



Interoperability approaches and implementations in current EU Projects

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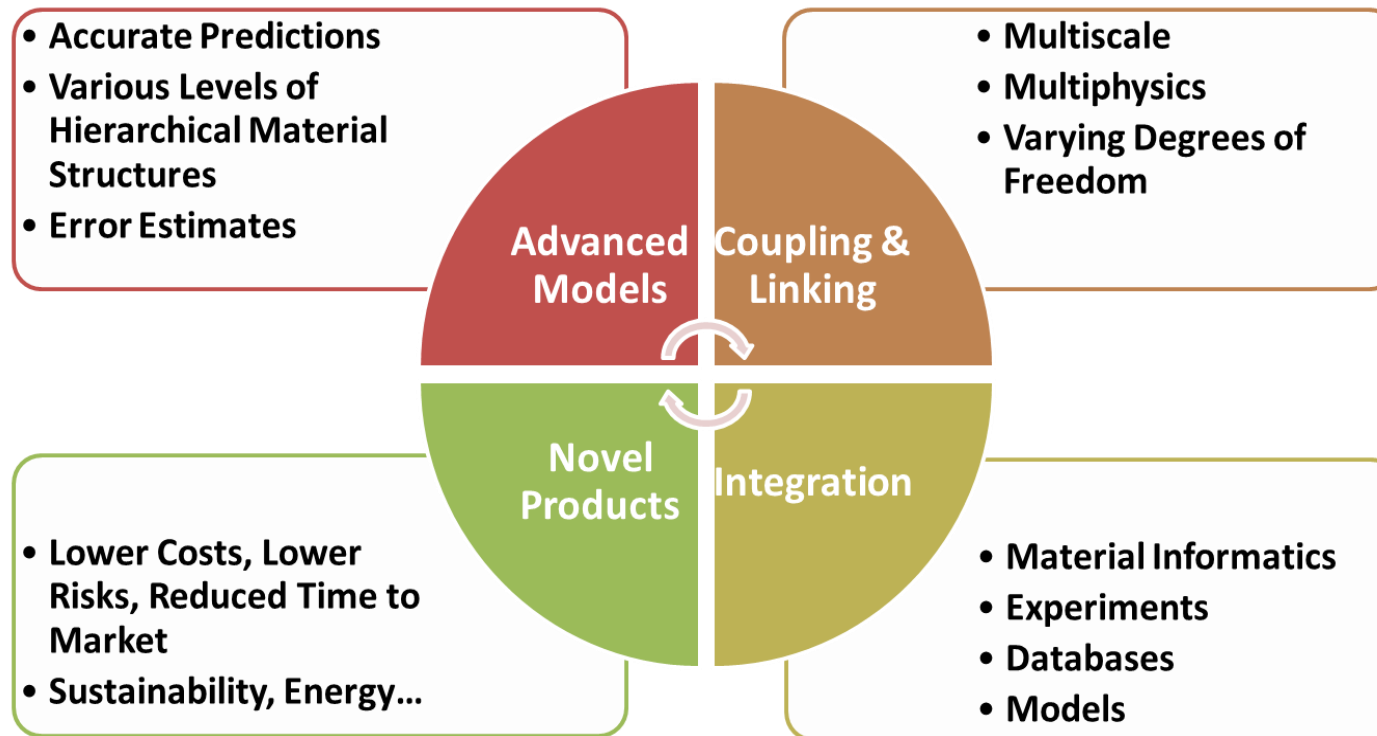
Outline

- Overview of EMMC past activities and EU projects with respect to interoperability
- Current and coming EU projects
- Future: Cross domain Interoperability materials modelling in the EU
 - *European Materials Modelling Ontology EMMO! And EMMO-schema*

