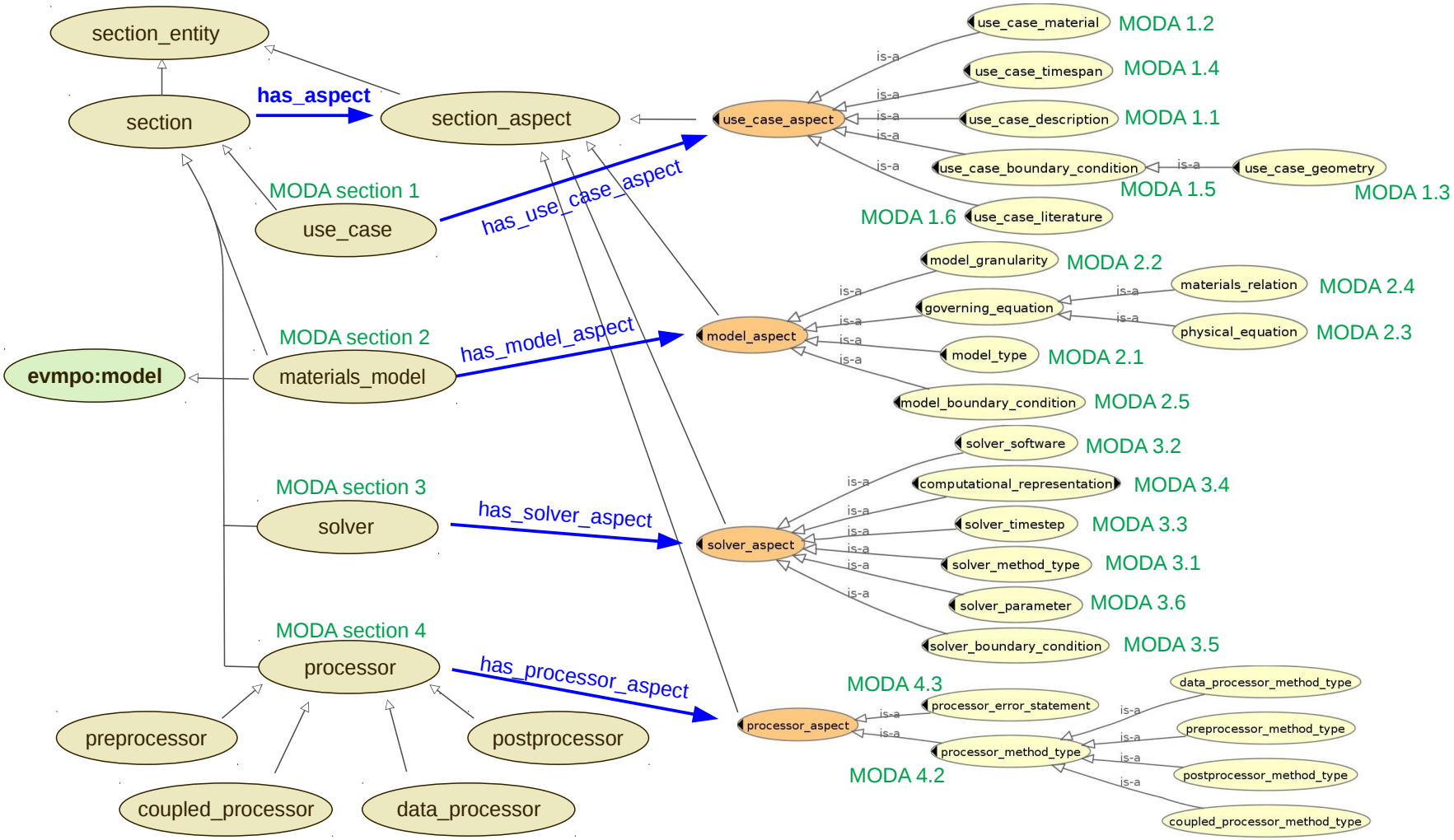
1	Aspect of the User Case/System to be Simulated	
1.1	Aspect of the User Case to be simulated	*Describe the aspects of the user case textually.* *No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation!* *The information in this chapter can be end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture.* *Simulated input which would have been calculated by another model should not be included (but in chapter 2.4)* *Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities van be documented here.*
1.2	Material	*Describe the chemical composition, ...and the values used for properties and from which database these are taken. If pre-processing was needed please specify the methodology.*
1.3	Geometry	*Size, form, picture of the system (if applicable)* *Note that computational choices like simulation boxes are to be documented in chapter 3.*
1.4	Time Lapse	*Duration of the case to be simulated.* *This is the duration of the situation to be simulated. This is not the same as the computational times to be given in chapter 3.*
1.5	Manufacturing process or in-service conditions	*If relevant, please list the conditions to be simulated (if applicable).* *These can be boundary, initial and global conditions.* *E.g. heated walls, external pressures and bending forces.* *Please note that these might appear as terms in the PE or as boundary conditions, and this will be documented in the relevant chapters.* *Note: These conditions will be expressed in physics relations in Ch 2.4* *Please specify the values used for parameters and from which database these are taken. If pre-processing was needed please specify the methodology.*
1.6	Publication on this data	*Publication documenting the simulation with this single model (if available and if not already included in the overall publication).*

