MATERIALS MODELLING MARKETPLACE FOR INCREASED INDUSTRIAL INNOVATION

Dirk Helm (Fraunhofer IWM) for the MarketPlace consortium

OntoCommons Workshop “Industry Commons Marketplaces”, April 29th , 2021

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The MARKETPLACE project is funded by Horizon 2020 under H2020-NMBP-25-2017
call with Grant agreement number: 760173

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Motivation

The Challenge	The Situation
• Extensive knowledge generated by simulations and experiments is not accessible but available	• Data stored at different locations, different labs/institutes, etc.
• Problems can be solved with similar solutions	• limited collaboration, hard to find expertise
• Data (results, information) is hardly curated	• calculations or experiments are often repeated with out a reason • it takes long time and efforts to find knowledge
• Numerous models and related software tools require different skills and conditions	• Tools require different expertise and knowledge
	• software deployment, operation and regular maintenance of tools

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The vision

Powerful modelling solutions in industry for **faster development** and market deployment of novel materials

Knowledge access and its exchange via **platform**

MATERIALS **MODELLING** data, modelling tools and expertise available at any time and at any place.

Simplified access to knowledge of existing models, data, and software solutions, translation services and validation capabilities.

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Our project goals

- To design, create and maintain a sustainable web-based platform,
- To open it to the entire materials modelling community,
- To include activities on databases, modelling, integrated open simulation platforms, as well as translation and knowledge services.

We provide the infrastructure (incl. overall rules).

You make it a marketplace.

The place is brought to life by the services and offers from suppliers and by visits from buyers.

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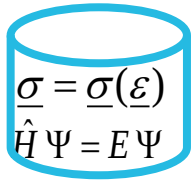
The key capabilities

> Search models, data, expertise…

Explore → Interact → Create → Execute → Curate

Explore: Search data and knowledge

- **Materials Models Data**



- **Software Tools**

- **Benchmarks**

- **Validation Data**

Interact: Get advice and support readily

- **Training and Education**

- **Expertise Discussions and User Feedback**

- **Translation Services**

Create & Execute: develop & deploy

- **Workflows Builders and Executers**

- **Integrated Open Simulation Platforms**

- **Databases of available tools Modelling App Store**

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The key capabilities

Knowledge services: find information and collaborate

- Search databases of experts, software solutions, show cases and use cases
- Semantic services enable semantic search and discovery
- Search numerical tools and/or providers of numerical simulations
- Find a Translator (Connection to OntoTrans: Open Translation Network)

Modelling and workflow services

- seamless integration of existing materials modelling solutions, open simulation platforms (OSP) and materials data from disparate databases into advanced materials modelling workflows
- Electronic, atomistic, mesoscopic and continuum models
- MarketPlace OSP-core (Open RESTful API)
- Integration of existing Platforms

