

OntoTrans 1st Open Workshop: Collaboration/Related Projects

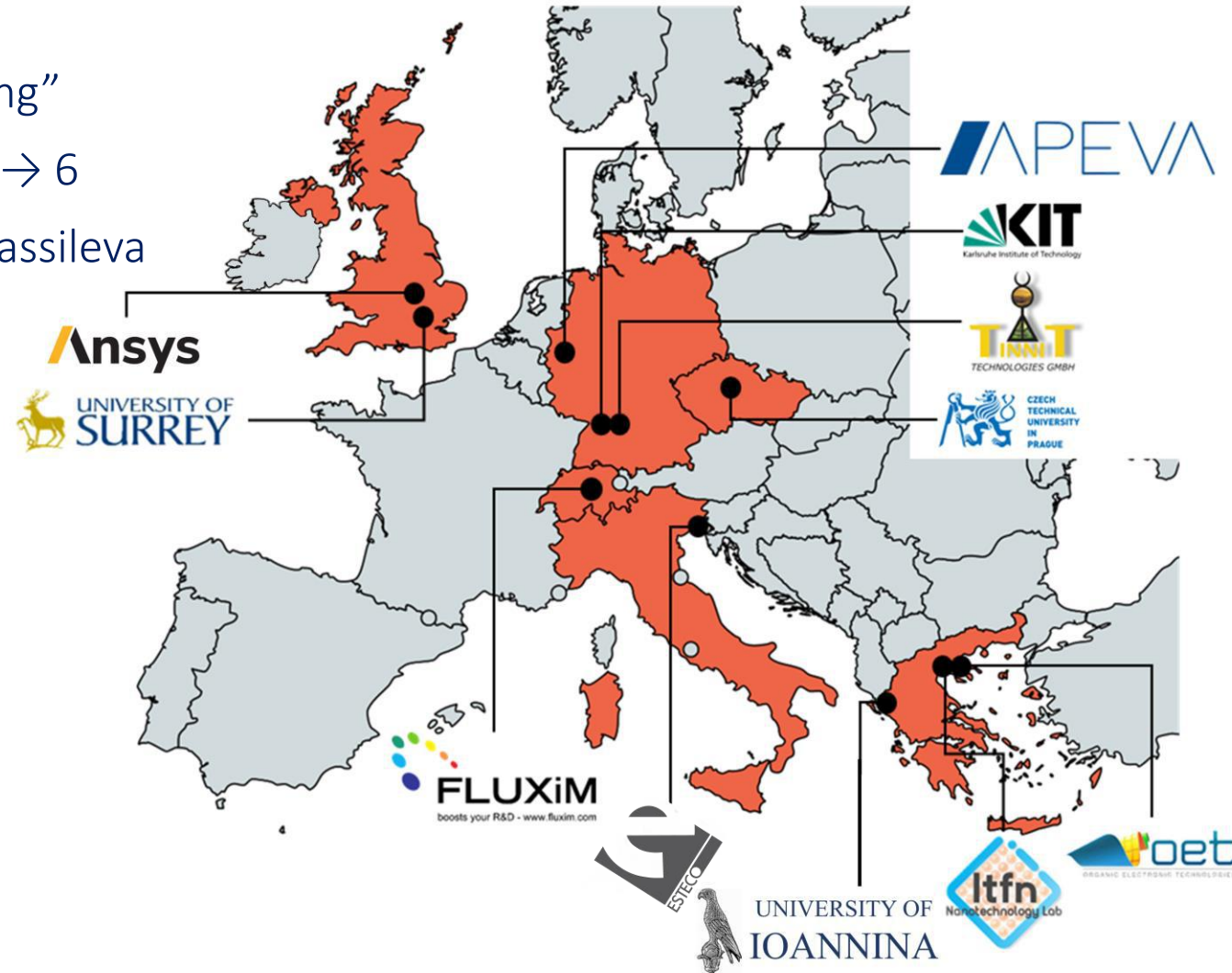
The MUSICODE project



The MUSICODE project at a glance

- **Type:** Research and Innovation Action (RIA)
- **Work programme:** H2020 call DT-NMBP-11-2020
“Open Innovation Platform for Materials Modelling”
- **Project No:** 953187, **Duration:** 2021-2024, **TRL:** 4 → 6
- **EC contribution:** €4,992,000 **EC PO:** Dr. Rossitza Vassileva
- **11 top European expert partners:**

- Academia
- University of Ioannina (Coordinator) 
 - Karlsruhe Institute of Technology 
 - University of Surrey 
 - Aristotle University of Thessaloniki 
 - Czech Technical University in Prague 
- Industry
- Fluxim AG 
 - TinniT Technologies GmbH 
 - Ansys 
 - ESTECO SPA 
 - Organic Electronic Technologies 
 - APEVA SE 