- Paradigm shift in the way materials are developed



<http://emmc.info>



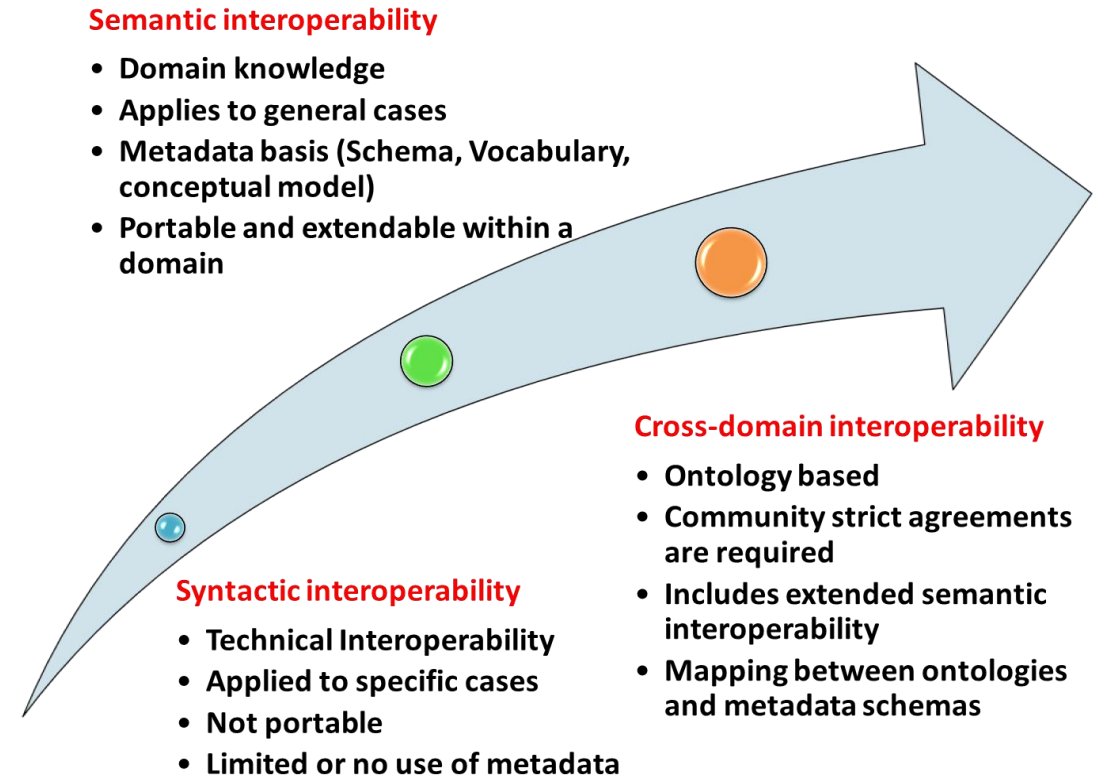


Approaches to interoperability

- In modeling, the focus is on integrating (existing) knowledge (**models and data**) to enable further progress in modeling
- Integration focuses on combining individually developed models/software tools into an integrated, complex workflows
- **Interoperability** is mutual capability to exchange and interpret the information
 - **By definition, it implies standards**
 - **Data:** Facts (elastic constants, colour, etc.)
 - **Information:** Data in a context (relations), describe what the data is
 - **Knowledge:** Our understanding/interpretation/analysis

Needs semantics
which demands
an ontology

- **Syntactic interoperability**
 - Data and operations are typically exchanged using specific protocols (e.g., input/output files)
 - Requires to develop and maintain **specific** conversion tools between each and every individual code/model
 - **Limited extensibility, high maintenance cost**
- **Semantic interoperability**
 - Exchanges data and meaning (**semantic knowledge**), requires agreed vocabularies (meaning) and relations → ontologies
 - Allows machine interpretation, automated translation, verification → **Knowledge bits**
- **Cross-domain interoperability**
 - Allows different systems, platforms from different domains to interact and exchange data
 - Requires upper ontology: BFO-EMMO





Practical Integration approaches & Interoperability

- **Object-oriented/Component based approaches**
 - standardization of operations on model (and data components)
 - common interfaces (e.g., API)
 - Examples: Corba, CCA (Common Component Architecture)
- **Service-oriented approaches**
 - standardization of services
 - Emphasis on internet technologies, services being remotely discoverable and executable.
 - Examples: webservices
- **Data-centric approaches**
 - standardization of data representation and conversion
- Each may be implemented in any level of interoperability
- Ontology-Based approaches are most **practical** in the long term!