AIX VIP MAP

SimPhoNy

AiiDA

SimphonyRemote

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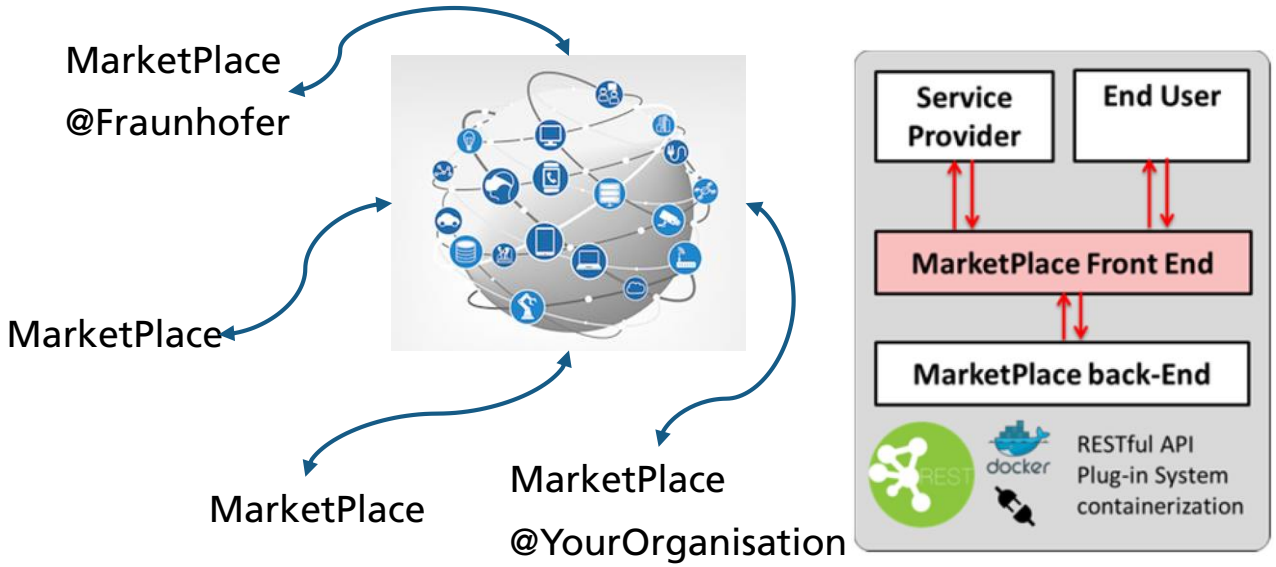
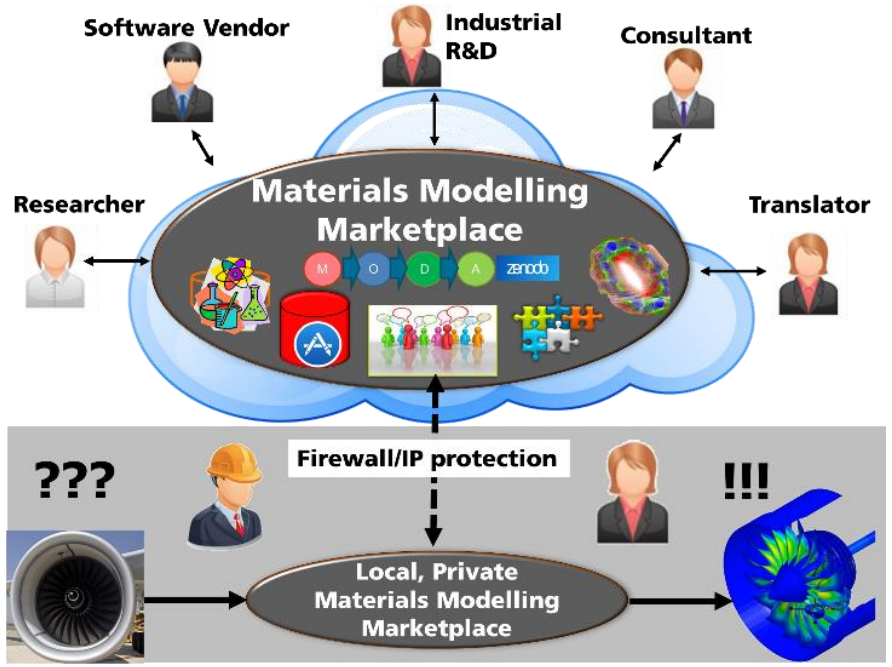
Fundamental concept of the MarketPlace Platform

- decentralized access to applications and disparate databases
- control and management of the extensive materials information
- data and knowledge scattered across Europe and beyond

Enabling more transparent access to, and vigorous utilization of, materials modelling and materials data for the European industry.





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Technical challenges

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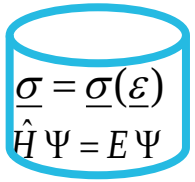

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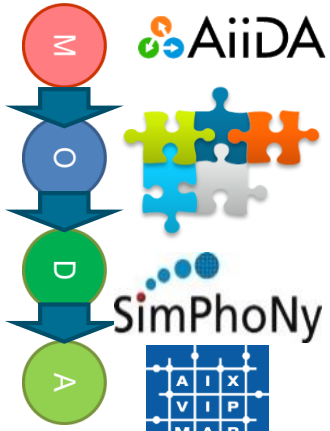

