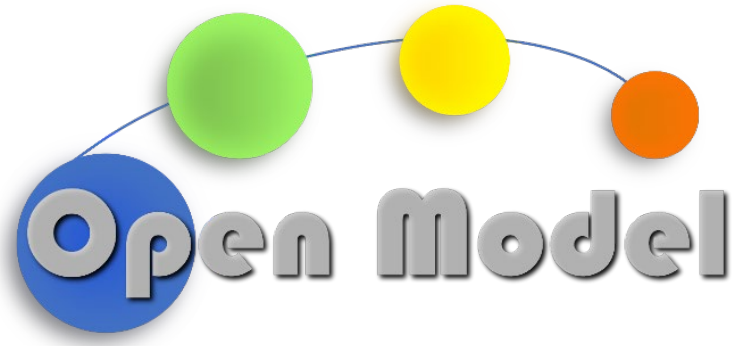
Jesper Friis (SINTEF)
Francesca Lønstad Bleken (SINTEF)
Welchy Leite Cavalcanti (FRAUNHOFER)



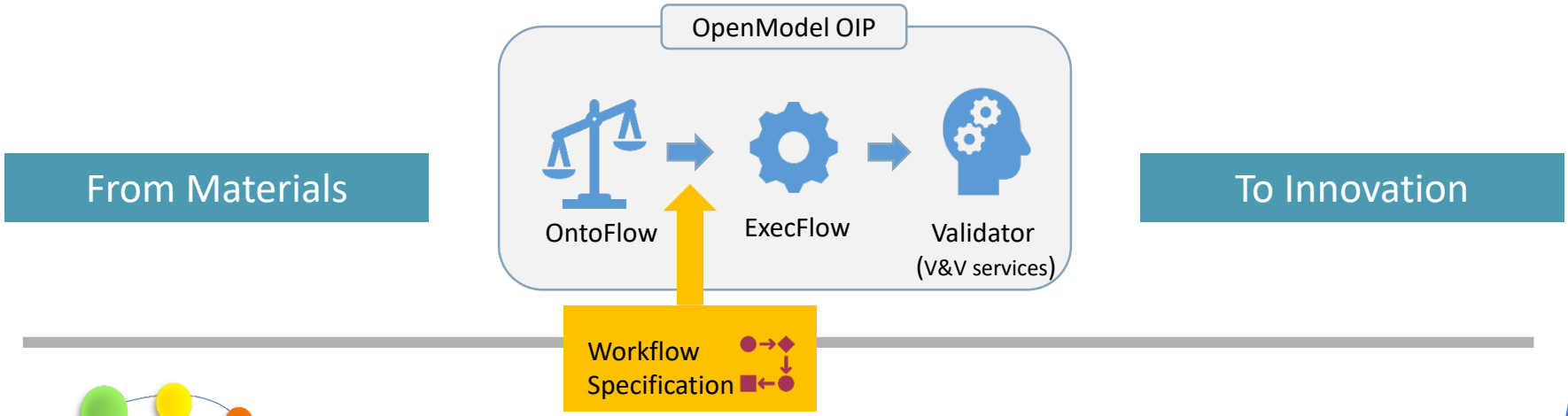
Introduction to the OIP projects: OpenModel

OpenModel Project

www.open-model.eu

- H2020 Project
  - Integrated Open Access Materials Modelling Innovation Platform for Europe - OpenModel (GA 953167)
  - H2020 (NMBP-11-2020)
  - 4 years project – started on 01.02.2021

An open-access materials modelling platform that aims to provide a comprehensive solution for Europe's materials modelling needs.
The ultimate goal is to standardise **materials modelling workflows**, provide easy access to data and foster innovation.