MUSICOE application domain: printing and gas transport in Organic Electronics

wet phase processing

Roll-to-Roll Printing (slot die) for OPVs



gas phase processing

Organic Vapor Phase Deposition for OLEDs

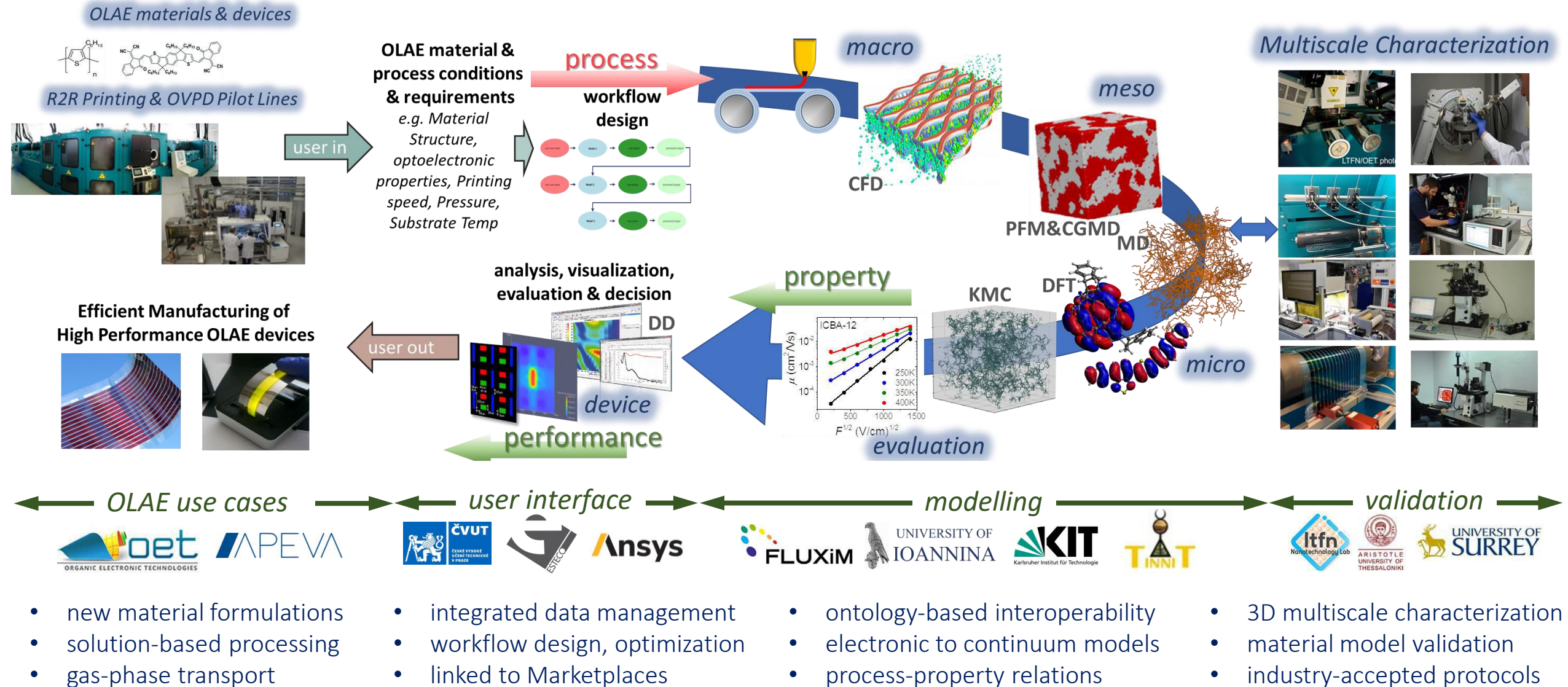


- Why to model:
 - gaining deeper understanding
 - screening of new materials
 - optimizing process flows
 - improving device efficiencies
 - exploring new device concepts

-> enabling virtual R&D

- Multiscale/Multiphysics models:
 - material properties
 - physical interactions
 - device functionality

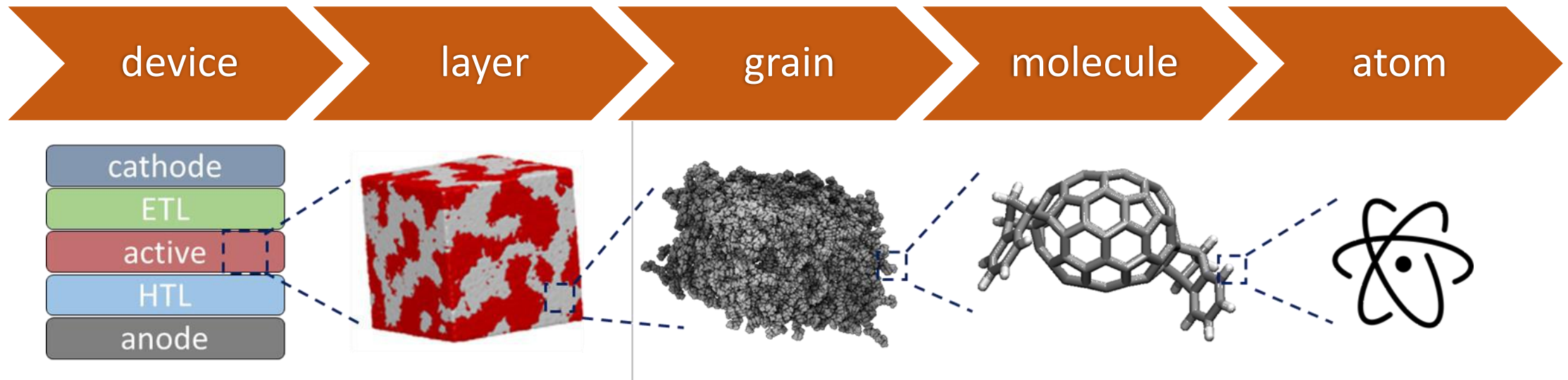
MUSICODE vision: an Open Innovation Platform for OLAE