Advantages
(with respect to syntactic):

- sustainability
- extendability
- low total cost of ownership
- enhanced collaboration between communities

- Initial efforts in previous activities within EU Multiscale Materials Modelling Cluster (5+1)
 - 5 modeling projects under NMP.2013.1.4-1 call: *Development of an integrated multi-scale modelling environment for nanomaterials and systems by design*
 - **NanoSim** <http://www.sintef.no/projectweb/nanosim/>
 - **SIMPHONY** <http://www.simphony-project.eu/>
 - **MMP**, <http://mmp-project.eu>
 - **MODENA**, <http://modena.units.it>
 - **DEEPEN** Nanostructures, <http://www.nmp-deepen.eu/>
 - ICMEg CSA (icmeg.eu)
- EMMC Interoperability and Integration and open simulation platforms working groups, <http://emmc.info>





Interoperability Approaches in EU Projects

Project	Object-oriented	Service-oriented	Data-centric	Syntactic – Semantic (1-5)
DEEPEN	No	Yes (Unicore)	Yes	3-4
MODENA	Yes (Fireworks)	No	No	2-3
NanoSim	Partially	No	Yes	4
COMPOSELECTOR MMP	Yes	Partially	No	3-4
FORCE SIMPHONY	Yes	Yes	Yes	3-4