- **Integrated Open Simulation Platforms**
- **Databases of available tools Modelling App Store**

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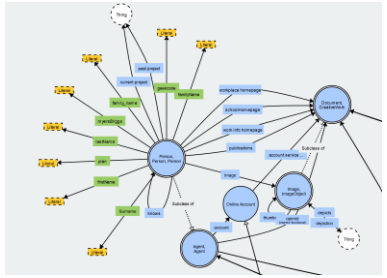
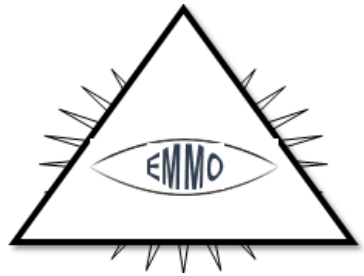
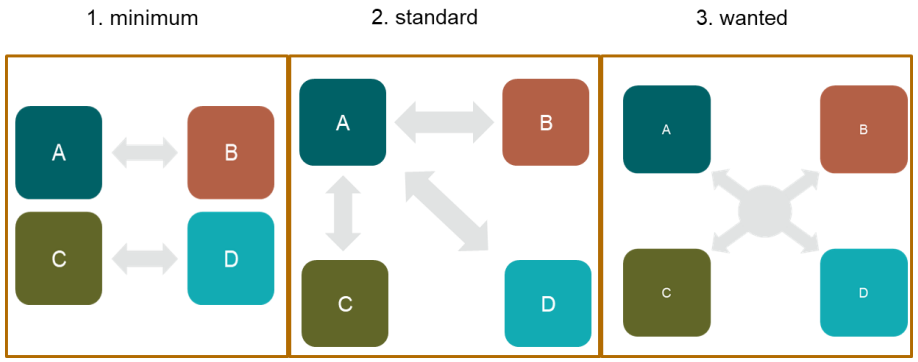
Technical challenges: Cross domain interoperability based on standards and ontology

- Ontology covers
  - MarketPlace services
    (Translation, Education, User Management, …)
  - Models and Modelling
  - Workflows, Simulations , Manufacturing
- Higher level common top level services service Ontology with other marketplaces: VIMMP
- Collaboration with multiple projects
  - simDOME, ReaxPRO, INTERSECT, FORCE, …







➞ seamless communication and information exchange across communities and tools

➞ make search and links between different databases effective and easy

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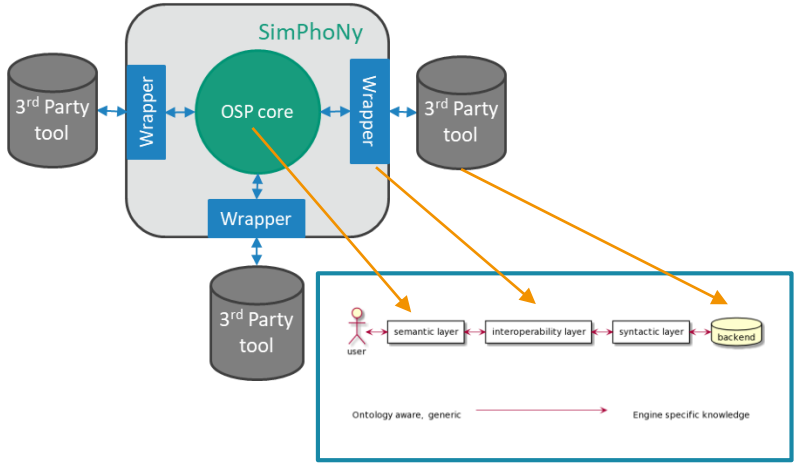
Fundamental concept of the MarketPlace Platform: Interoperability

- **SimPhoNy** is a Python package that aims to power interoperability data across multiple 3rd-party software tools
- Consists of two main components:
  - **OSP-core:** enables the user to perform CRUD operations Create, Read, Update and Delete) on ontology-based representation of data
  - **Wrappers:** a plug-in mechanism for 3rd-party tools that interactively converts between an ontology-based representation of data (CUDS) and an ontology-free one
- The notion of CUDS is used to uniformly represent data using an ontology
  - CUDS class – represents an ontology class/concept
  - CUDS object – represents an ontology individual
  - Provided with API for CRUD functionalities (Create, Read, Update and Delete)
  - CUDS is a recursive data structure in that a CUDS object may contain other CUDS objects