Ontologies

Data requirements and ontologies for OE materials

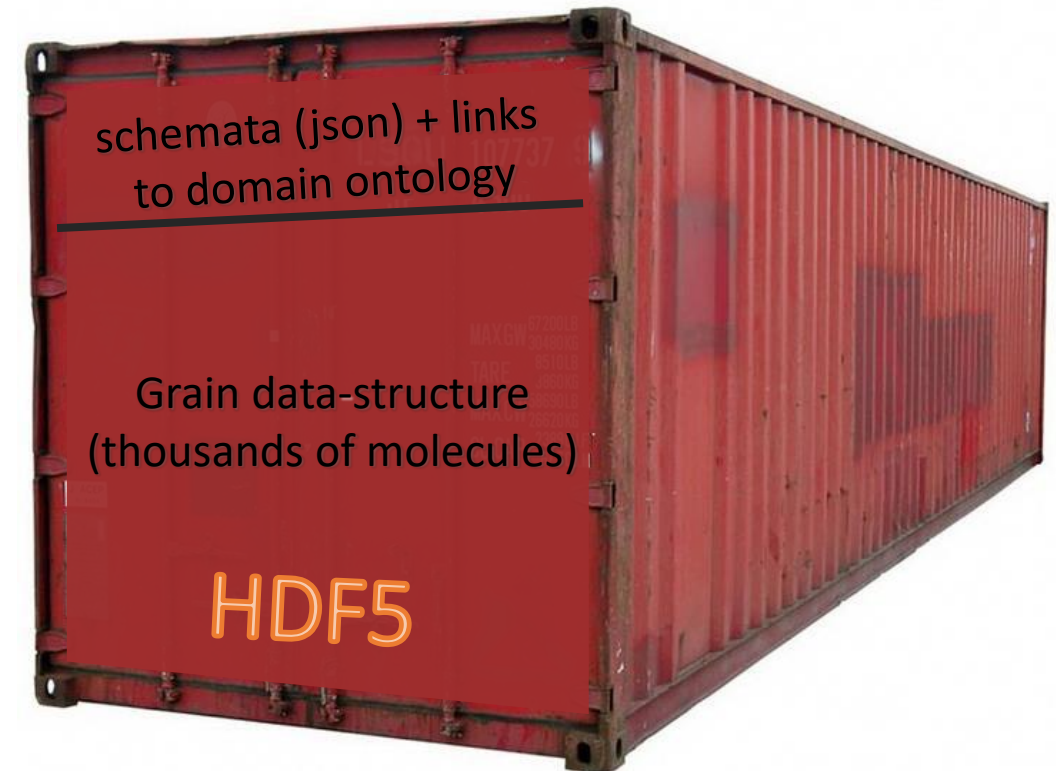
- Semantically related data structures



- Semantically structured data schemata:
 - 'General Info', 'Properties', 'Structure', 'Parts', 'Computational Info', 'Links'
- Semantic representation of entities (models and data) and their services

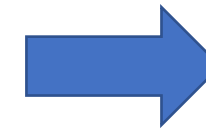
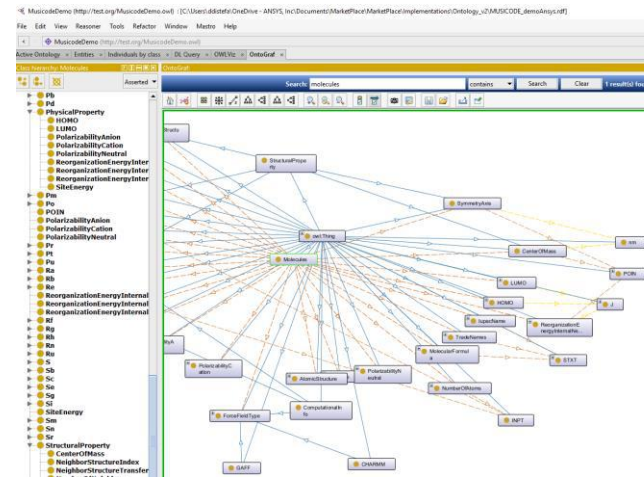
Data schemata → data services

```
{
  "_schema":{
    "name": "gr.uoi.musiccode.grain",
    "version": "0.5"
  },
  "_datasetName": "grains",
  "GeneralInfo":{
    "material":{ "dtype": "a" }
  },
  "Properties":{
    "reorganizationEnergyExternal":{ "dtype":"d", "unit":"J" }
  },
  "Structure":{
    "cellSize":{ "dtype":"d", "shape":[3],"unit":"m"}
  },
  "Parts": {
    "schema":"gr.uoi.musiccode.molecule" }
  },
  "ComputationalInfo":{
    "boundaryCondition": { "dtype": "a" }
  },
  "Links":{
    "other":{ "dtype":"l", "shape": "variable" }
  }
}
```