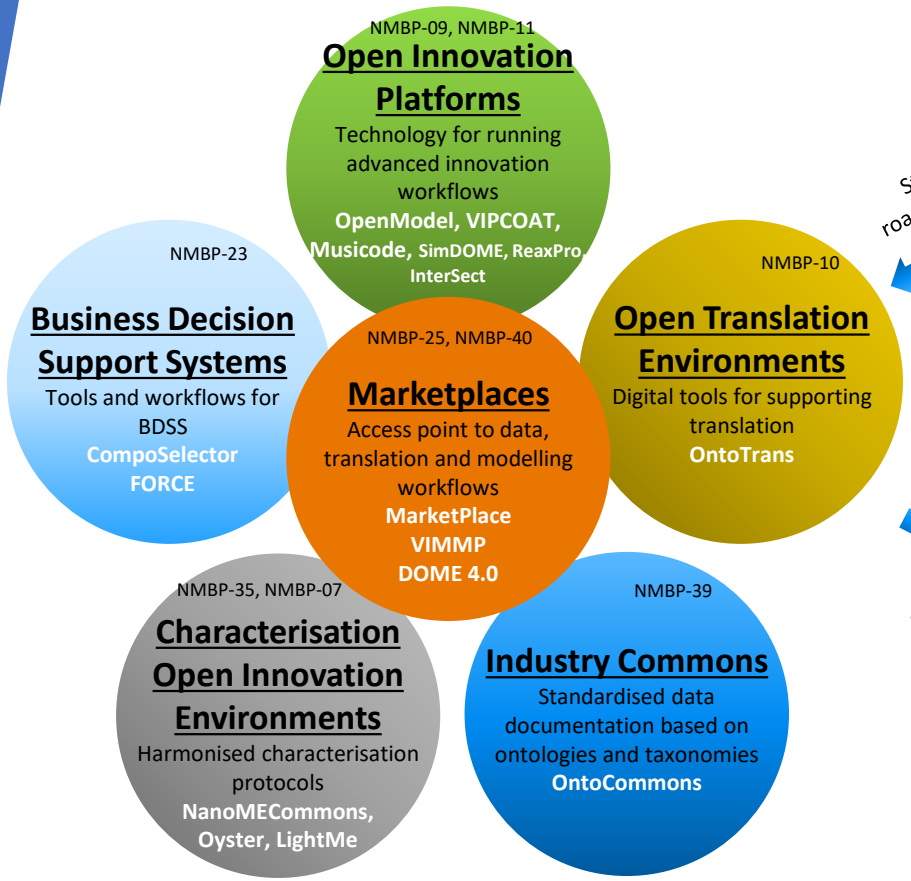


OpenModel partners

OpenModel PARTNERS: Comprising all stakeholders type

OPEN MODEL MOTIVATION

Provide technology for running advanced innovation workflows



Strategies, roadmaps, overall picture

