EMMC: A Community Advancing Materials Modelling and Digitalisation in Europe

Gerhard Goldbeck (EMMC Executive Secretary)

History

2014: Informal Association of European Stakeholders

2016: EU funding (H2020 NMBP Coordination and Support Action)

2019: Established in Brussels (Belgium) as non-profit association, **EMMC ASBL**

FACILITATE INTEGRATED MATERIALS MODELLING & DIGITALISATION

OVERCOME OBSTACLES TO UPTAKE BY INDUSTRY, INCREASE IMPACT

SUPPORT INDUSTRIAL DEPLOYMENT OF SOFTWARE

COORDINATE ACTORS, IMPROVE INTERACTIONS & COLLABORATION

N° d'entreprise :	0731621312
Nom (en entier) :	**EMMC**
(en abrégé) :	
Forme légale :	Association sans but lucratif
Adresse complète du siège :	Avenue Louise 54 1050 Bruxelles
Objet de l'acte :	CONSTITUTION

www.emmc.eu

EMMC ASBL, since 2019

- Member driven, inclusive organisation
- Free Associate Membership for all
- Full Individual Members form the AGM
- Organisational Members represented in Org. Assembly

Organisational Assembly Chairs:

Natalia Konchokova (Hereon), Costas Charitidis (NTUA)

<u>Board of Directors</u>
Nadja Adamovic (TU Wien) - Chair
Malgorzata Celuch (QWED)
Jesper Friis (SINTEF)
Adham Hashibon (UCL)
Peter Haynes (Imperial College)
Kersti Hermansson (Uppsala)
Esther Hurtós (EURECAT)
Patrycja Polińska (Goodyear)
Ilian Todorov (UKRI -STFC)

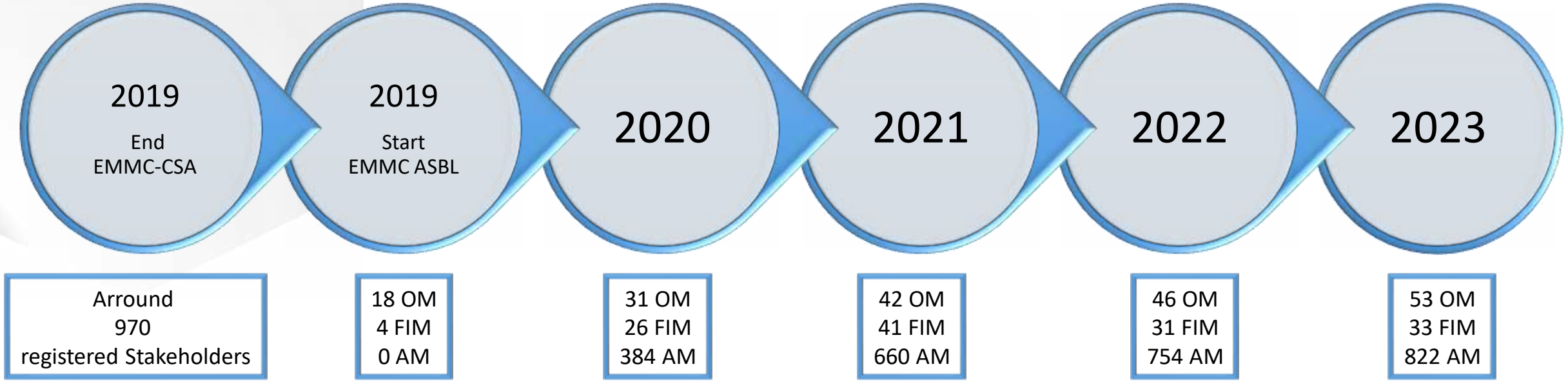
<u>Executive Secretary</u>
Gerhard Goldbeck

The EMMC considers the <u>integration of materials modelling and digitalisation</u> critical for more agile and sustainable product development.

EMMC International Advisory Board Members

- Abhijit Chatterjee, 3DS Biovia, **Japan**
- Alejandro Strachan, Purdue University and NSF nanoHUB, **United States**
- Detlef Hohl, Shell, **Netherlands**
- James Warren, NIST, **United States**
- Jonathan Mueller, Volkswagen, **Germany**
- Kwang-Ryeol Lee, Korea Institute of Science and Technology, **Korea**
- Paulo Noronha Lisboa-Filho, UNESP - São Paulo State University, **Brazil**
- Phuti Ngoepe, University of Limpopo, **South Africa**

Membership development



EMMC ASBL Founding Organisational Members

TU WIEN

GOLDBECK CONSULTING

materials design

Fraunhofer

ANSYS GRANTA

SYNOPSYS®

access

DPI
The Polymer Research Platform

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

SINTEF

UKRI Science and Technology Facilities Council

institute IMDEA

JM Johnson Matthey
Inspiring science, enhancing life

AC²T research

SCM
Software for Chemistry & Materials

MARVEL

esi

LUXEMBOURG INSTITUTE OF SCIENCE AND TECHNOLOGY | LIST

All Members, see:
https://emmc.eu/members/

EMMC related projects acknowledgement

https://emmc.eu/emmc-related-projects/

MarketPlace

VIMMP
VIRTUAL MATERIALS MARKETPLACE

SimDOME

INTERSECT

Open Model

COMPOSELECTOR
Polymer Composites Business Decision Support System

OYSTER

VIPCOAT

Nano Bat

nanoMECommons

ONTO COMMONS

FORM PLANET

ONTOTRANS

FORCE

i-TRIBOMAT
Intelligent Open Test Bed for Materials Tribological Characterisation Services

SUBLIME

ZEOCAT-3D

ReaxPro

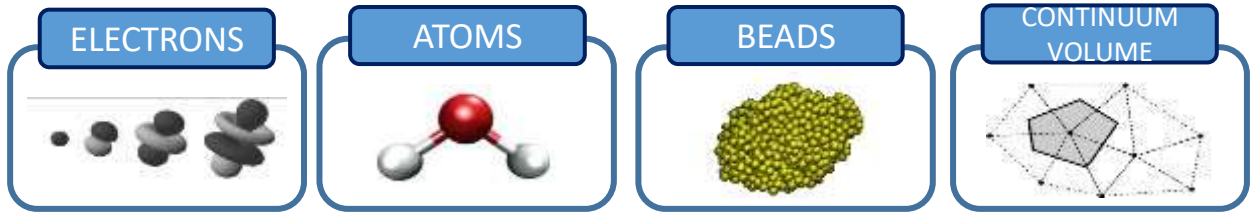
NICKEFFECT

CHARISMA

…. and more

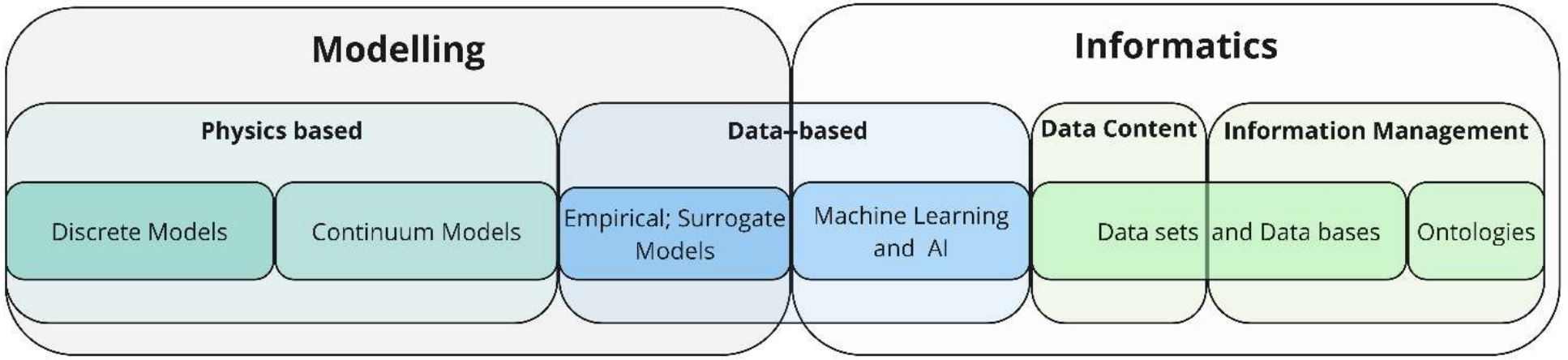
What is special about EMMC?