Sections and aspects of a simulation from MODA

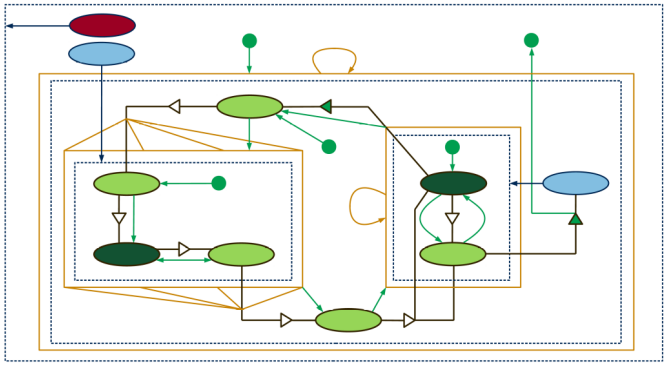


Logical data transfer in simulation workflows

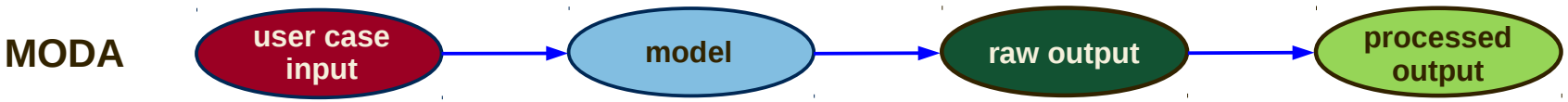
Logical (i.e., non-technical) workflow description following the approach from MODA

Reduced ambiguity of relations between the sections

Alignment with section description from MODA



MODA and logical data transfer in simulation workflows



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

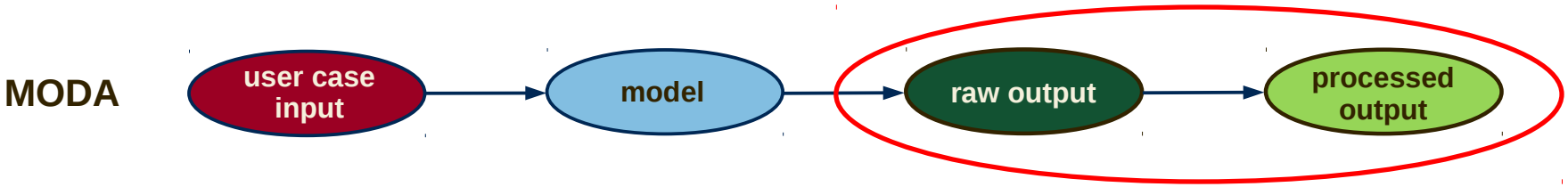
Examples

A **model** can **apply to** a part of the workflow; relation "osmo:applies_to".

The model can be parameterized at workflow execution time; then the arrow represents **logical data transfer**; n.b., technical data transfer such as file I/O may or may not occur.