Data exchange in HDF5 container
Data schema is contained in the container
Semantic representation of data
Data services automatically generated by schema
Service-based model APIs (wrappers)
Missing link: data schema → domain ontology

MUSICODE schemata - ontology



ontology

Molecule schema

A screenshot of the MUSICODE Molecule representation in MI (Molecular Information) format. The interface shows a table with columns for 'Molecule ID', 'Molecular Formula', 'IUPAC Name', 'Trade Names', 'Generic Name', 'Molecular Weight', 'Atoms', 'Number Of Atoms', and 'Atomic Structure'. The example molecule is Methane (CH₄).

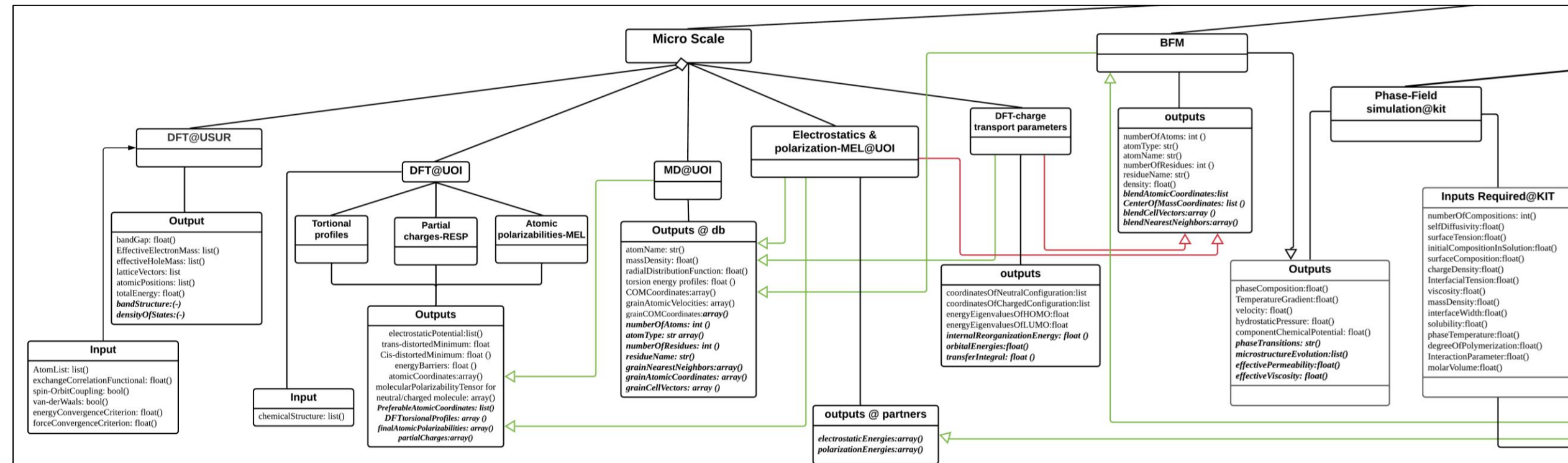
Methane - example	
Molecule ID	CH ₄
Molecular Formula	CH ₄
IUPAC Name	methane
Trade Names	
Generic Name	Methane
Molecular Weight	16
Atoms	H, C
Number Of Atoms	5
Atomic Structure	CH ₄ of
Physical Property	
HOMO	
LUMO	
Polarizability Anion	
Polarizability Cation	
Polarizability Neutral	
Reorganization Energy Internal Neutral	
Reorganization Energy Internal Anion	
Reorganization Energy Internal Cation	
Site Energy	