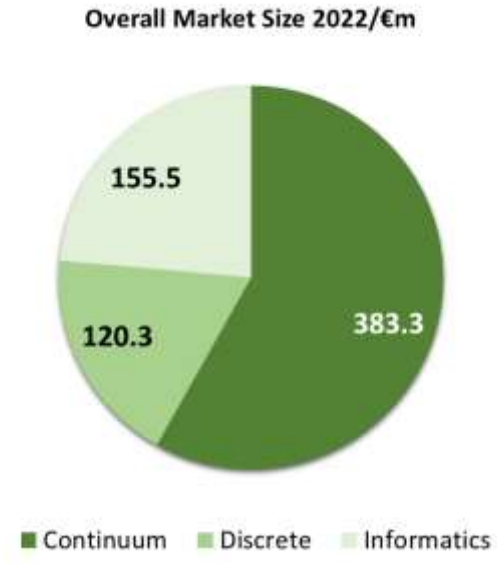
- Includes **ALL** types of modelling Physics and data based



- Includes **ALL** chemical/material and application fields
- Includes **ALL** types of roles: Code authors/software owners (academic & commercial), modelling expert and materials manufacturers, consultants and so-called translators etc.
- Supports harmonisation and standardisation in terminologies, taxonomies and ontologies for improved communication and interoperability (Human-human, machine-machine)

Fields covered by EMMC





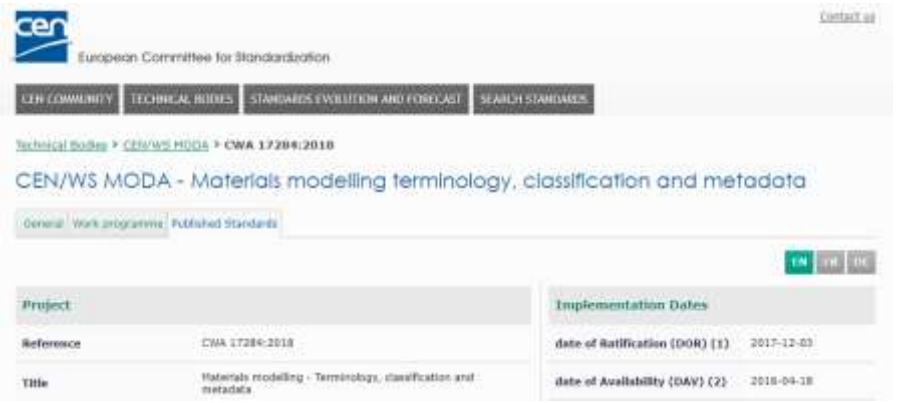
Fields of modelling and digital representation of materials and their software market size.
From:
Goldbeck, Gerhard, Simperler, Alexandra, & Roscioni, Otello. (2023). Materials Modelling and Informatics Software Market. Zenodo. https://doi.org/10.5281/zenodo.8101869

Terminology standards and EMMO ontology

EMMO (Elementary Multiperspective Material Ontology)

https://github.com/emmo-repo/

A knowledge management framework for natural sciences and engineering



https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/RI/cwa17284_2018.pdf

Started by practitioners in Materials Science in order to produce a framework consistent with scientific principles and methodologies

Developed and used in a number of projects with **governance by the EMMC**, including:

SimDOME

ONTOTRANS

Open Model

ONTO COMMONS

nanoMECommons

BIG-MAP

Battery Interface Genome - Materials Acceleration Platform

EMMC working with the community; member benefits

Workshops: Since 2014 in total more than 55 EMMC events

https://emmc.eu/news/emmc-2023-highlights/

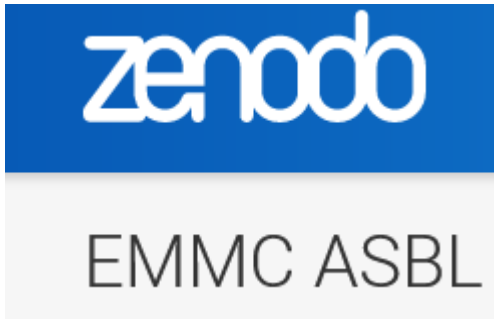
Surveys and professional development

https://emmc.eu/simulation-success-stories/

EMMO Ontology

https://github.com/emmo-repo/EMMO

https://github.com/EMMC-ASBL/

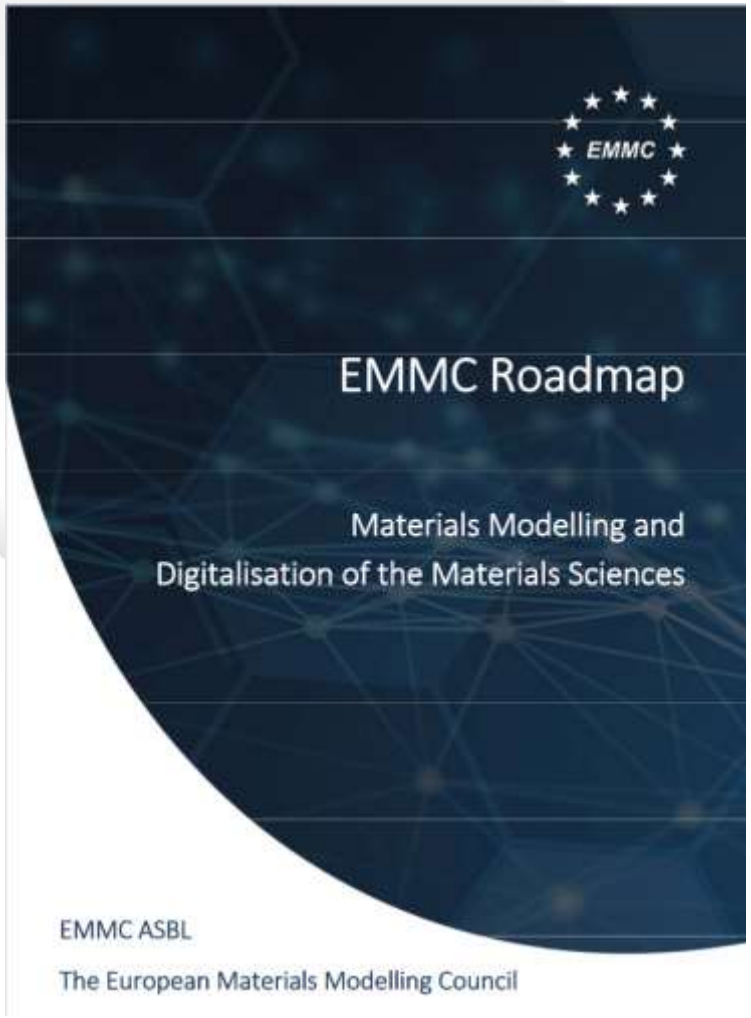


https://zenodo.org/communities/emmc

4th EMMC International Workshop 2023, Vienna

Materials & Digitalisation: the backbone of the Green Transition

EMMC RoadMaps



2023 update to be published soon

Previous versions : 2020, 2018, 2016, 2015

2023 RoadMap Status

Available for internal feedback of EMMC members

https://emmc.eu/emmc-roadmaps/

EMMC contribution to H2020 funding calls

NMBP WP 2016-2017

Computational Materials Modelling for the Development of Nanotechnologies and Advanced Materials

- NMBP-23-2016: Advancing the **integration of Materials Modelling in Business Processes** to enhance effective industrial decision making and increase competitiveness
- NMBP-24-2016: **Network to capitalize on strong European position in materials modelling** and to allow industry to reap the benefits
- NMBP-25-2017: Next generation **system integrating tangible and intangible materials model components** to support innovation in industry

NMBP WP 2018-2019

Materials Characterisation and Computational Modelling

- DT-NMBP-09-2018: **Accelerating the uptake of materials modelling software** (IA)
- DT-NMBP-10-2019: **Adopting materials modelling in manufacturing processes** (RIA)

NMBP WP 2020

- DT-NMBP-11-2020: **Open Innovation Platform for Materials Modelling** (RIA)
- DT-NMBP-39-2020: **Towards Standardised Documentation of Data through taxonomies and ontologies** (CSA)
- DT-NMBP-40-2020: **Creating an open market place for industrial data** (RIA)

EMMC contribution to HORIZON EUROPE calls

EMMC directly related

- HORIZON-CL4-2022-RESILIENCE-01-19: **Advanced materials modelling and characterisation** (RIA)
- HORIZON-CL4-2023-DIGITAL-EMERGING-01-12: **Adaptive multi-scale modelling and characterisation** suites from lab to production (RIA)
- HORIZON-CL4-2023-RESILIENCE-01-39: **Coordination and knowledge sharing** across materials development communities (CSA)

EMMC related to due to topic and/or including EMMO ontology

- HORIZON-CL4-2022-RESILIENCE-01-12: Functional multi-material components and structures (RIA)
- HORIZON-CL5-2023-D2-01-03: Advanced digital twins for battery cell production lines (Batt4EU Partnership)
- HORIZON-CL4-2023-RESILIENCE-01-23: Computational models for the development of safe and sustainable by design chemicals and materials (RIA)

EMMC Focus Areas: Reflect EMMC strategic directions

https://emmc.eu/activities/emmc-focus-areas/

Model Development	Interoperability Digitalisation	Software deployment	Impact in Industry	Policy Roadmap
Capabilities and qualities of models	Semantic foundation, platforms	Robust, well-documented, maintained	Integration into R&D processes Translation, Value	Inform and shape R&I policy and EU actions
Annual eSSENCE-EMMC Workshop	EMMO Ontology Governance	Best Practice, Success Stories	Translator Guide Tools for industry	EMMC Roadmaps AMI 2030