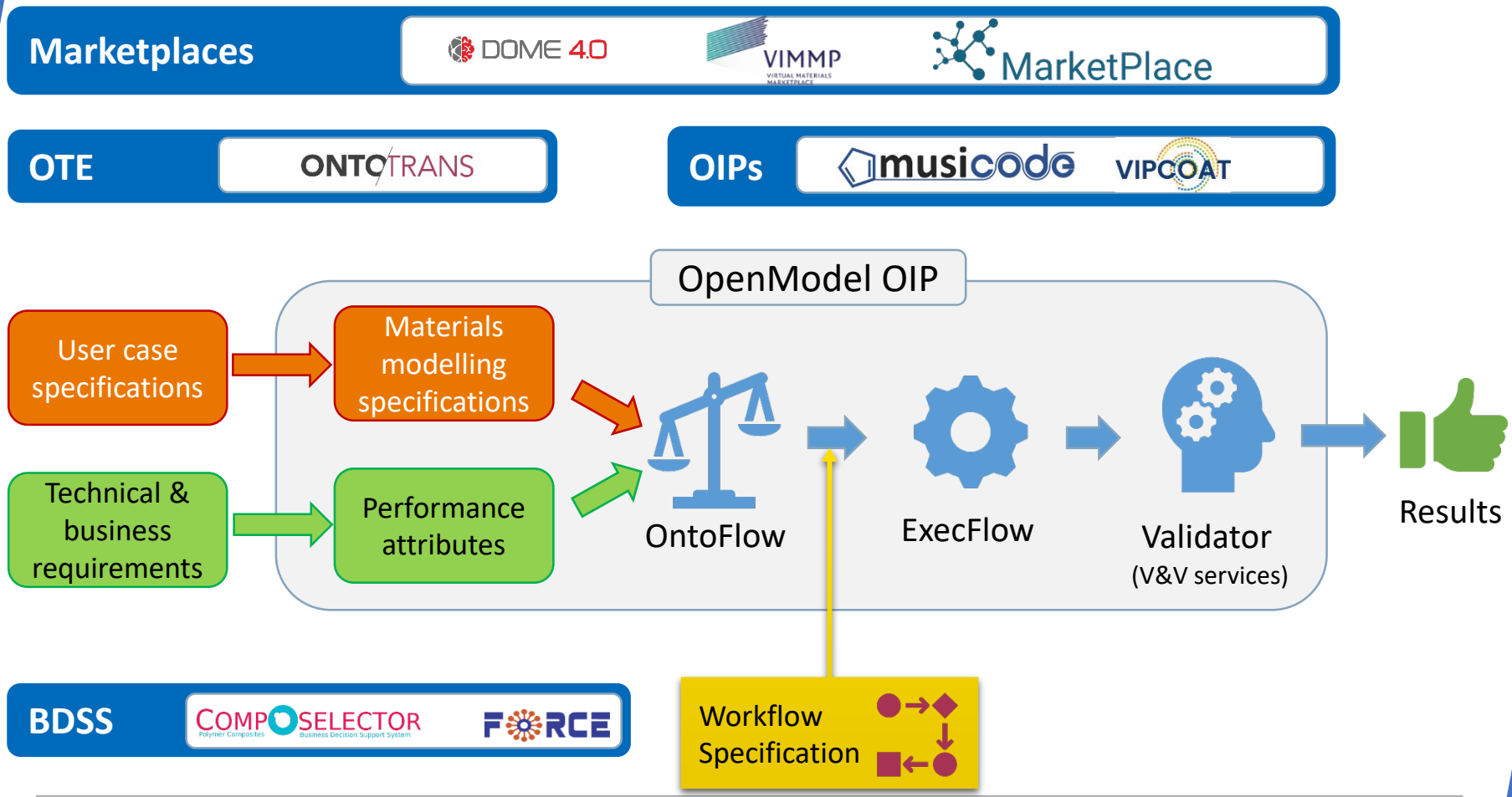
EC
Promotes European interests (peace, sustainable development, …)
Means: Creates calls and provide funding

EMMC
Supports industrial uptake of materials modelling.
Means: Workshops, roadmaps, standardisation efforts (e.g. EMMO)