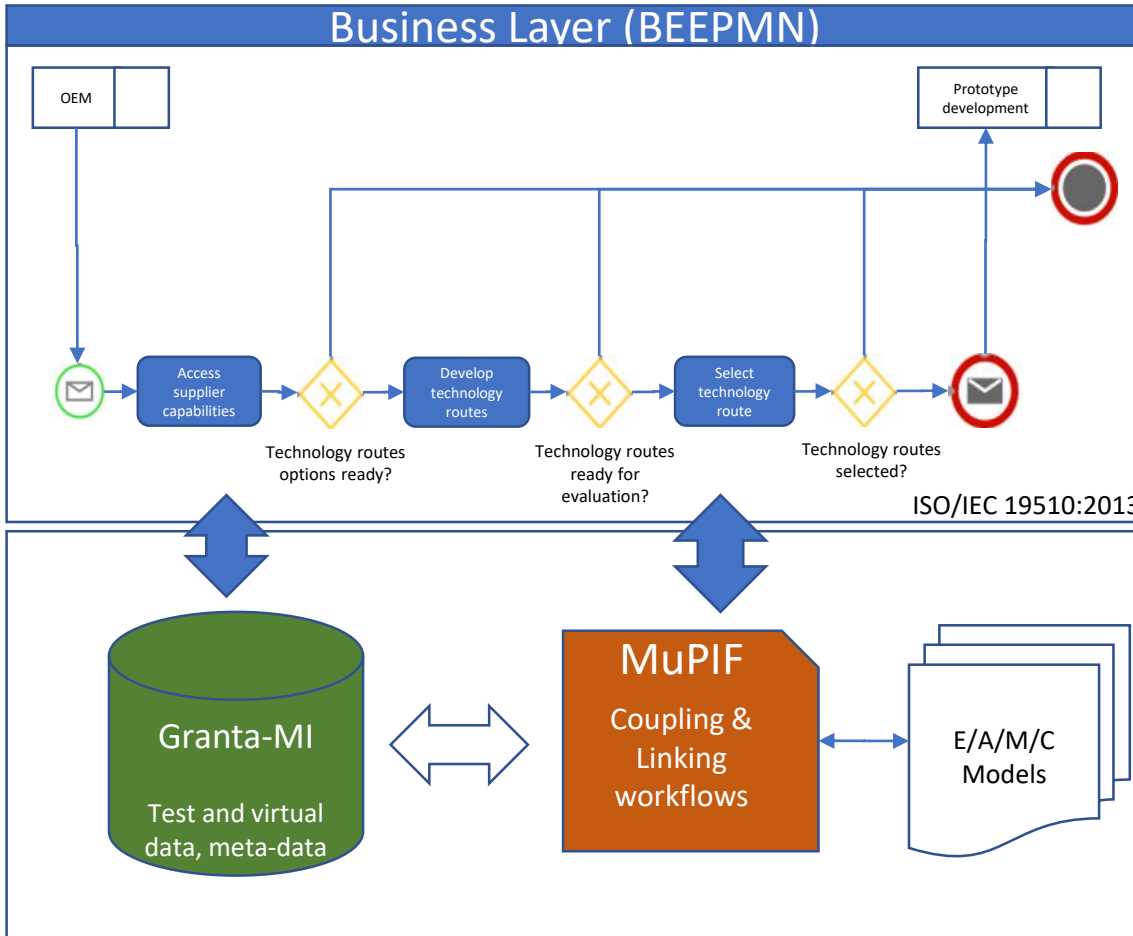
Current EU projects

- The EMMC EMMO activity (see presentation by Emanuele Ghedini later)
- Two new RIA projects under NMBP-23-2016 - Advancing the integration of Materials Modelling in Business Processes to enhance effective industrial decision making and increase competitiveness
 - **FORCE project**
 - Formulations and Computational Engineering (FORCE)
 - Develop a integrated Business Decision Support System (BDSS) based on open standards for industries engaged in formulating chemical ingredients, <https://www.the-force-project.eu/>
 - **COMPOSELECTOR**
 - Multi-scale Composite Material Selection Platform with a Seamless Integration of Material Models and Multidisciplinary Design Framework, <https://www.composelector.net/>
- **NanoSim** (last year)
- And more to come (see presentation by Welch Leite Cavalcanti later)

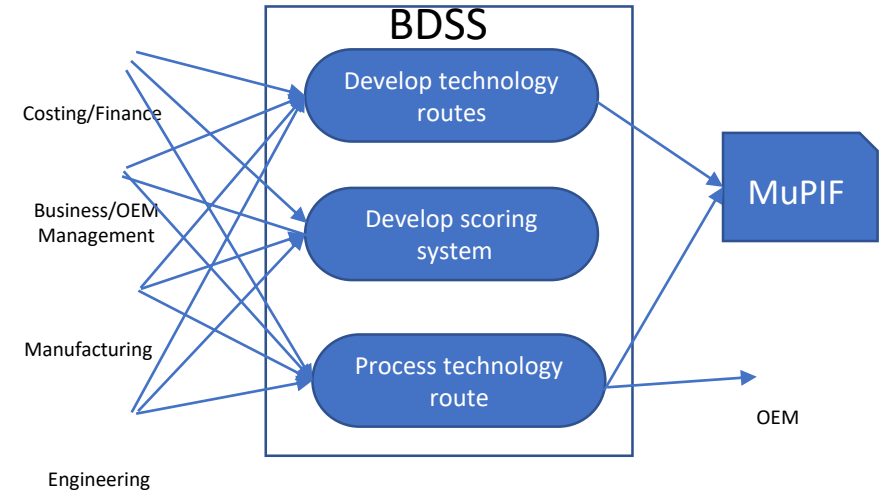


Composelector project

Multidisciplinary optimization, uncertainty, model selection

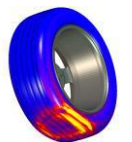
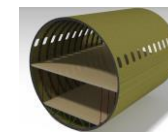


DECISION SUPPORT APPS
LCE, Light Weighting, Visualization Costing, Res Subs Assessment. etc...



Application cases

- Material and Process Selection of fuselage thermoplastic frame
- Material and manufacturing of Composite Leaf Spring
- Material and process selection of tire