Molecule representation in MI



Molecule representation in MuPIF datatypes

Data requirement (or workflow) ontology for OE materials

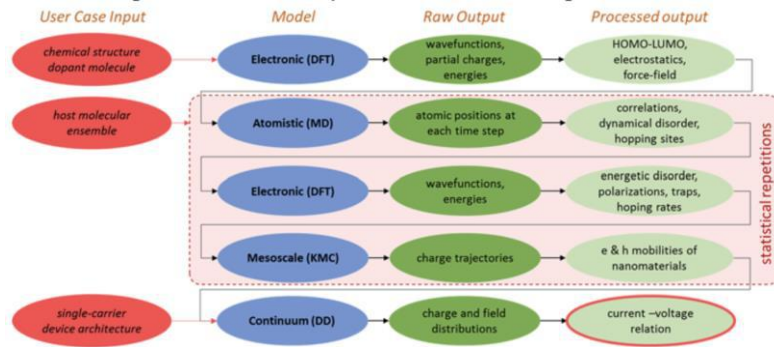


WORK IN PROGRESS

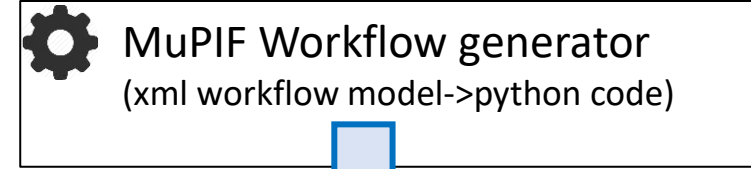
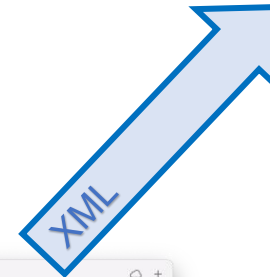
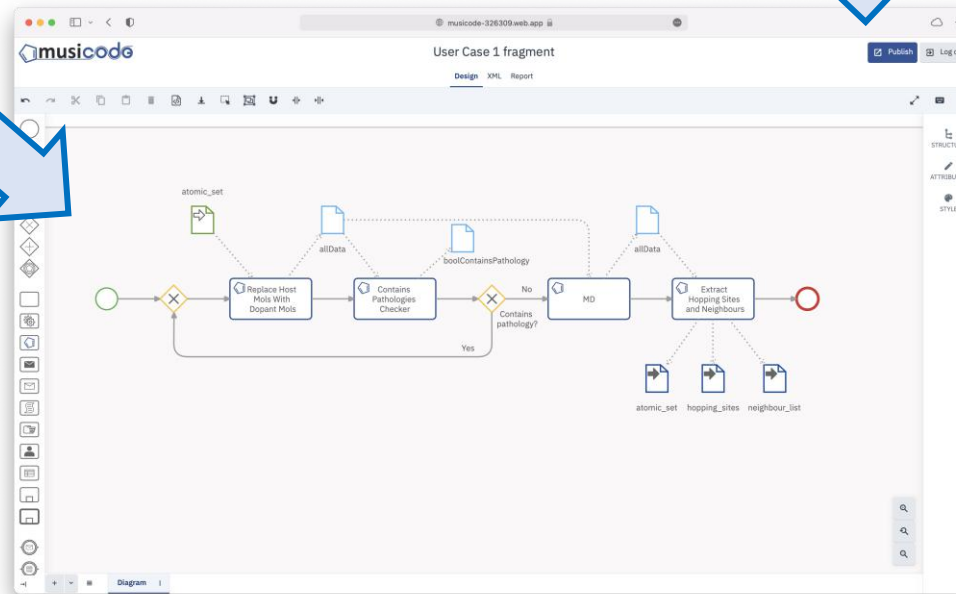
Workflows