Model development

- Robust reliability and benchmarking
- Sufficient accuracy for complex systems
- Verification & Validation & Uncertainty Quantification protocols
- Easier access to and re-usability of modelling workflow solutions
- See also https://emmc.eu/simulation-success-stories/
- Compare with Engineering: e.g. NAFEMS benchmarks
  - Introduced in 1986 as a first set of independent "standard“ tests which could be applied to any Finite Element System.

https://www.nafems.org/community/working-groups/education-and-training/nafems_benchmark_challenge/

https://www.nafems.org/publications/resource_center/p18 /

“Modelling Capabilities” Case examples concerning material properties

Elastic Coefficient (in GPa)

System: polymer with complete cross-linking :

a) Resin: Diglycidyl ether of bisphenol A (DGEBA) resin cured with 4,4’ diaminophenylsulfone (DDS)

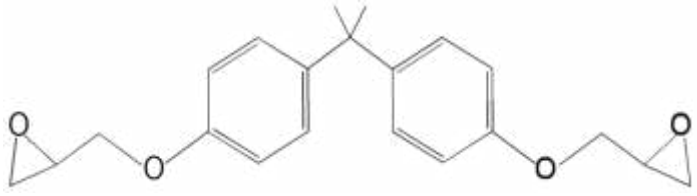
b) Resin: Tetraglycidyl diaminodiphenylmethane (TGDDM) cured with DDS

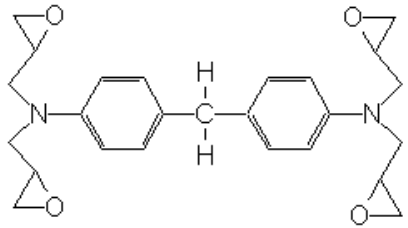
Conditions: ambient T and p

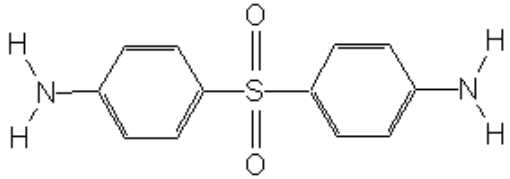
Experimental Data:

a) S. R. White, P. T. Mather, M. J. Smith, Characterization of the cure-state of DGEBA-DDS epoxy using ultrasonic, dynamic mechanical, and thermal probes, Polymer Engineering and Science, vol. 42 (1), 51-67 (2002) https://doi.org/10.1002/pen.10927

b.Shabnam Behzadi & Frank R. Jones (2005) Yielding Behavior of Model Epoxy Matrices for Fiber Reinforced Composites: Effect of Strain Rate and Temperature, Journal of Macromolecular Science, Part B, 44:6, 9931005, DOI: 10.1080/00222340500393881 https://doi.org/10.1080/00222340500393881







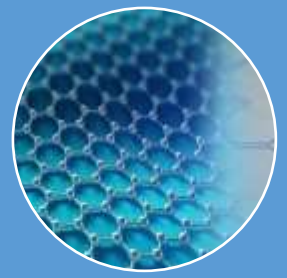
Type	Resin	Calculated Bounds (GPa)	Experiment (GPa)
RA_4+RB_2	DGEBA	3.49-3.53	2.4-3.2 [a]
RA_4+RB_4	TGDDM	5.18-5.19	5.103±.033 [b]

Breaking down silos

Lack of processing, engineering and production requirements as design parameters

Lack of information integration

Lack of virtual materials that can act as design variables



Materials Science

Materials Processing

Materials Engineering

Materials Production

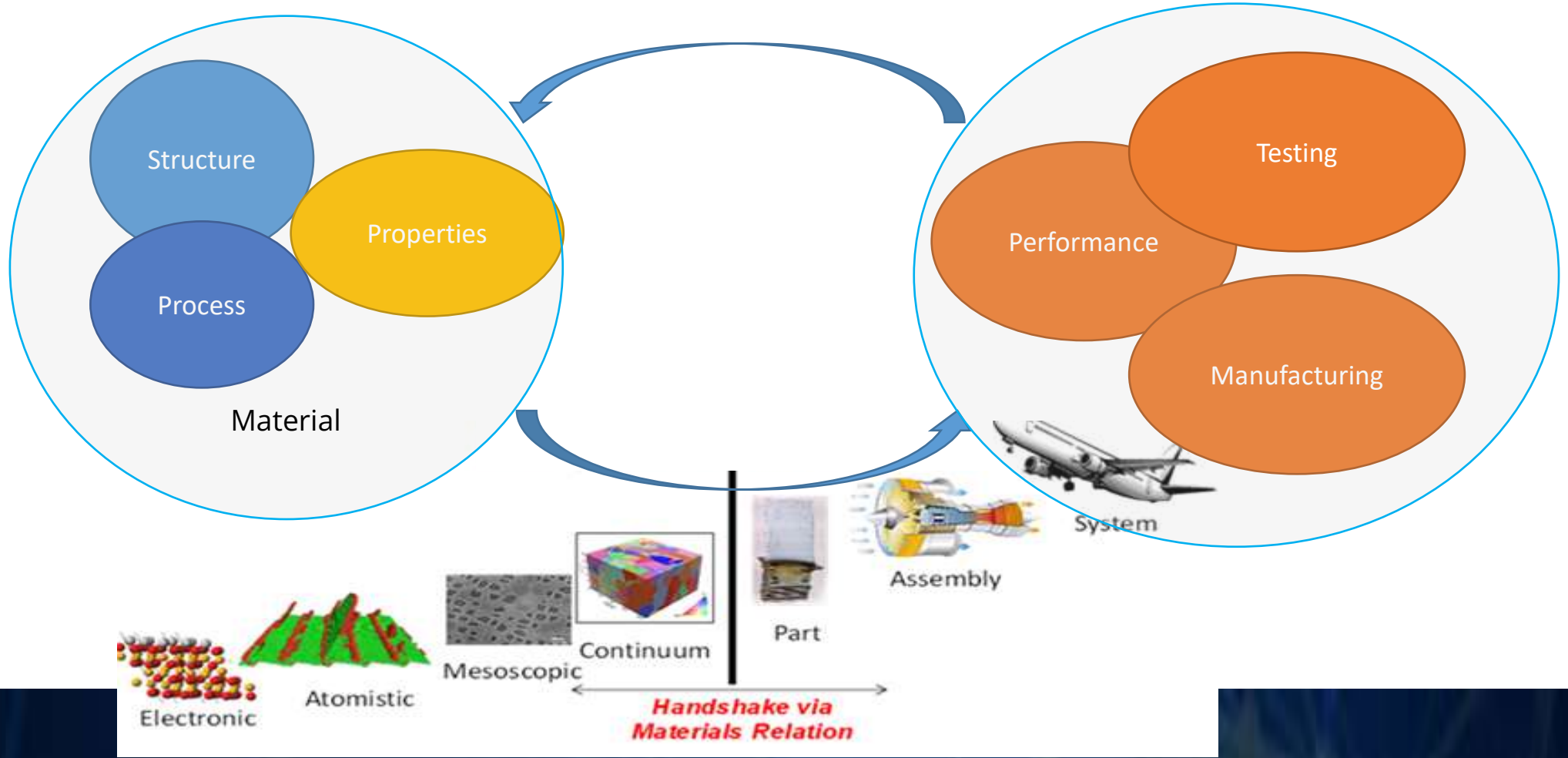
Flow of information, interconnected modelling and characterisation, feedback loops