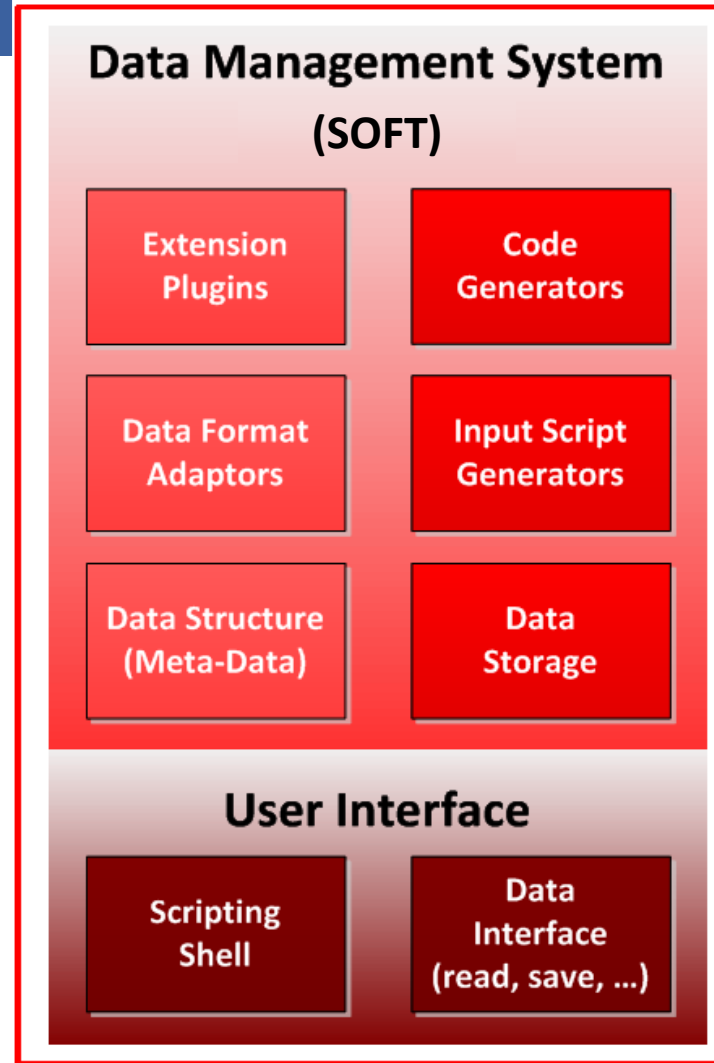




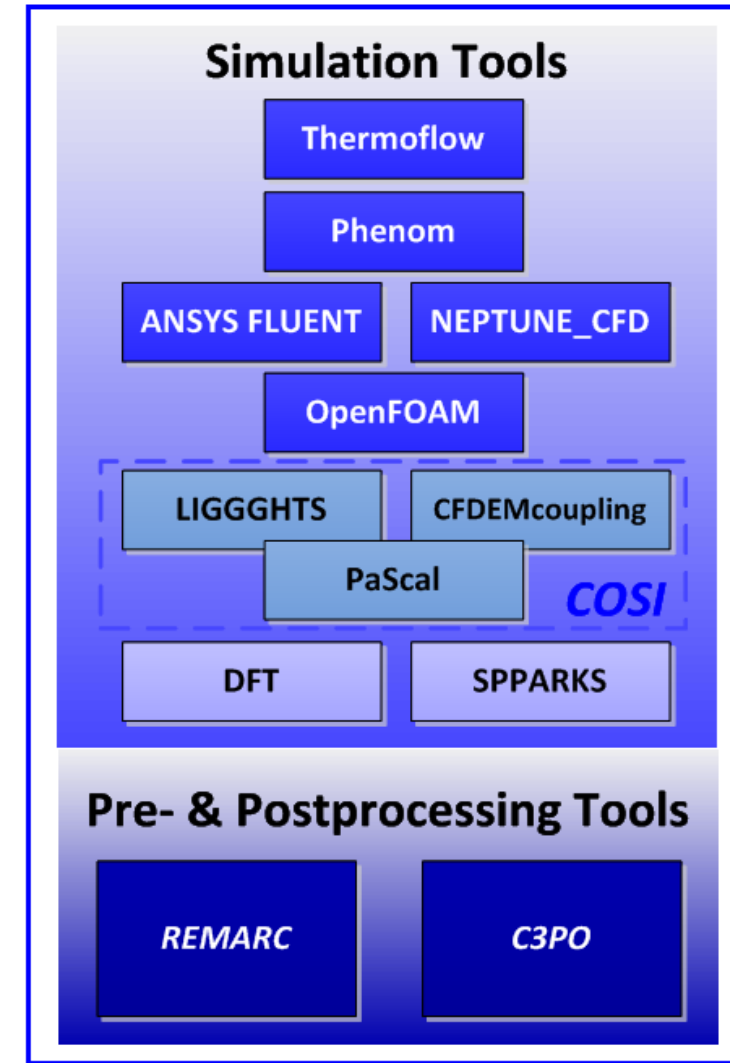
Multi-scale Simulation-Based Design Platform for Cost-Effective CO₂ Capture Processes using Nano-Structured Materials