Infrastructure solutions and components

Industrial uptake and related projects utilising the infrastructure

OpenModel MAIN CONCEPTS



OpenModel Ontologies

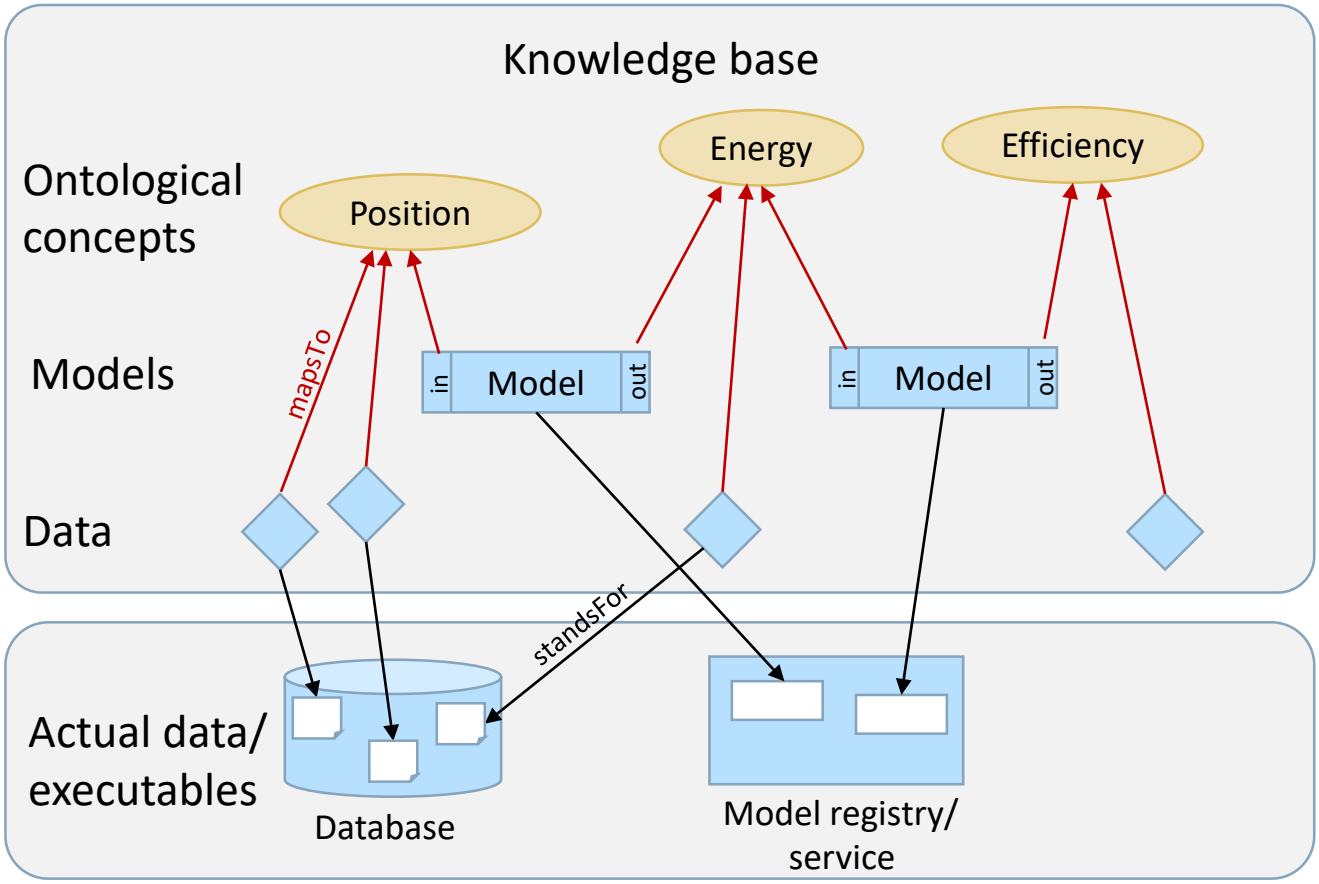
- Currently developing workflow and model basics in EMMO-middle, jointly with OntoTrans.

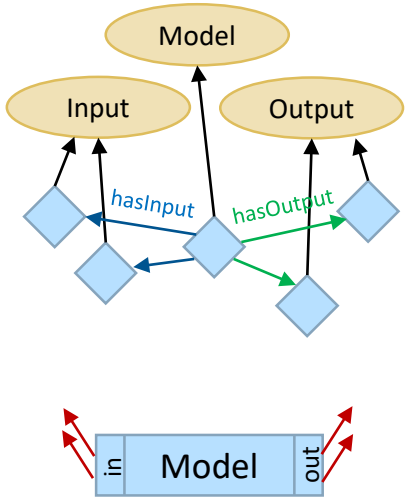
- Workflow Ontology
- Performance Attribute Ontology
- Generic V&V ontology

- Forming an EMMC task group focused on workflow ontologies.