Workflows in MUSICODE: from MODA workflows to MuPIF workflows

MODA



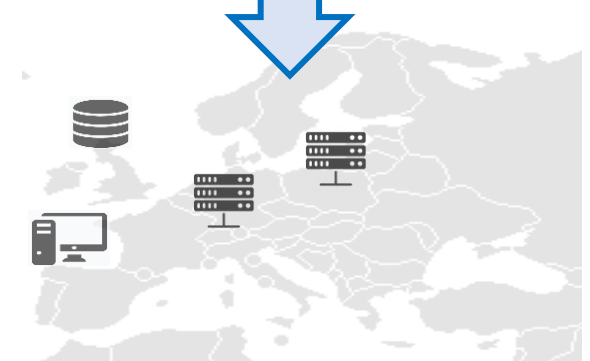
BPMN workflow editor



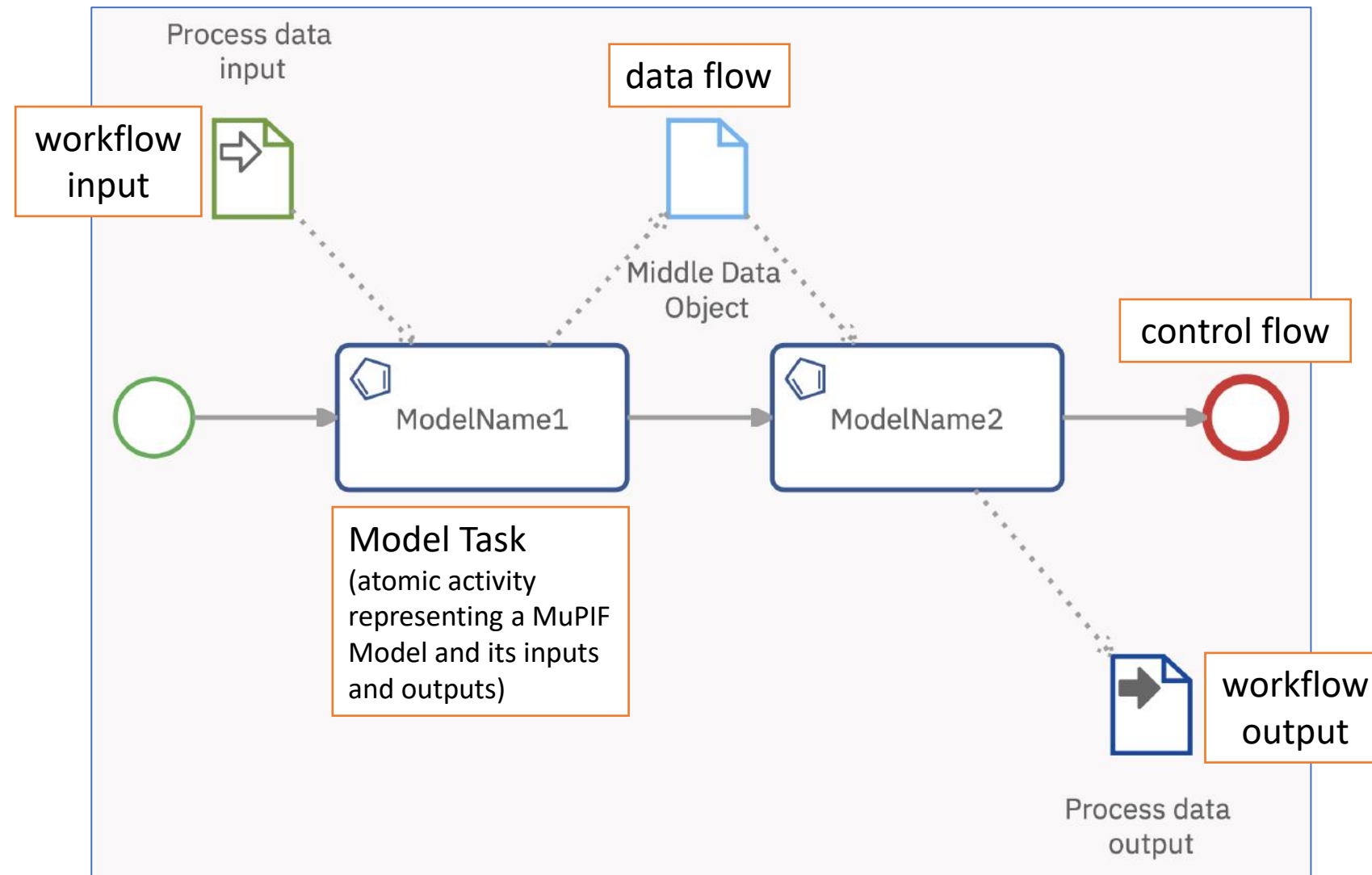
Executable MuPIF Python workflow



Execution



Workflow representation: BPMN 2.0 standard




- **Model Task**
 - Tailored for MuPIF Models
 - Other kinds of building blocks
- **Gateways**
 - Loops and branching
 - Other control-flow patterns
- **Hierarchical construction**
 - Sub-workflows & pools
 - Data flows

Interfaces

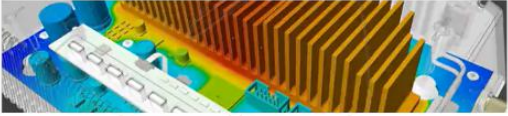
Data Management System

MI Home



Modelling


Modelling activities



Access Monitor


Modelling Workflows

Search, Select and execute



Access Button 2 Button 3

Workflow editor



Access Button 2 Button 3

Explore

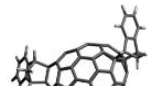
Quick Search

Text search over the entire platform

Search... Refresh Showing 0

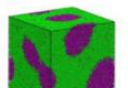
Name

Molecules



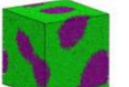
Access

Grains



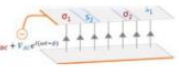
Access

Layers




Access

Devices




Access

Data Curation System



Template Import Help

Resources



Software Hardware

Other Tools..

Contents

Musicode

Indene C70 bis-adduct 2 isomer (IC70BA-2 isomer)

General Info

Molecule name

Molecular Formula

Generic Name

Molecular Weight

Atoms

Number Of Atoms

Atomic Structure

Physical Property

HOMO

LUMO

Polarizability Anion

Polarizability Neutral

Reorganization Energy Internal Neutral

Reorganization Energy Internal Anion

Computational info

Force Field File

Force Field Type

MI Viewer

Read Mode

Edit Mode

Contents

Musicode

Indene C70 bis-adduct 2 isomer

Simulation Templates

Simulation Executions

Software tools

Hardware

Molecules

Grains

Subset Grains (Default)

Example grains

IDIC-CR300

Layers

Subset Layers (Default)

Layer

MAPSi3

PCDTBT - PC70BM

testLayer

Devices

MI Viewer

Read Mode

Edit Mode

Contents

Musicode

IDIC Crystalline Sample 300K (IDIC-CR300)