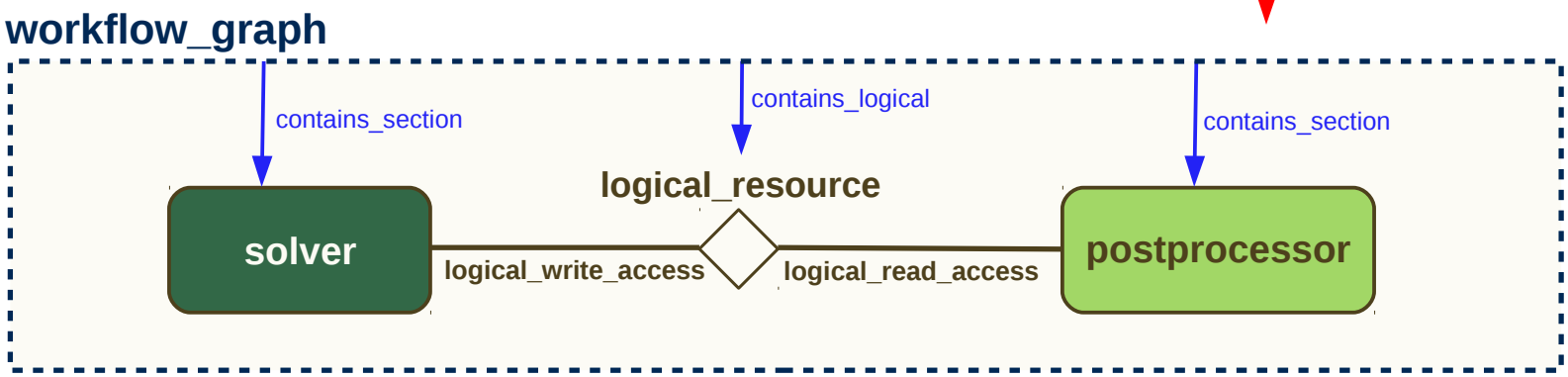
Workflows may contain conditional or iterative operations that are active only under certain conditions; in OSMO, such elements are referred to as **virtual resources**. The relation "osmo:instantiates" relates a concrete to a virtual resource.

MODA and logical data transfer in simulation workflows



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

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



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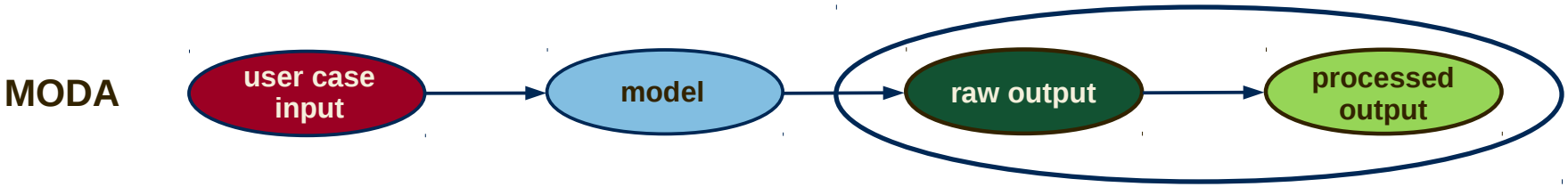

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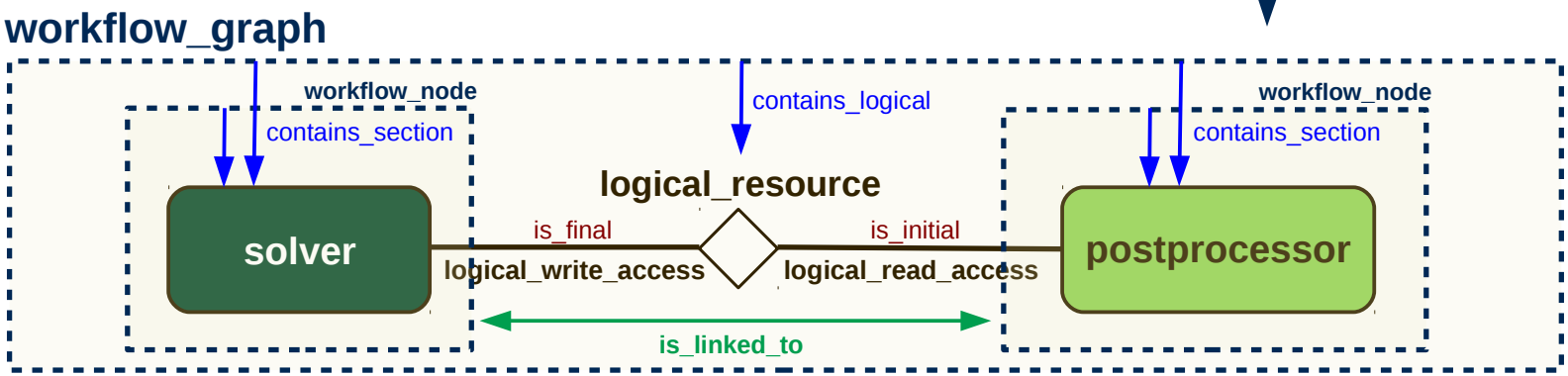