- Porto:
 - open-source computational platform based on SOFT
 - <https://github.com/NanoSim/Porto>

Common Environment Software Platform (*Porto*)



Simulation Software Platform



Users & Developers
(students, researchers, engineers)



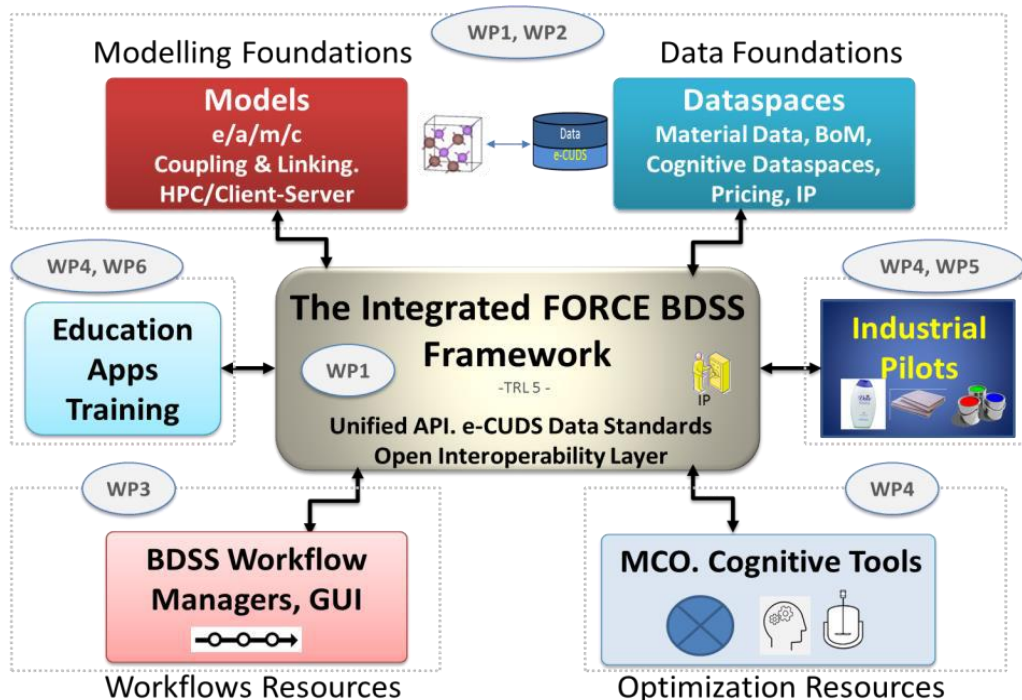


Force project

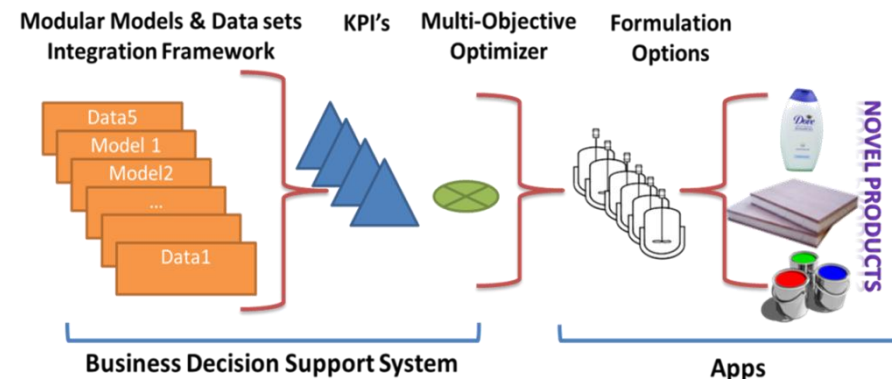


<https://www.the-force-project.eu/>

CO: Dr. Adham Hashibon, Fraunhofer IWM.