Materials Modelling and Digitalisation

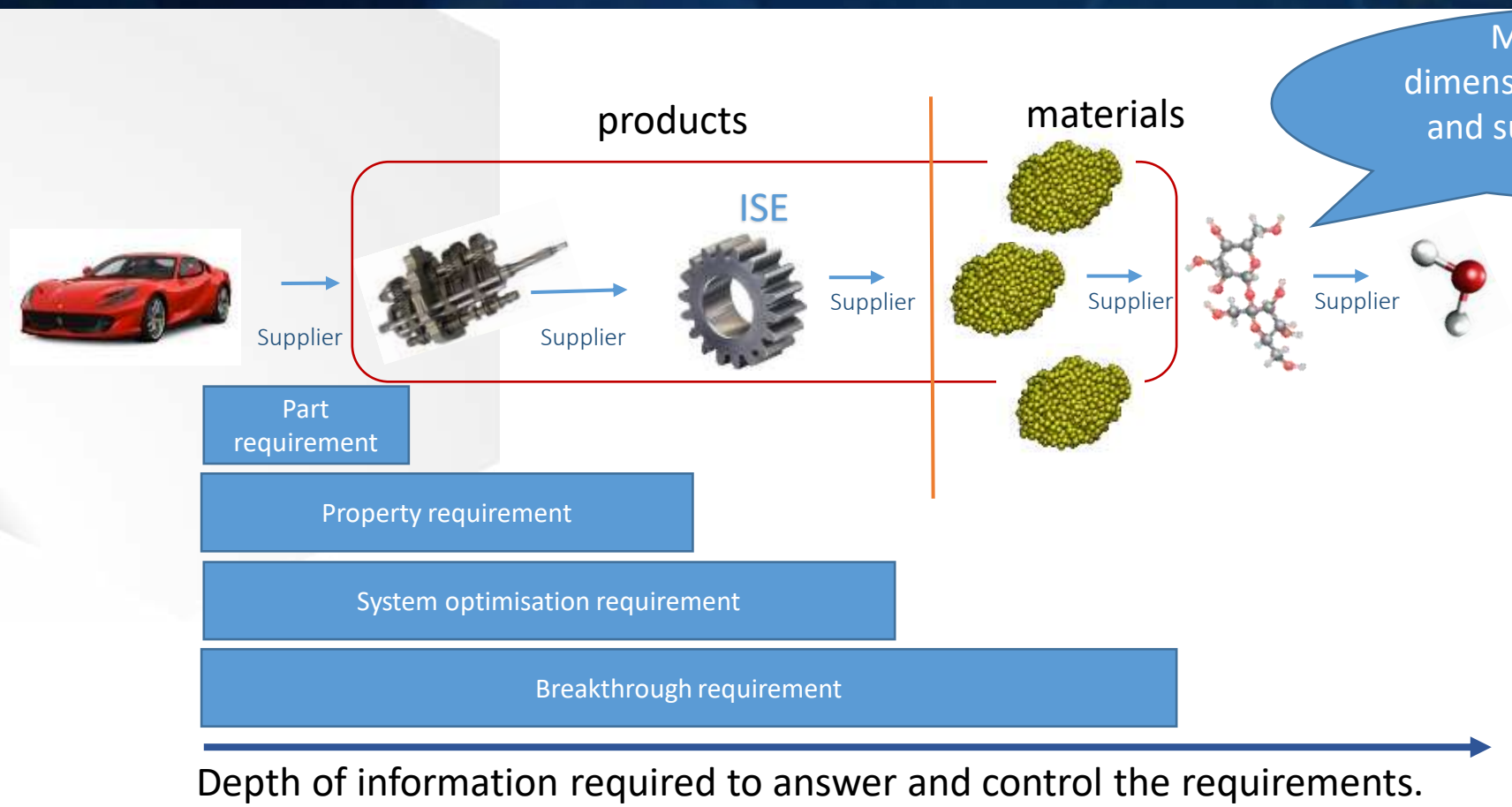
Integrate material/product life cycle management

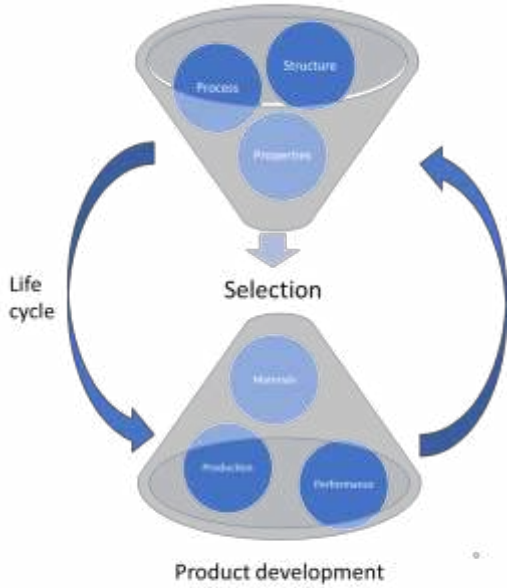
Design of the Material for Products

Design Product with the Material



Knowledge based materials integrate depth of design, sustainability and support breakthroughs

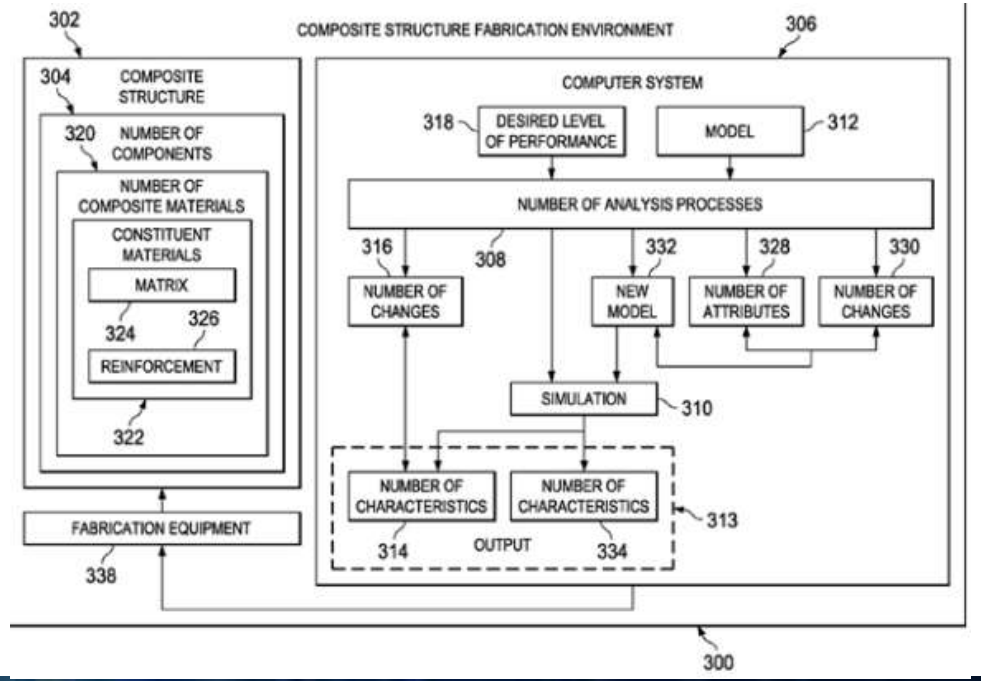




Requires: Interoperability of models and a common ontology

Nothing new, see e.g. Boeing patent: Product Chemical Profile System

- A system that is able to pull together and **query all levels of information about a product down to the chemistry level**
- "A **product-to-chemical continuum** is generated …. to traverse the product-to-chemical continuum through the callout-context pathway segments that **span the plurality of levels**."
- "The product information that matches the set of context search parameters is extracted from the product-to-chemical continuum."

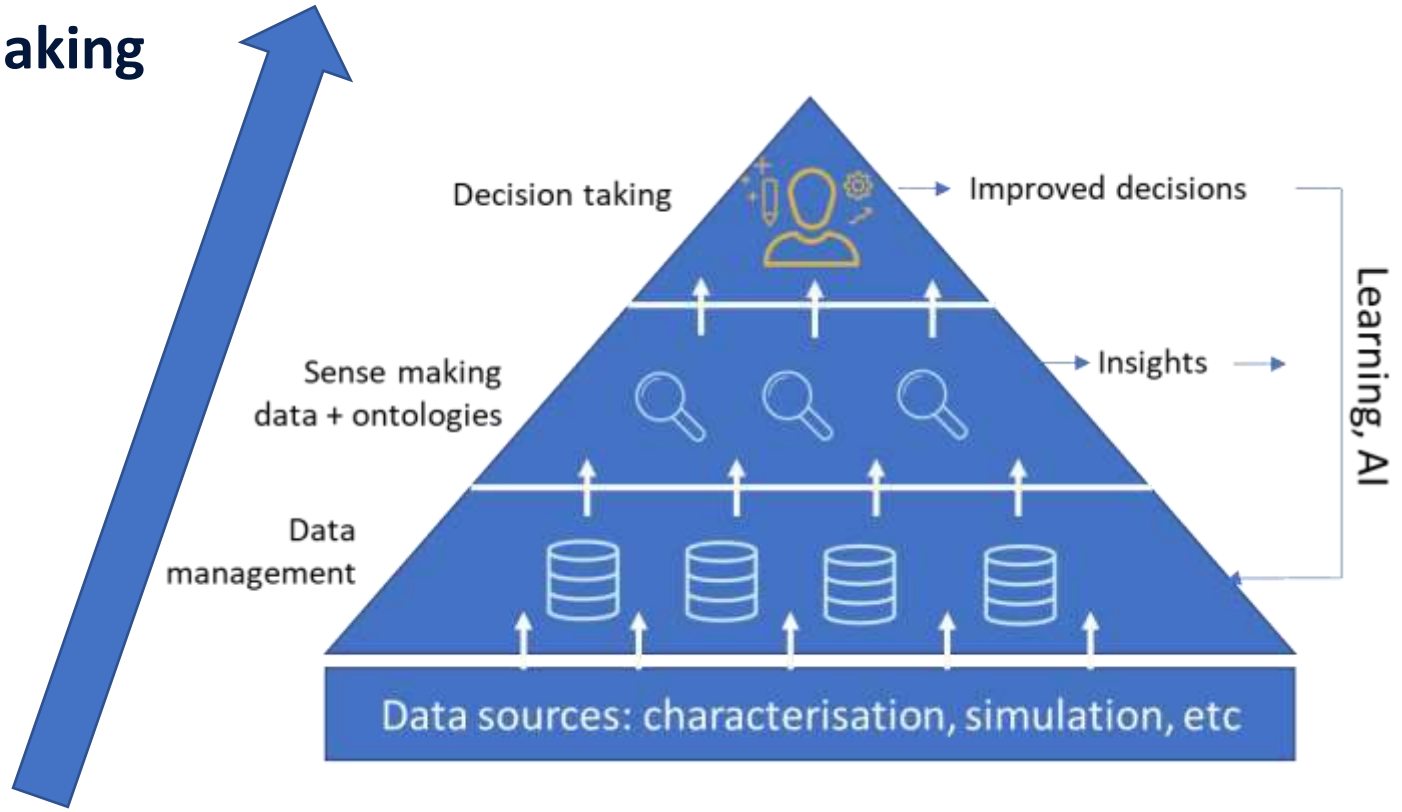


Patent [WO2015060960](WO2015060960) (Filed on 18 Sep 2014)