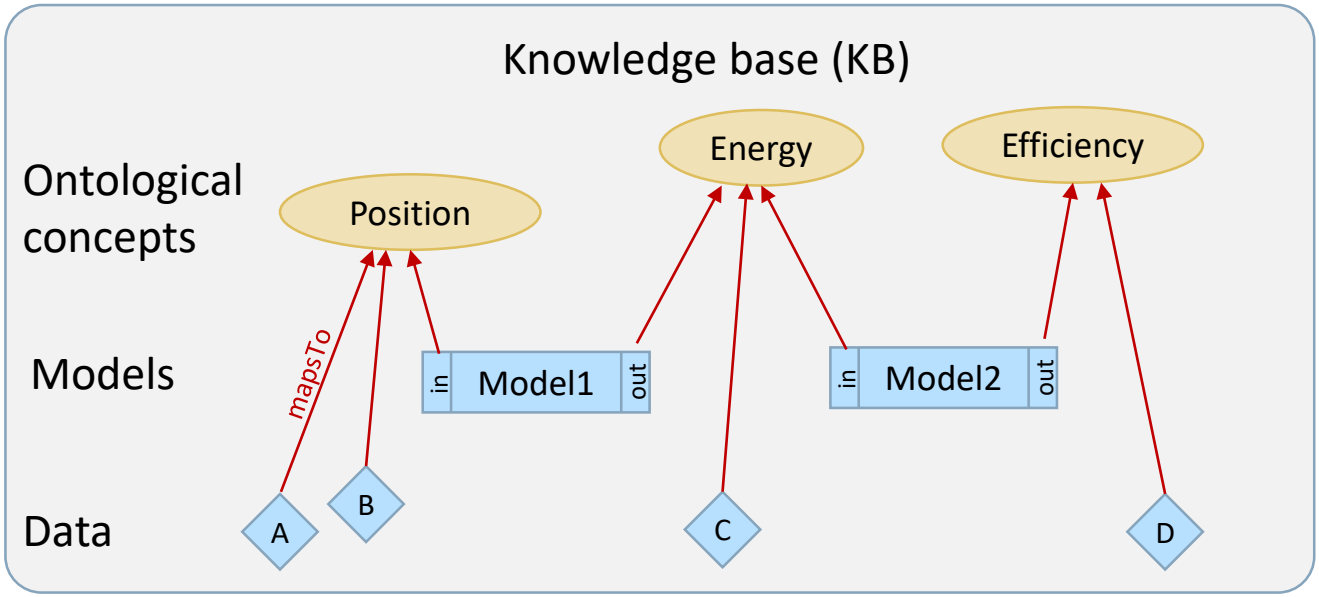
- Application ontologies
  - Specified (workflow, attributes, V&V)
  - Domains
  - Application

OpenModel Semantic workflow builder / OntoFlow





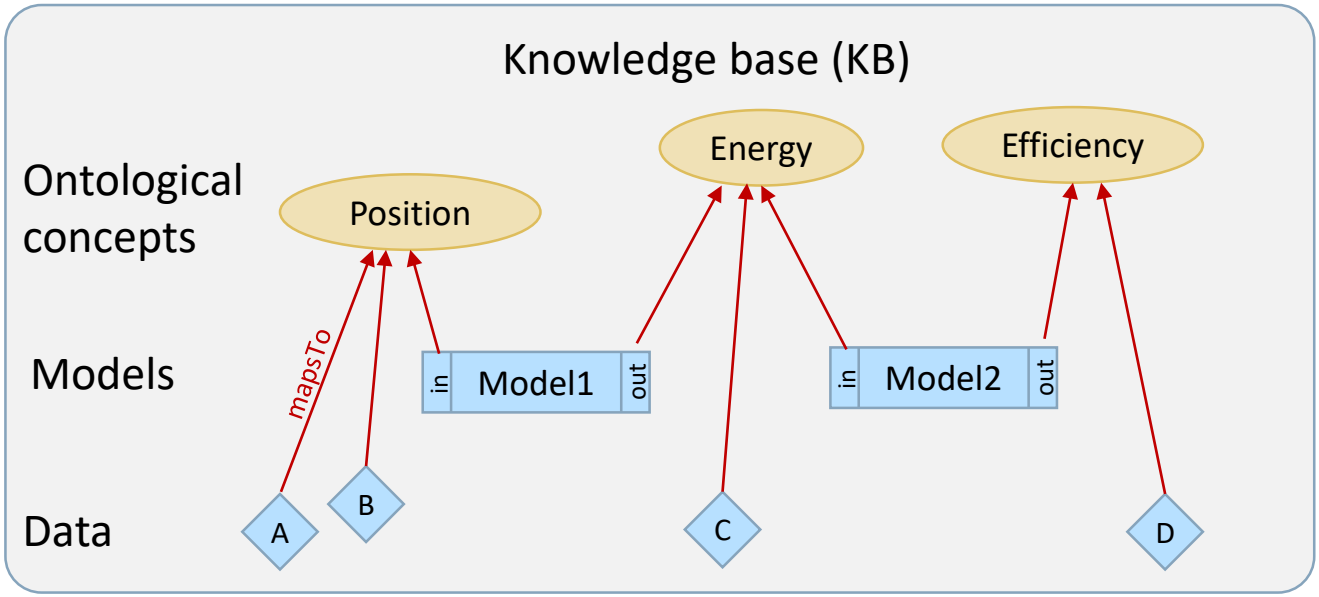
OpenModel Semantic workflow builder / OntoFlow