CUDS container view

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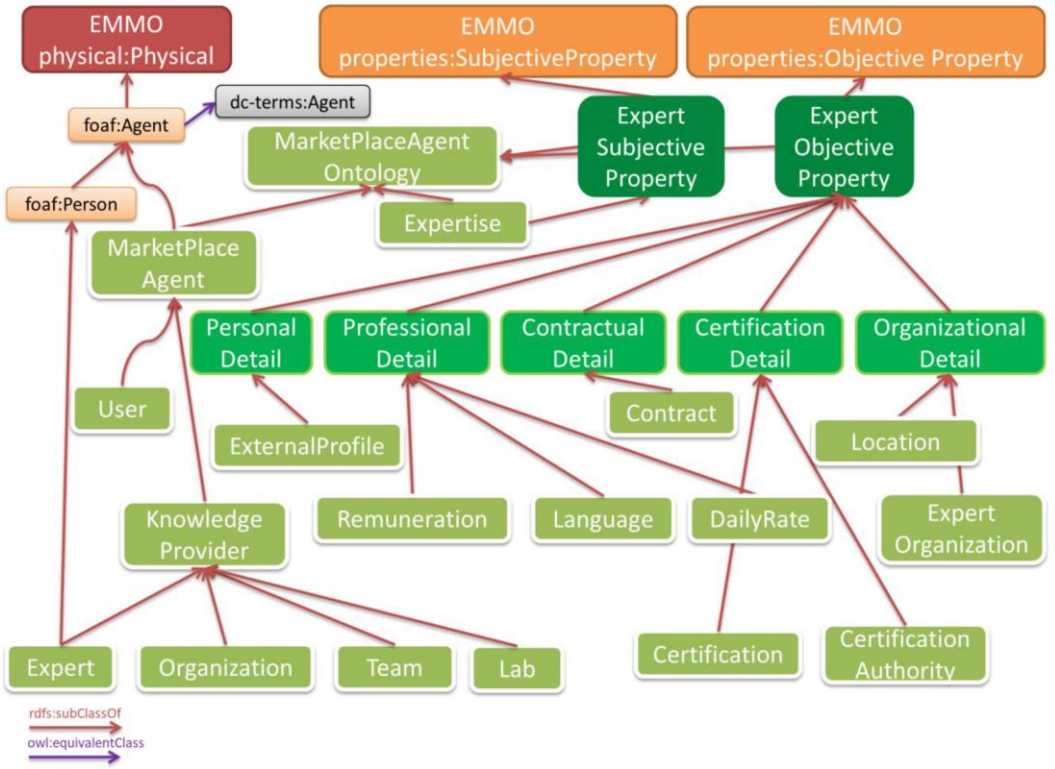
Fundamental concept of he MarketPlace platform: Ecosystem of Ontologies

- Ontologies with emphasis on MarketPlace's operations
  - **Expert** ontology – characterises an expert for matching operation.
  - Software ontology – taxonomy for software
  - Material ontology – taxonomy for material
  - Manufacturing ontology - taxonomy for manufacutring
  - Application handling ontology
  - European Virtual Marketplace Ontology (EVMPO) – interoperability VIMMP and MarketPlace
- Interoperability foundations, ontologies and metadata standards
  - Ontology for workflows
  - Applied math adding application mathematics to base EMMO math