Vision:
Shared knowledge generation and exploitation

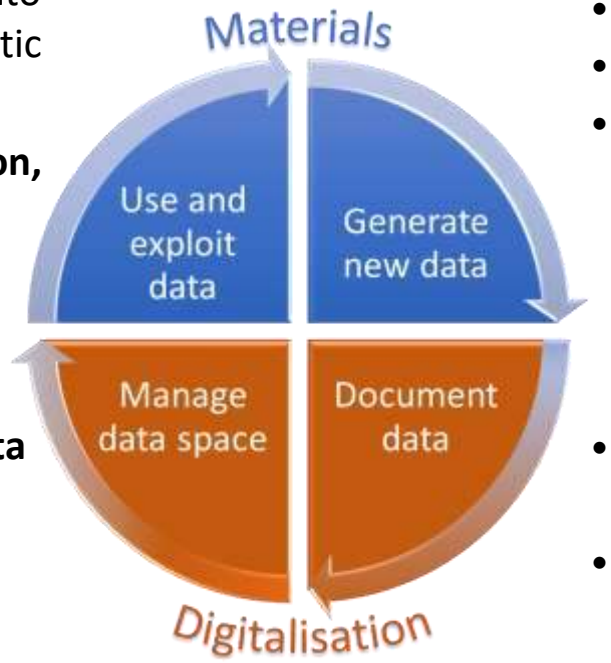
Towards outcome-driven, accelerated materials design, development and use

- **Knowledge exploration and decision making**
  - Exploration of complex information
  - Support multi-criteria decision making
- **Enhanced knowledge generation**
  - AI boosted by ontologies
- **Data documentation**
  - FAIR data, metadadata and ontologies
- **Data/knowledge generators**
  - Materials models (physics and data-based)
  - Characterisation, sensing



Materials Digitalisation: virtuous cycle of activities

- Processing data from multiple sources into **information of added value**, using semantic technologies, ML/AI.
- Methods for **materials data exploration, query, evaluation** (Knowledge graphs etc)



- **Advanced physics-based modelling and AI/ML**
- **Harmonised materials multi-technique workflows**
- **Autonomous labs**

- Development, implementation and governance of **a federated Materials Data Space**
- New set of repositories for **curated materials data** (human and machine)

- **Common "semantics":** materials terminologies, schema and ontologies
- **Standardisation of digital documentation** for all materials data generation technologies

EMMC Roadmap

Advanced Materials Initiative: AMI 2030

1 Lead G. Goldbeck (EMMC)

Activities to accelerate digitalisation in product innovation

- Management of data
- Data-driven development of advanced materials

EMMC contributing to AMI2030; www.ami2030.eu

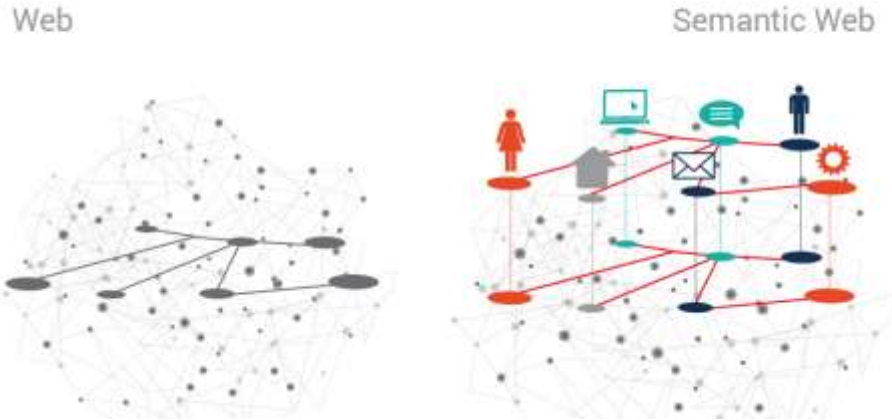
Semantic data management: what and why?

Applying semantic web technologies to the management of data

- **Flexible** Data Model
- **Interconnects** data siloes
- **Saves time, cost, and improves maintainability** relative to e.g. relational databases
- Provides ability **emergent insights** due to reasoning on semantically integrated data

Technology stack includes Ontologies (concepts and their relations)

https://en.wikipedia.org/wiki/Semantic_Web

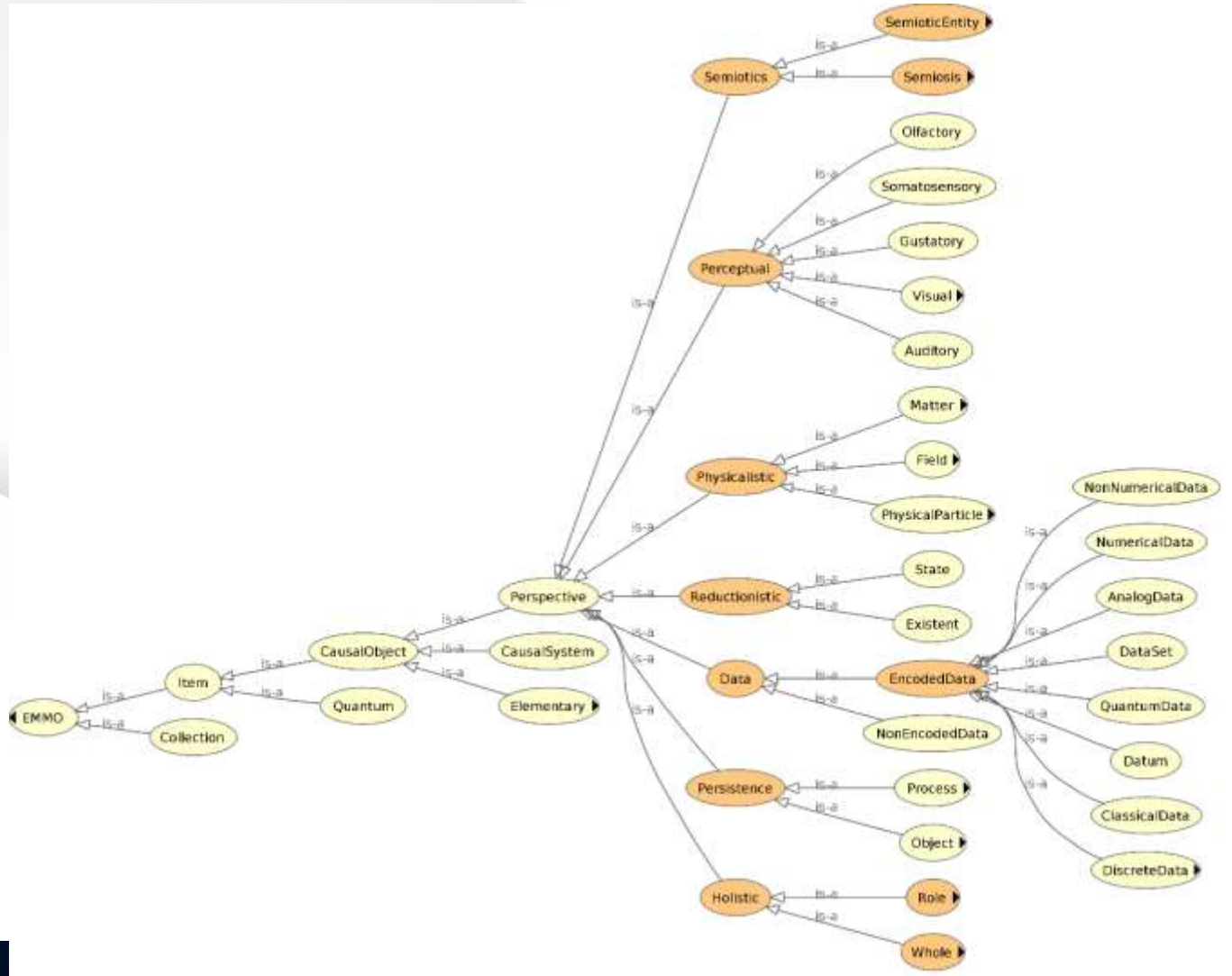


https://devopedia.org/semantic-web

Berners-Lee in 2014

Born	Timothy John Berners-Lee 8 June 1955 (age 68) London, England
Other names	TimBL TBL
Education	The Queen's College, Oxford (BA)
Known for	Invention of the World Wide Web
Spouses	Nancy Carlson (m. 1990; div. 2011) Rosemary Leith (m. 2014)
Children	2 children; 3 step-children