OntoFlow traverse the KB and find all mapping routes to instantiate D:

- $D_1 \leftarrow M_2 \leftarrow C$
- $D_2 \leftarrow M_2 \leftarrow M_1 \leftarrow A$
- $D_3 \leftarrow M_2 \leftarrow M_1 \leftarrow B$

OpenModel Semantic workflow builder / OntoFlow



Desision support:

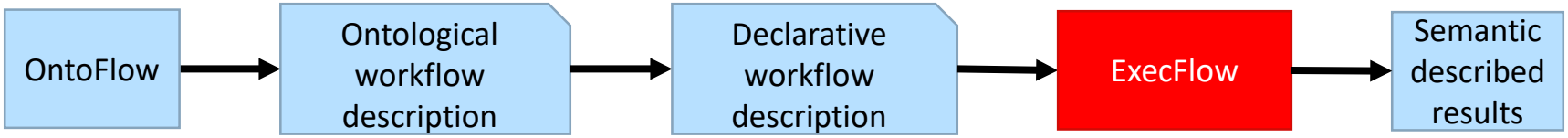
Associating costs to mapping steps

$cost_A = 1$
$cost_B = 2$
$cost_C = 4$
$cost_{M1} = 10$
$cost_{M2} = 3$

OntoFlow traverse the KB and find all mapping routes to instantiate D:

- $D_1 \leftarrow M_2 \leftarrow C$ *cost = 7*
- $D_2 \leftarrow M_2 \leftarrow M_1 \leftarrow A$ *cost = 14*
- $D_3 \leftarrow M_2 \leftarrow M_1 \leftarrow B$ *cost = 15*

OpenModel Workflow Executor / ExecFlow

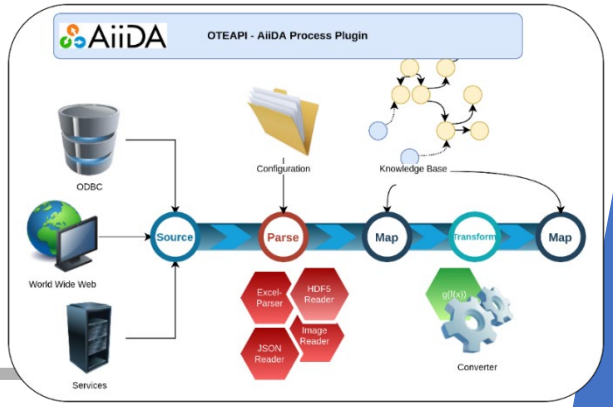


AiiDA
Automated Interactive Infrastructure and Database for Computational Science

Workflows · Data provenance · Plugin framework · HPC Interface · Open Science · Open source