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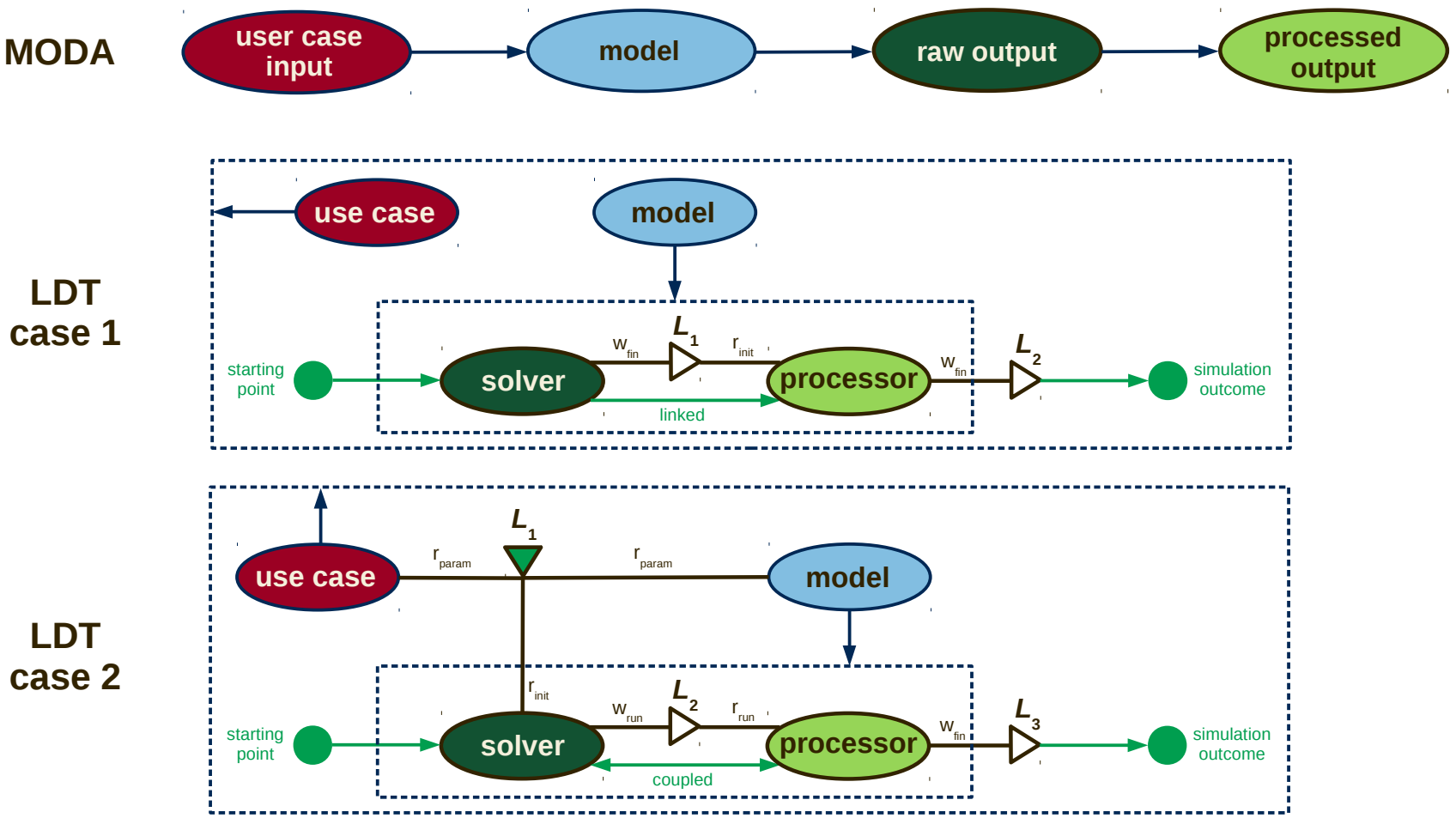
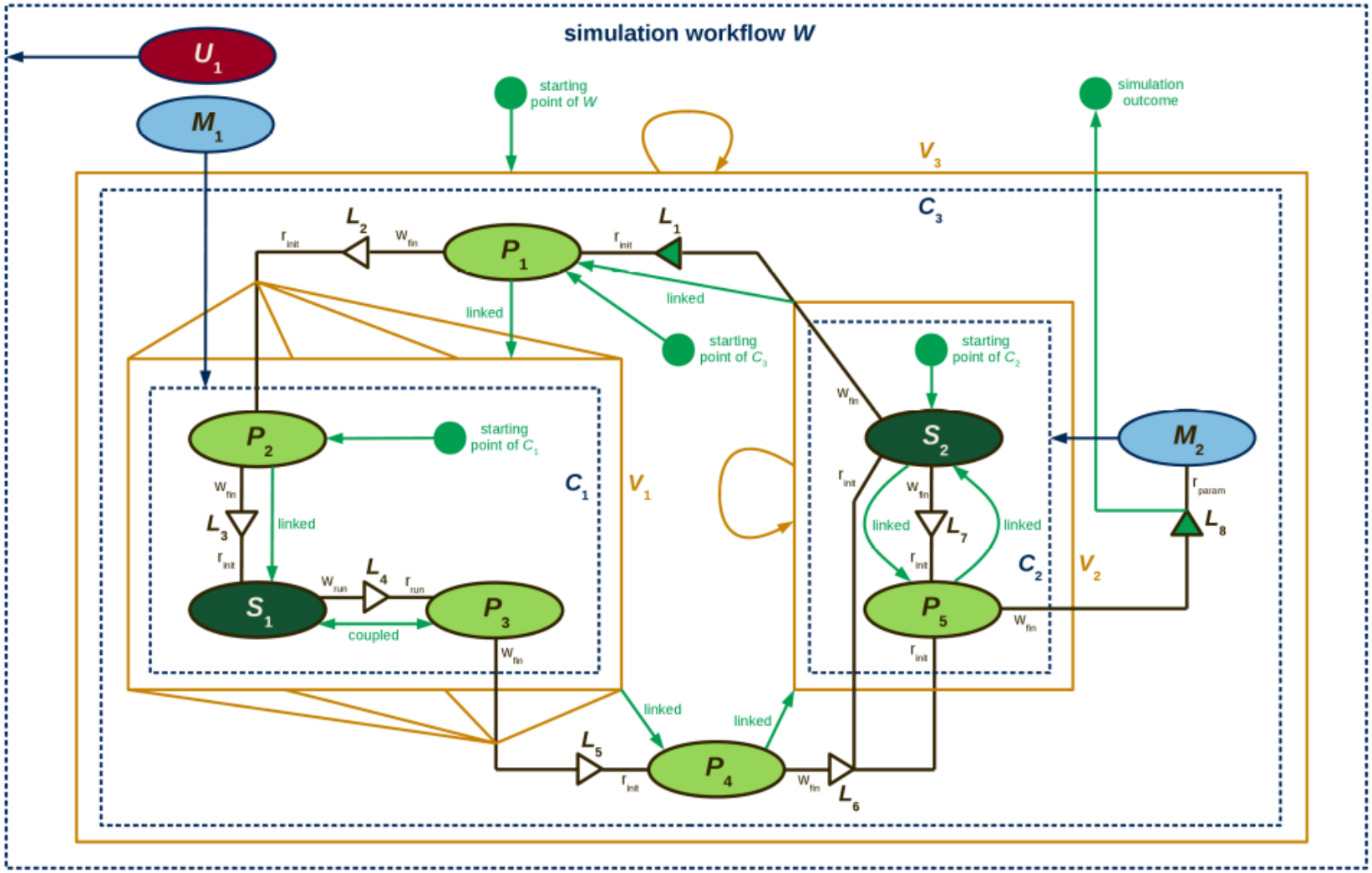