Benefit of an Ontology (in short)



Reasoning:
- possibility to apply constraints to data documentation improving the quality of your databased documentation (consistency)
- inferring new knowledge (e.g., types, relations) from existing one

Interoperability:
- between disciplines, providing a network of relations between entities, and placing them under different perspectives

Expressivity:
- taxonomy, annotations, and relations provides a way to express meaning for a dataset, much powerful than a simple keyword

The Need for a Materials Ontology

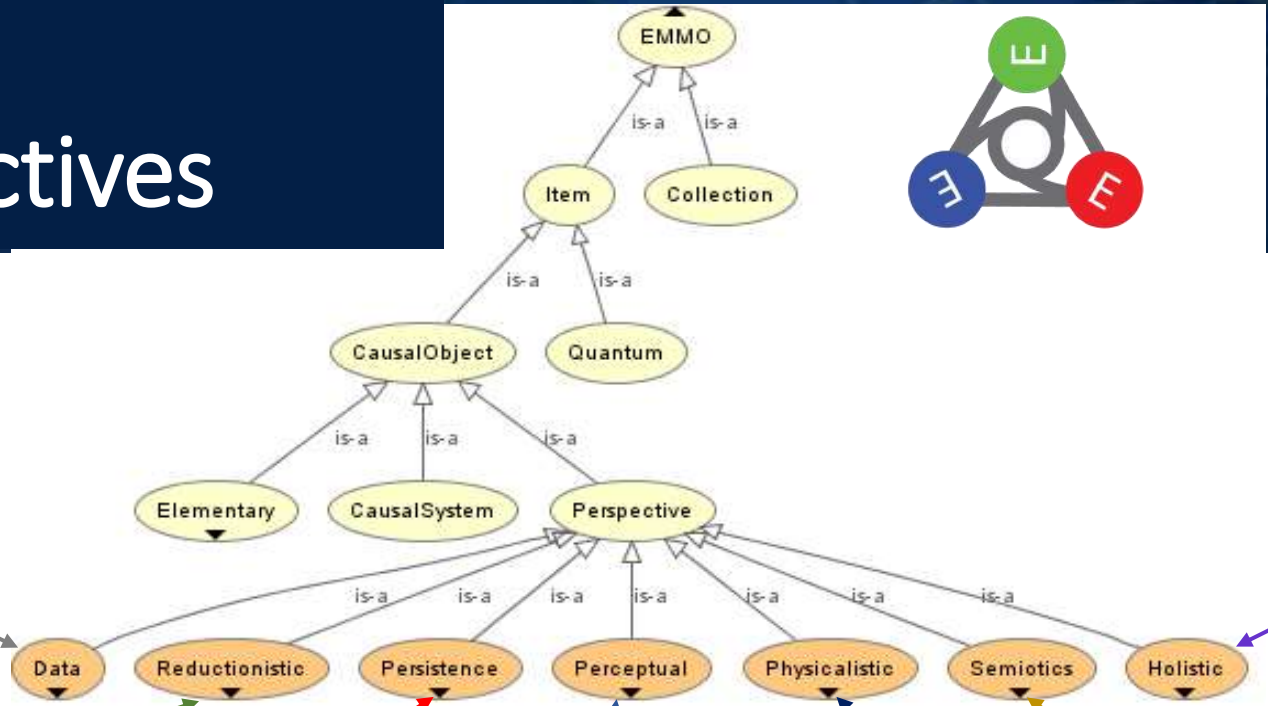
In 2018 several European practitioners in Materials Science under the **governance** of the **EMMC** expressed the need to develop a **knowledge framework** consistent with **scientific principles and methodologies** to complement the **existing physical-mathematical approach.**

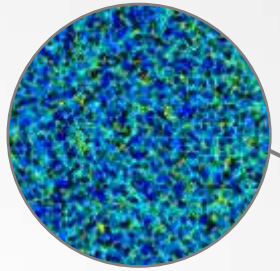
https://emmc.eu/)

The **Elementary Multiperspective Material Ontology (EMMO)** is an ontology developed to represent such knowledge framework.

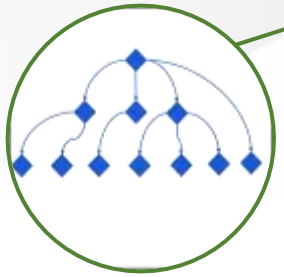
https://github.com/emmo-repo/EMMO

EMMO Perspectives





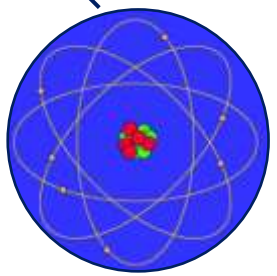
Data
- Contrasts
- Encoded data
- Information



Reductionistic
- Direct parthood
- Countability
- Ordering

Persistence
- Process
- Objects

Perceptual
- Audio
- Visual
- Olfactory etc



Physicalistic
- Matter
- Field
- Material

Semiotics
- Signs/Icons
- Models
- Properties

Holistic
- Whole
- Parts (roles)

Multiperspective example

Physicalistc
A solid which is an aggregate of organic and inorganic molecules

Book

Holistic	Persistence
A whole and an object	

Physicalistic	Reductionistic
A hierarchy of physical entities book -> pages -> paper -> fiber -> …	

Symbolic	Reductionistic
A hierarchy of book -> chapters -> paragraphs -> words -> symbols	

Semiotics
A sign that stands e.g. for the life of a person

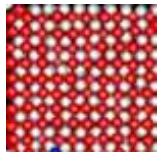
Reductionism: multiscale perspective

has_part

has_part

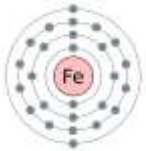
has_part

has_part

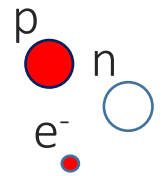


has_part

has_part



has_part

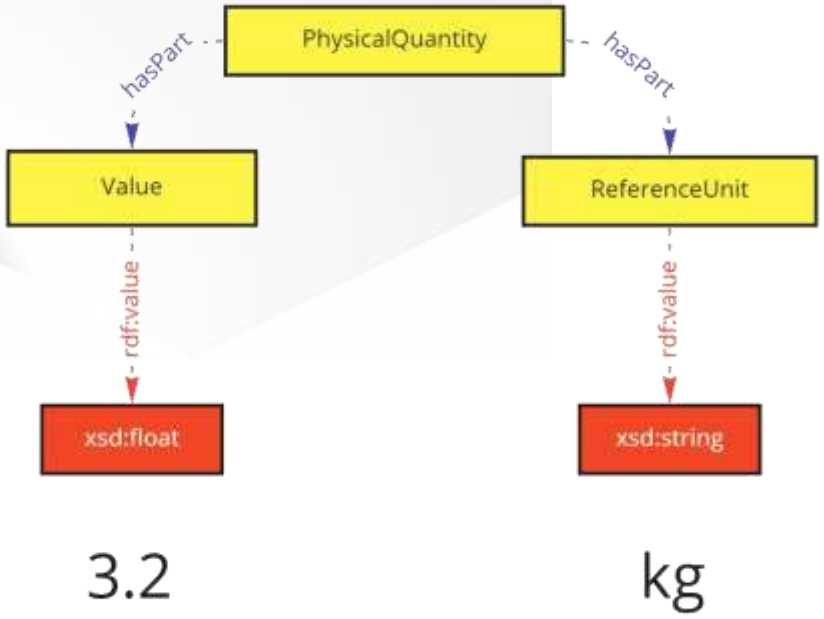


Material can be represented at different levels of granularity, depending on **perspective**.