ExecFlow

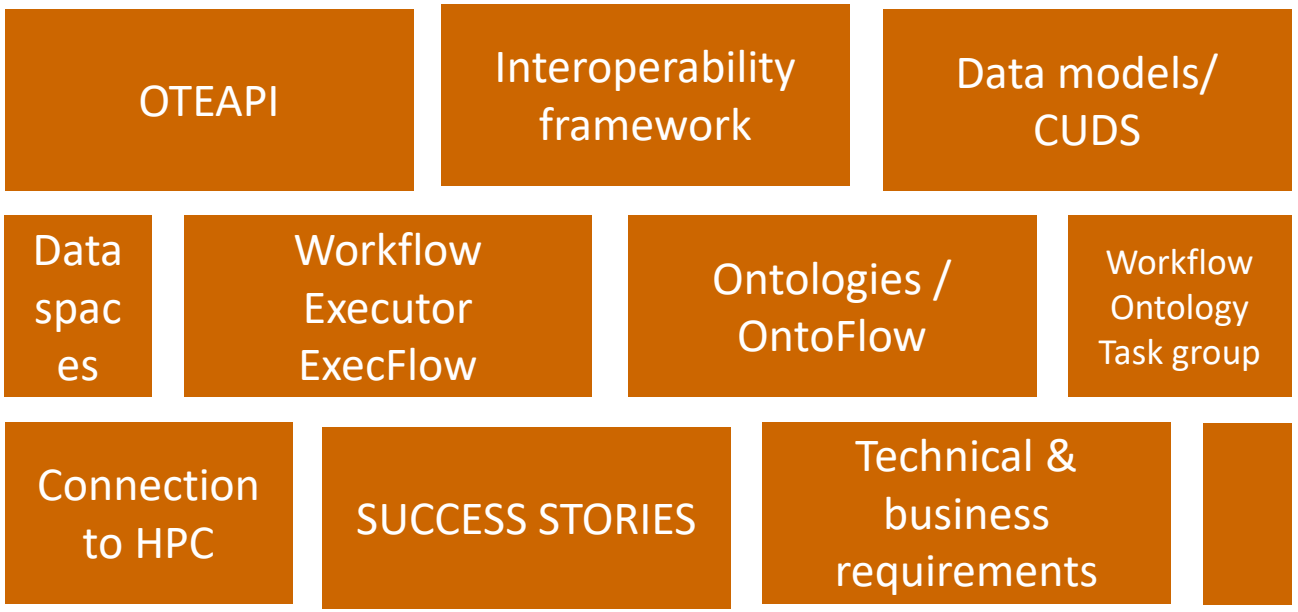
- Workflow execution is handled with AiiDA
- (Auto)generated AiiDA workflow from declarative workflow description (WrapperSDK)
- Dataflow is handled with OTEAPI



DEMONSTRATED VIA 6 SUCCESS STORIES

Success story	Long-term goals	Partners
SYNAPTIC ELECTRONICS [1]	Development of next-generation memory devices	CNR, AMAT
COMPOSITE MANUFACTURING [2]	Virtual manufacturing for automotive composite components	SISW
ALUMINIUM REINFORCED CONCRETE [3]	Competitive and environment friendly constructions with aluminium reforcement	Hydro, SINTEF, HEREON
METAL FORMING [4]	Resource efficient metal processing and manufacturing	HEREON
DIGITAL POWDER TESTING [5]	Development of efficient catalytic powders	CMCL
FUEL CELL TECHNOLOGY [6]	Improved hydrogen fuel cells for transportation	DCS, TOYOTA, HEREON

AVENUES FOR EAB PARTICIPATION AND OPENMODEL CURRENT DEVELOPMENTS



Some possibilities for collaborations

- Ontologies
  - Methodology for ontology development
  - Workflow ontology (EMMC task group) **(already decided)**

- Interoperability software components
  - SOFT/DLite
  - OTEAPI
  - Data spaces
  - Mappings & building of workflows
  - Declarative workflow description & execution

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 953167.