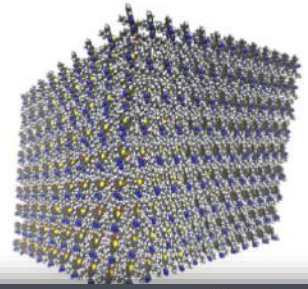
General Info

Grain Name

Number Of Residues

Grain Type

Atomistic Grain Image



MI Viewer

Read Mode

Edit Mode

Contents

Musicode

PCDTBT - PC70BM blend

Electrical properties

Thickness

Constant Electron Mobility

Constant Hole Mobility

Density of States HOMO

Density of States LUMO

HOMO

LUMO

Dielectric Constant

Langmuir Rec Prefactor

Optical Gen Eff

Electron Trap Density

Electron Trap Depth

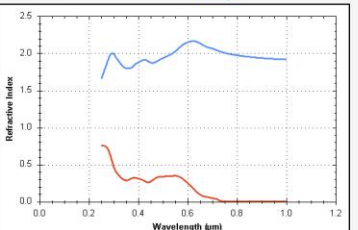
Electron Electron Trap Capture Rate

Hole Electron Trap Capture Rate

Optical properties

Refractive Index

Hide Graph

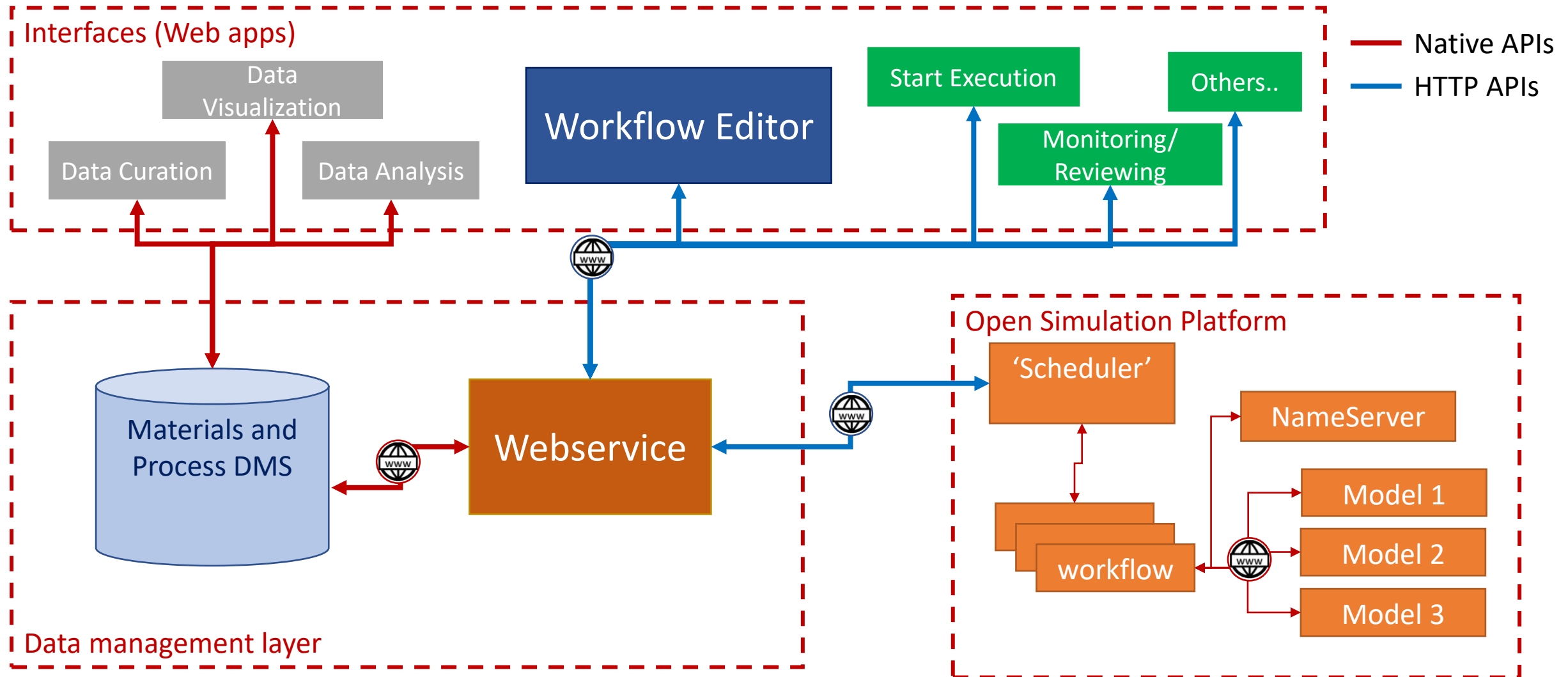


Part

Real

Imaginary

Interfaces in MUSICODE

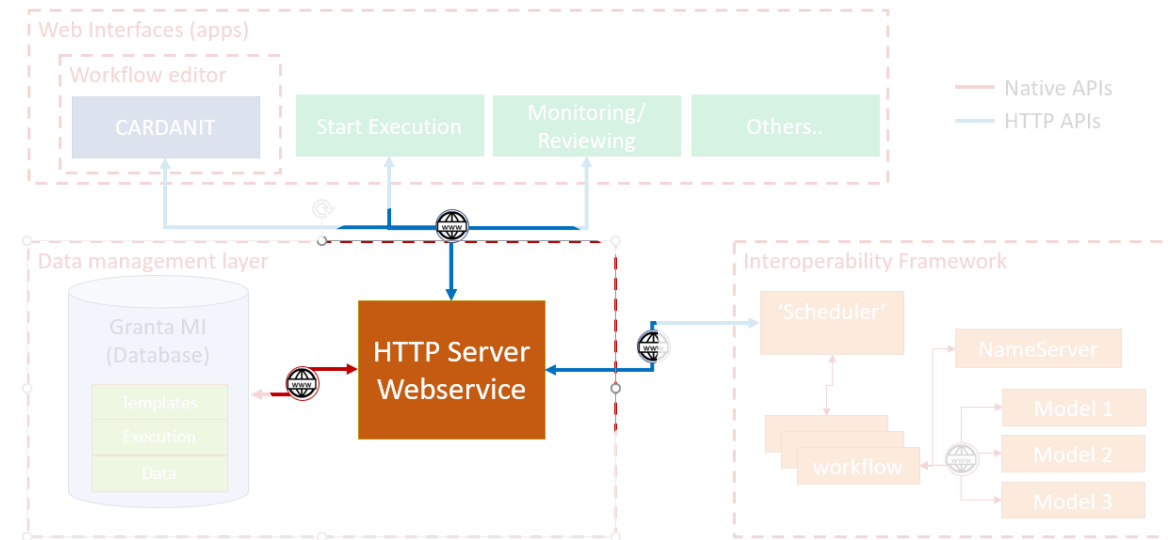


MUSICODE OIP: Webservice

- **Communication among components through HTTP APIs:**

- Standardization of interfaces
- Application independent communication
- Distributed architecture
- Allows independent developments
- And customized deployment

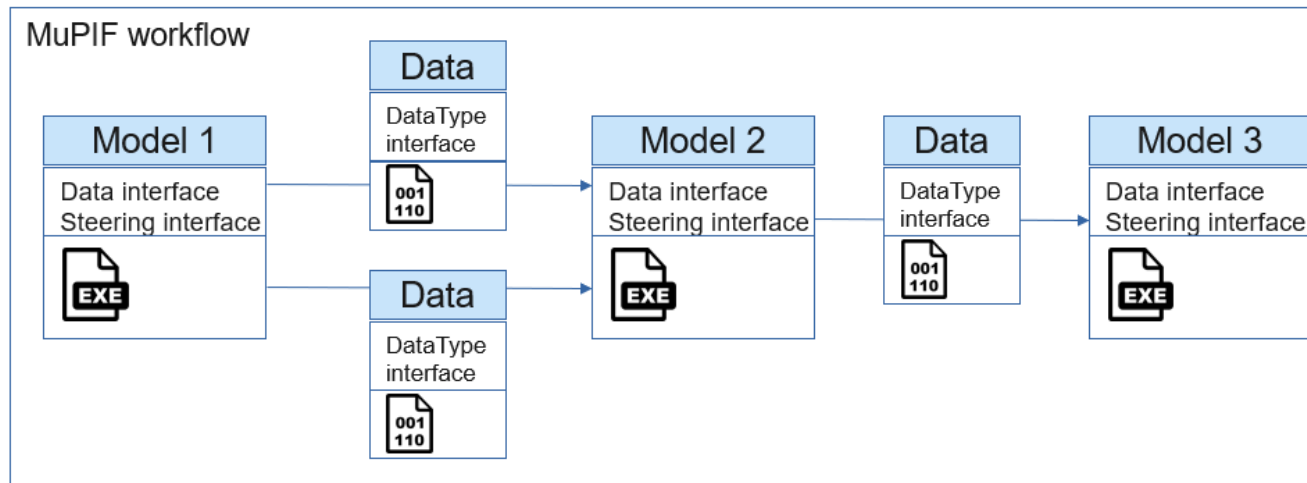
Executions	
GET	/executions/ List Executions
POST	/executions/ Create Execution
GET	/executions/{execution_guid} Read Execution
PATCH	/executions/{execution_guid} Update Execution
POST	/executions/{execution_guid}:save Propagate Execution Results
POST	/executions/{execution_guid}:start Start Execution
Templates	
GET	/templates/ List Templates
POST	/templates/ Create Template
GET	/templates/{template_guid} Read Template
PATCH	/templates/{template_guid} Update Template



- **APIs will be documented in openAPI standard**
 - De-facto standards
 - Allows automated code generations
 - Facilitate interoperability with other platforms

Open Simulation Platform: MuPIF

- Standardized http-based interface to DMS
- Abstract representation of entities: components with standardized interfaces
- Component based design
 - Entities represented by abstract class with standardized abstract interface
 - Model entity: generating, consuming or transforming data
 - DataType entities: representing data exchanged
- MuPIF is standardizing component interfaces rather than data structures
- Platform supports any type of workflows (weakly and strongly coupled)



Challenges

- Extend (EMMO based) ontology with the concept of services
- Develop workflow ontologies
- MuPIF Models/DataTypes with interfaces to 3rd party datasets
 - onboarding external data as a complement to DMS
- Provide semantic based data access to DMS
- Enable schema (data and services) interoperability through ontology
 - inference, mappings, transformations

Thank you for your attention!



This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Call DT-NMBP-11-2020 "Open Innovation Platform for Materials Modelling"