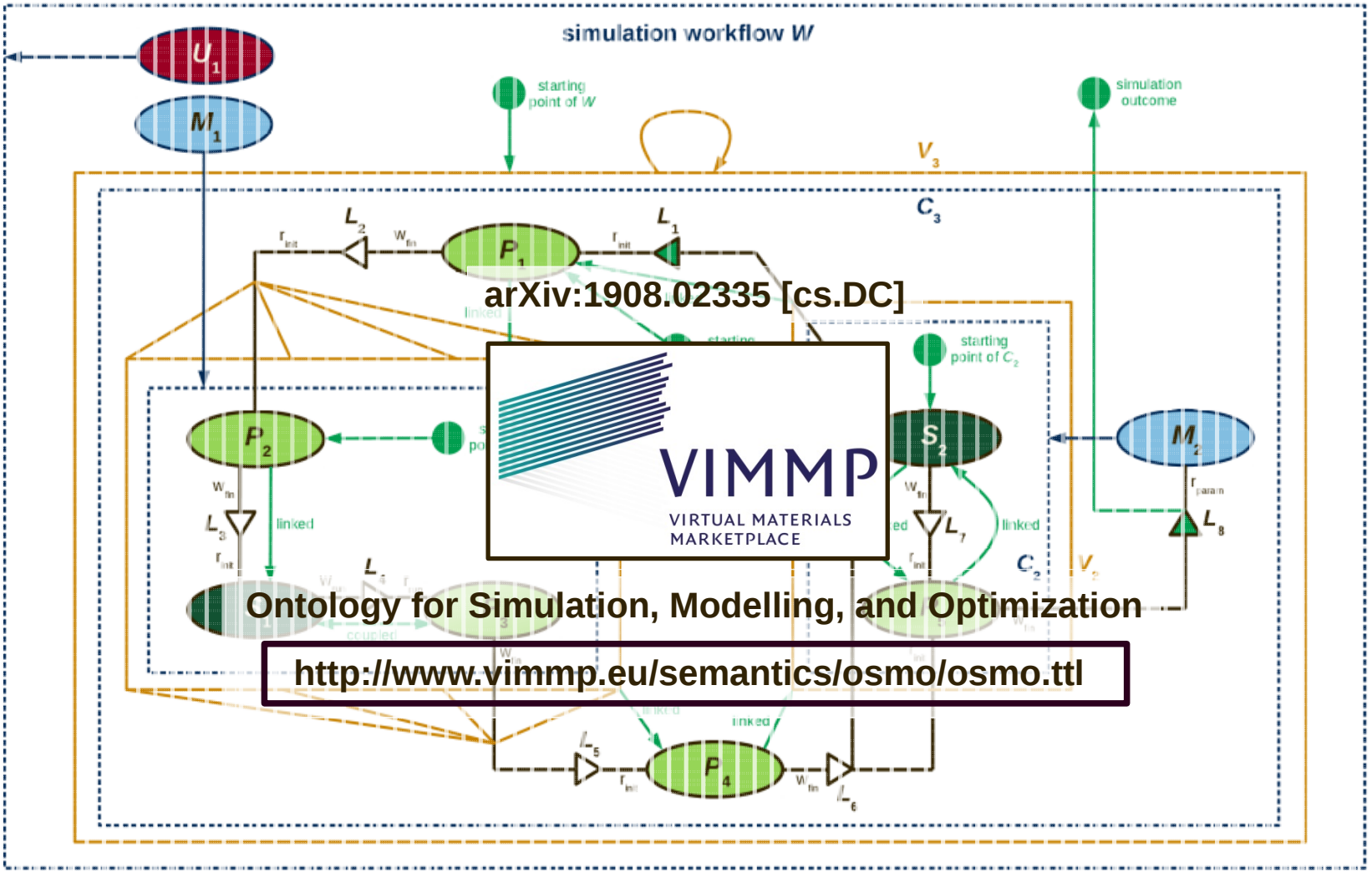


MODA and logical data transfer in simulation workflows



Ontology for Simulation, Modelling, and Optimization



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Hamburg	–	Philipp Neumann
Stuttgart	–	Christoph Niethammer

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