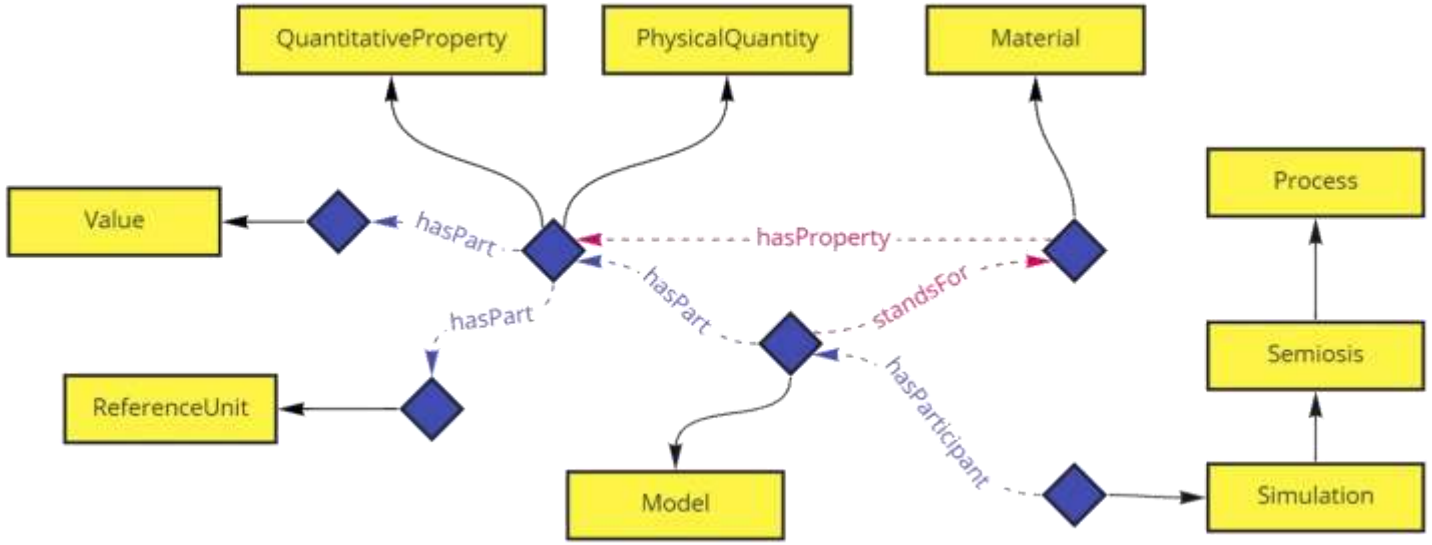
The ontology gives information about the **direct upper and the direct lower levels types**.

Materials properties

Physical Quantities are represented as **syntactical structures** of numbers and strings, and **stored in RDFS format**.

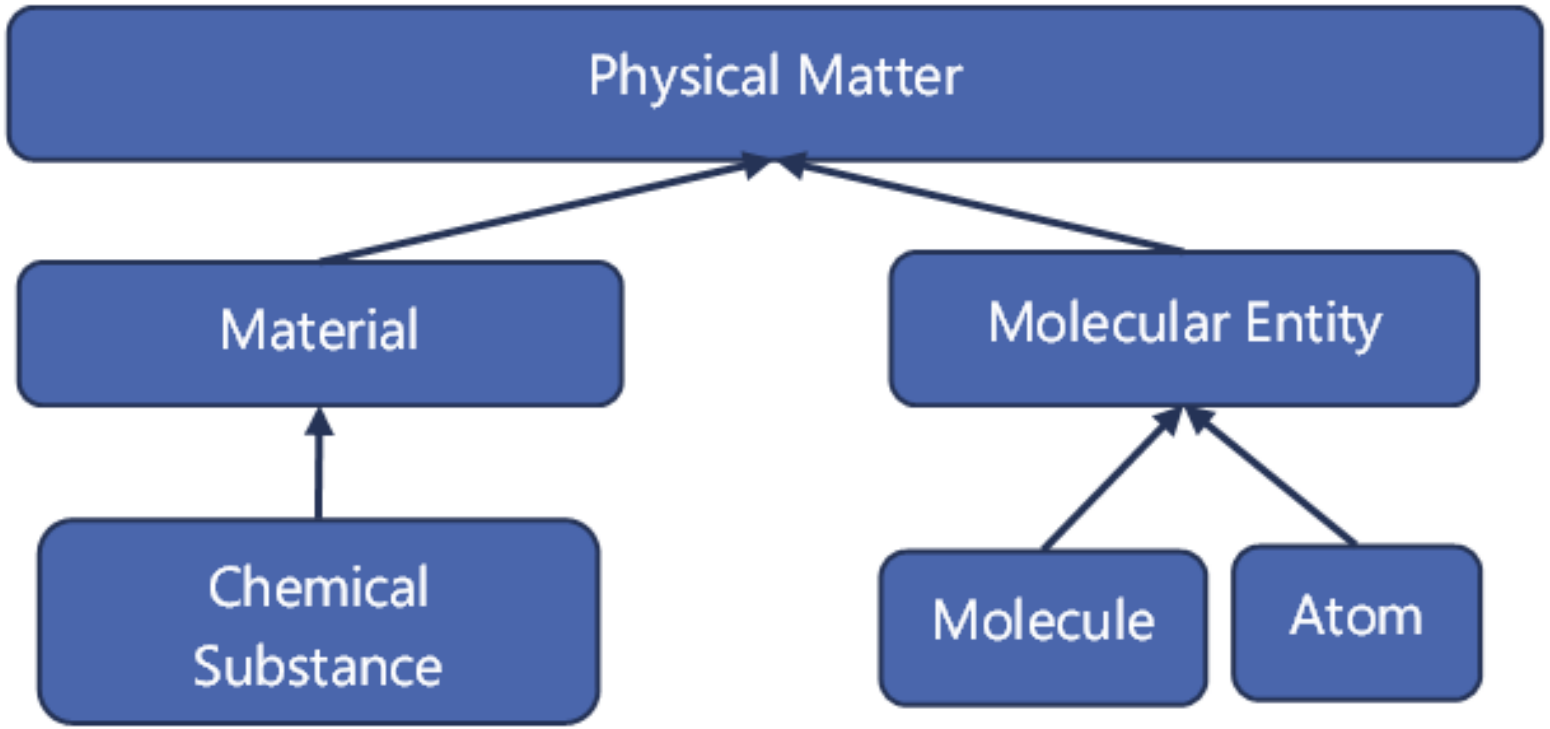


QuantitativeProperties are physical quantities that are connected to a material through a **semiotic process** of **simulation**.

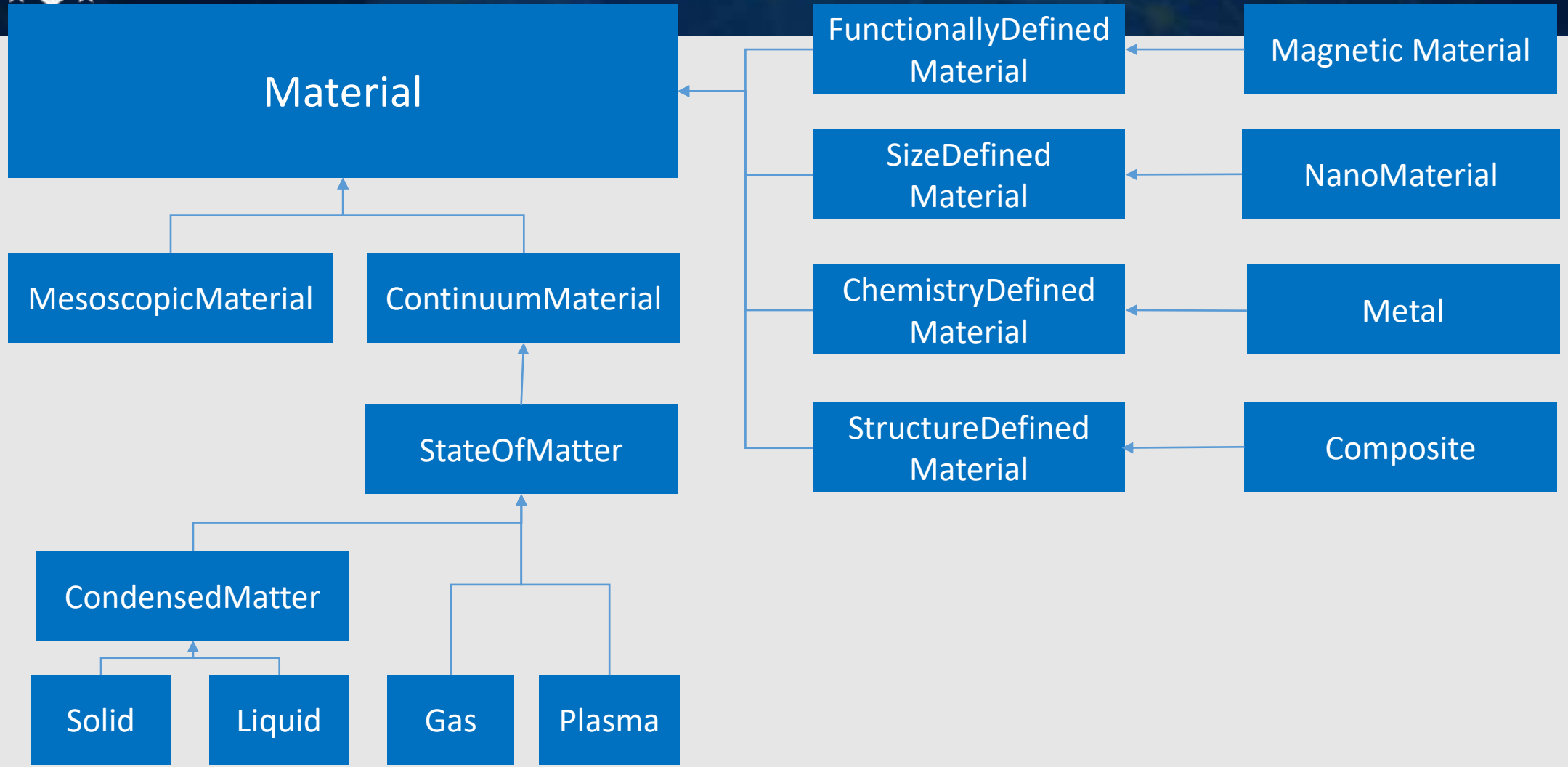


EMMO also includes SI and QUDT Units Ontology, VIM etc, i.e. all de facto standards