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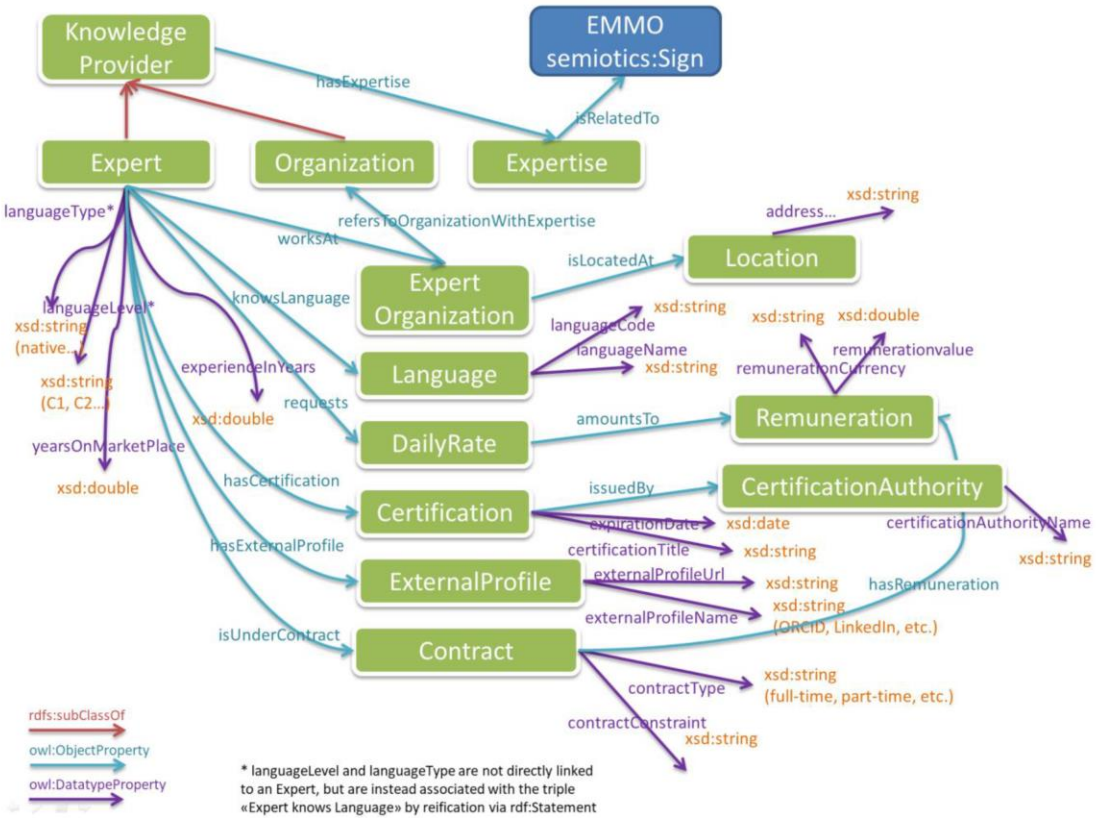

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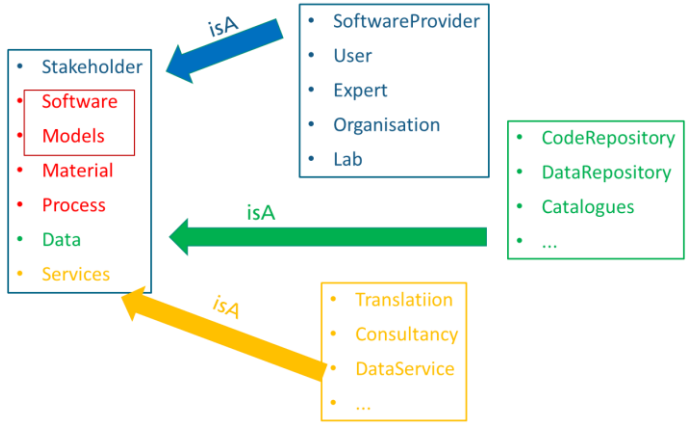