CUDS of SimPhoNy → EMMC EMMO-Schema



Personal care liquids:
Design consumer segmented personal care fluids

Rigid PU foams:
Low K-value PU insulation

Fast curing inks:
PU process optimisation & ink formulation design

Project Info Box	
Project Website:	http://The-FORCE-Project.eu
Project Acronym	FORCE
Project Email:	info@the-force-project.eu
EC Grant Agreement No.	721027
Start date	1.1.2017, duration 4 years
Coordinator	Dr. Adham Hashibon, Fraunhofer IWM (DE)
Email:	Adham.hashibon@iwm.fraunhofer.de



Reuse of existing tools and established codes

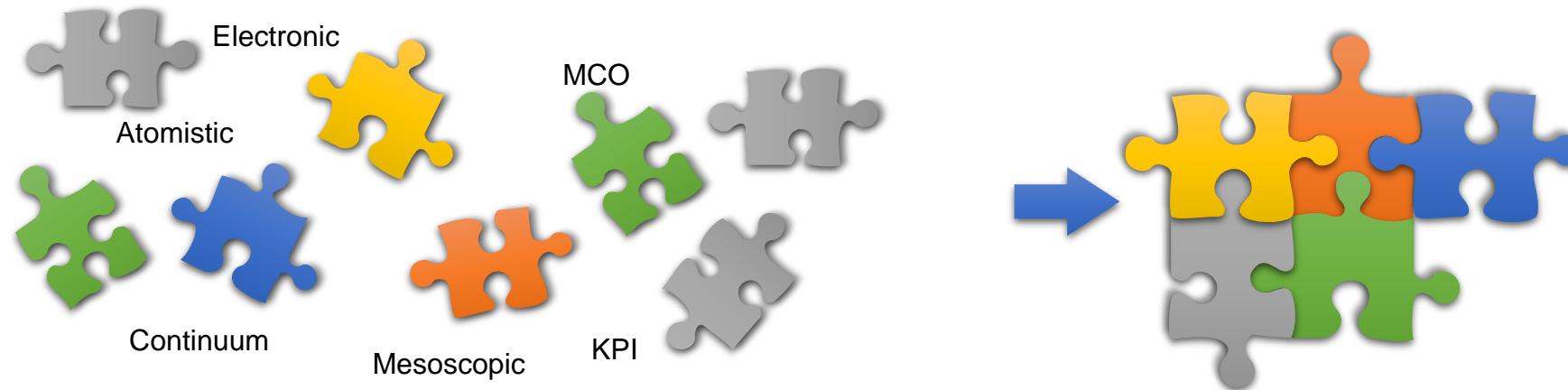
Open data standards and Common API

Interoperability supported by EMMO ontology

Object Oriented, Data centric, Service Oriented

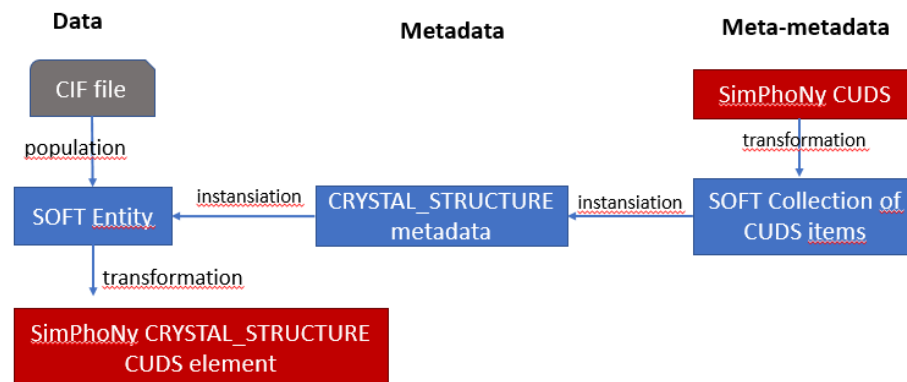
- Standard API providing CRUD operations (Create, Read, Update, Delete)
- EMMO-based metadata schema for annotating data (metadata)
- Extensive use of MODA and extended MODA to extract standards

CUDS of SimPhoNy → EMMC
EMMO-Schema



The goal is semantic, cross-domain interoperability

- Preliminary work in the cluster 5+1, EMMC provides proof of concept connection between NanoSim and SimPhoNy (A demo showing how a CIF file can be read by SOFT to generate a SimPhoNy CRYSTAL_STRUCTURE)
- Work ongoing between COMPOSELECTOR and FORCE
 - Extend ontology to describe methods
 - Achieve platform level Interoperability





Thank You