Materials and Chemistry Classes in EMMO



Materials classes in EMMO



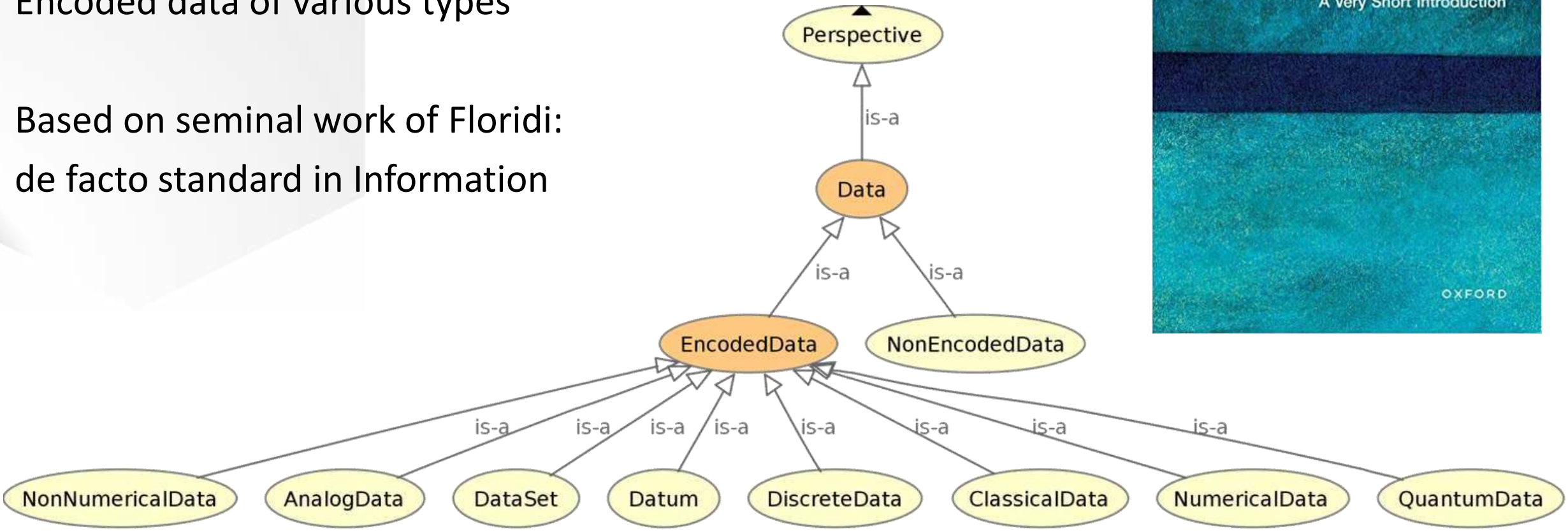
DATA

Data as physical patterns in general

Encoded data of various types

Based on seminal work of Floridi:

de facto standard in Information

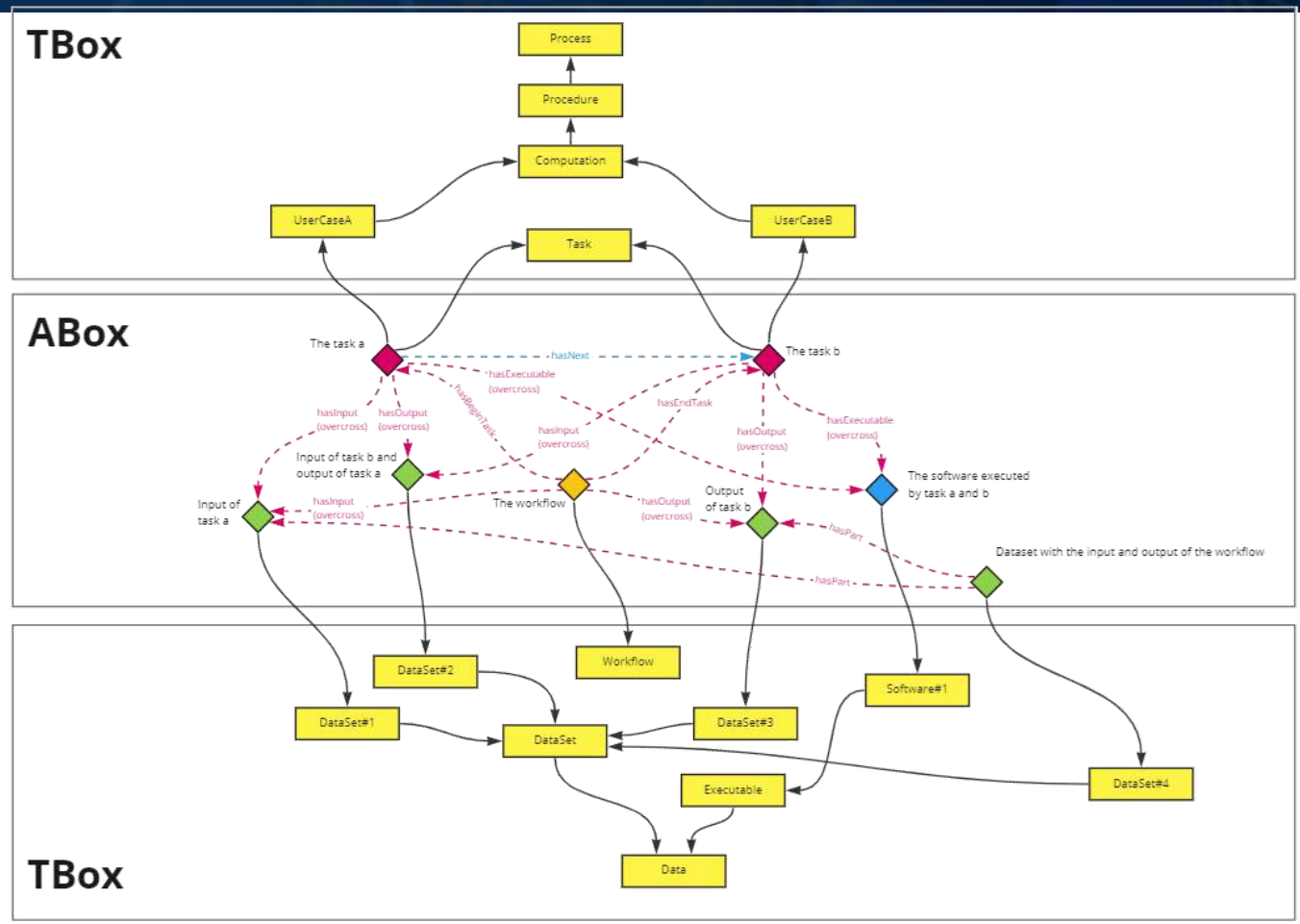


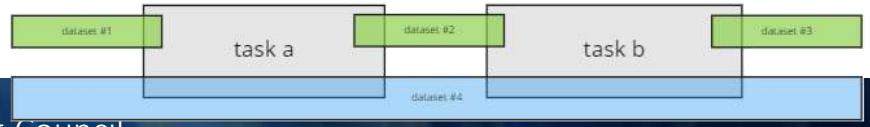
Simulations

Representation of **executables workflows**.

Process and Data Perspectives combine to represent different aspects.

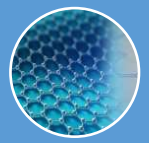
Tasks in a workflow are treated in a **multigranular** way.





Conclusions

- EMMC is the community for materials modelling and semantics: “digital materials”
- EMMC supports all stakeholders in responding to ever more complex requirements for materials and products addressing.
- Activities include
  - Materials modelling for innovation and as reliable data/knowledge sources
  - Data/knowledge integration via terminology standards and ontologies


Materials Science


Materials Processing


Materials Engineering


Materials Production

Flow of information, interconnected modelling and characterisation, feedback loops

Contributing projects acknowledgement

Join us: https://emmc.eu/register/

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Many EMMC Members contributed via inputs to roadmaps, workshops, position documents that have been used as a basis for this presentation