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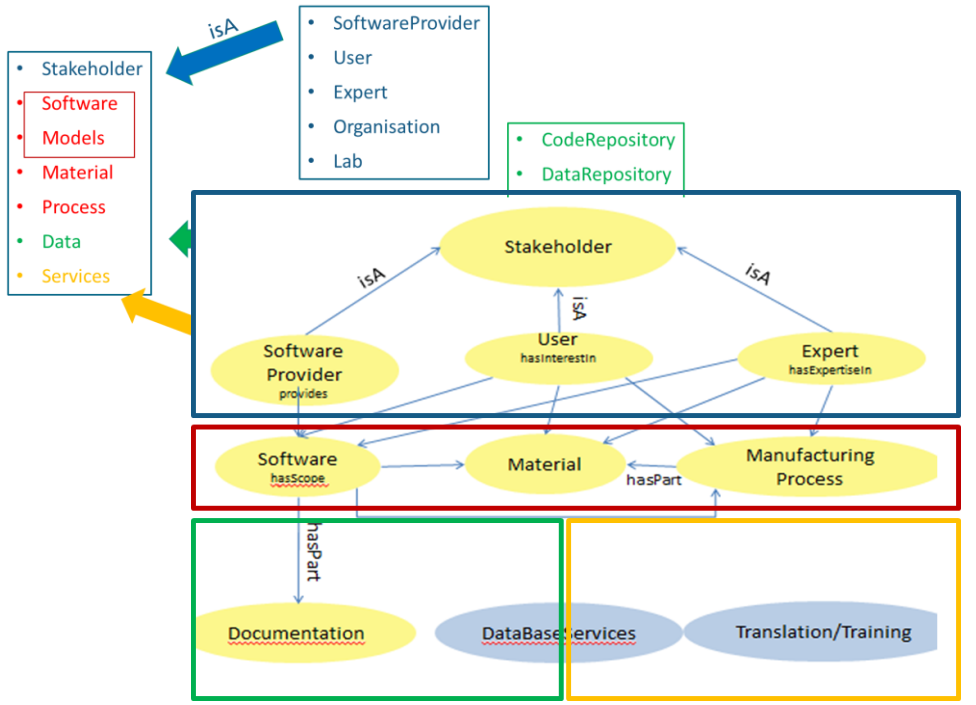

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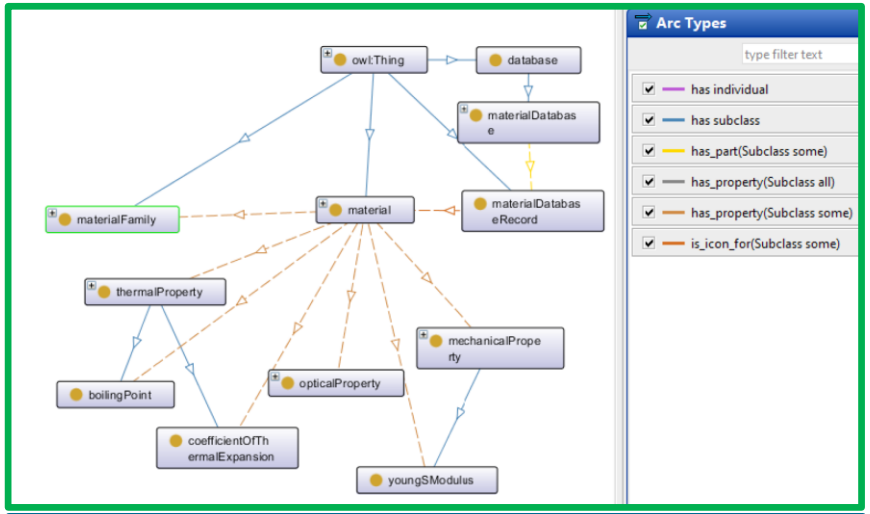
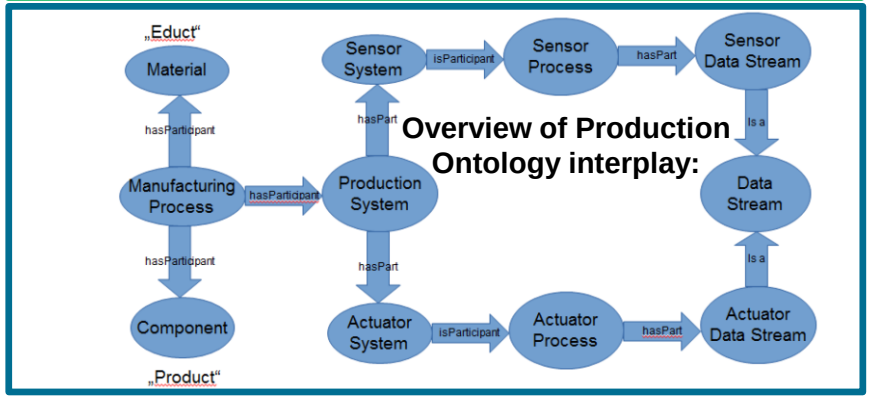
- Ontologies for materials
  - Ontology module for wetting experiments
  - Material composition ontology
  - **Material database ontology**
  - **Material properties ontology**
  - Mechanical testing
  - Crysallography domain ontology
  - Atomistic & electronic ontology
- Ontologies with emphasis on applications
  - Manufacturing processes ontology
  - **Production systems ontology**
  - Application ontology





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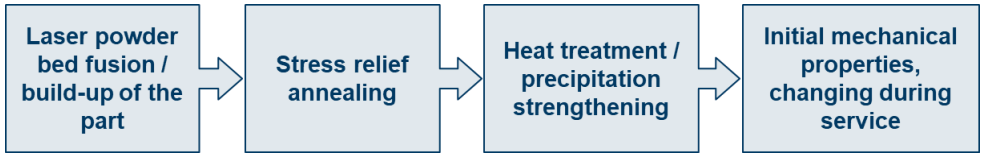
Use Cases in the MarketPlace to demonstrate the capabilities

- Industrial applications are used to
  - guide the development, test usability
  - ensure relevance to industrial use cases
  - train and demonstrate
  - produce initial content to populate the platform with
    - initial set of Apps
    - additional databases,
    - initial set of services: translation, education, training, etc.

Create a seed for an ecosystem that promotes, attracts and leads community participation from vendors and users!

- **User Case 1:** Additive manufacturing of superalloys



- **User Case 2:** Simulation of screen printing of functional layers
- **Use Case 3**: Nanomaterials for catalyst, energy and coating applications
- **Use Case 4 :** Ceramic Injection Molding (CIM) for medical applications
- **Use Case 5:** Printing of Photovoltaic Thin Film
- **Use Case 6:** 3D printing of Metals, “open” App

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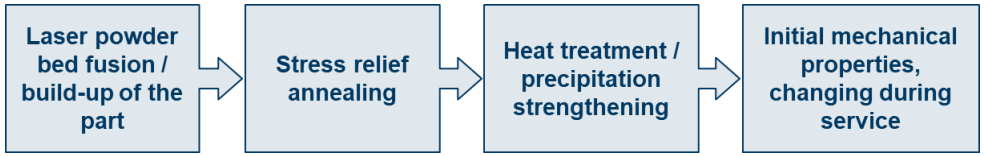

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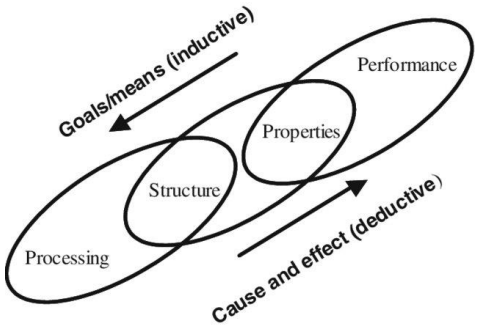
Use Cases 1: Additive manufacturing of superalloys

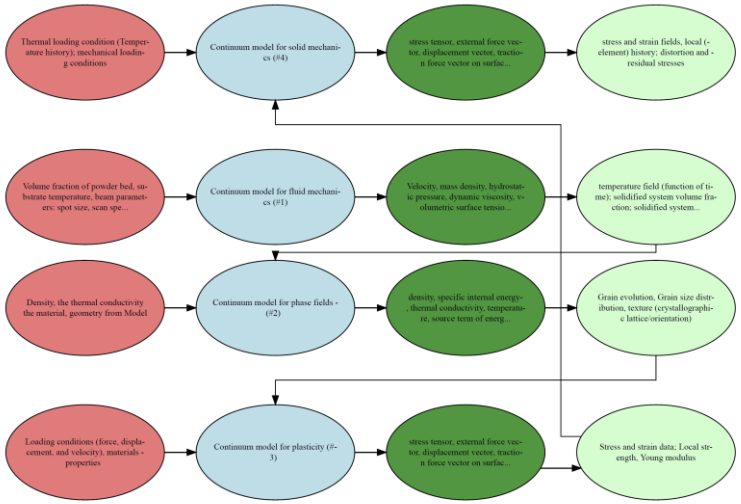
- **Overall goal:** Material- and process design for addtitive manufacturing of superalloys (polycrystalline metal)
- **Technical goal:** Determine the process-structure-property relationship for additive manufacutred metals
- **Translation** to a solveable problem from modelling and simulation point of view by using MODA (MOdelling DAta generalisation) and select appropriate simulation tools for the required simulation tool chain

Material- and process design

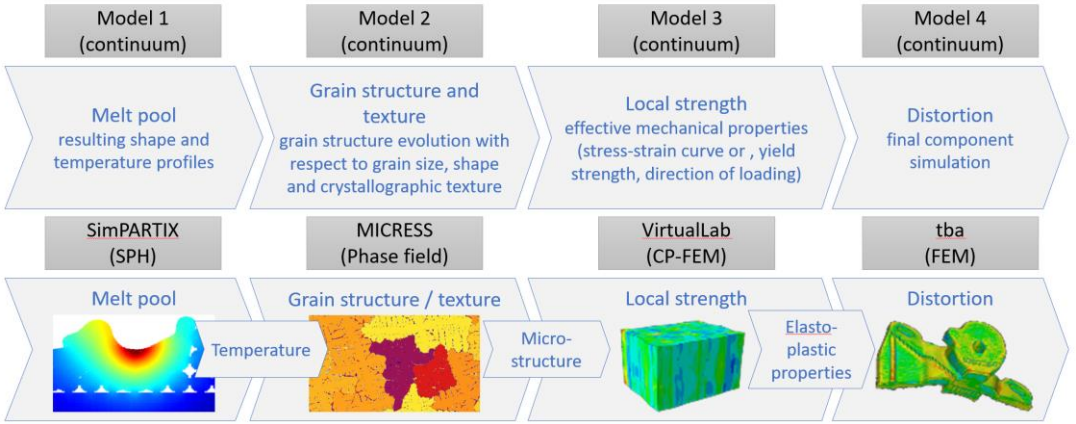


Olson (1997)

MODA for UC 1



simulation tool chain



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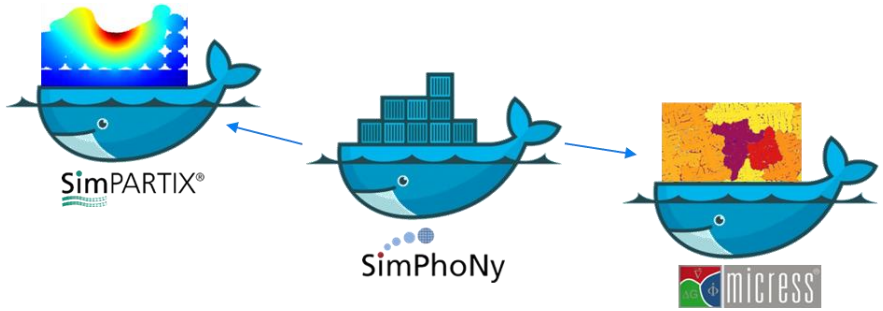
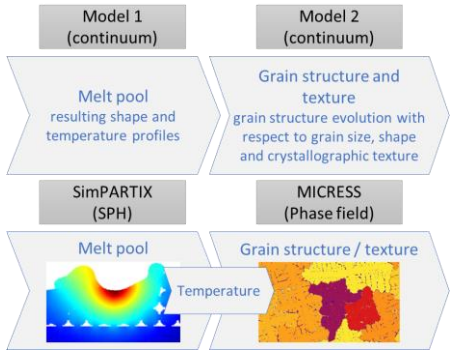
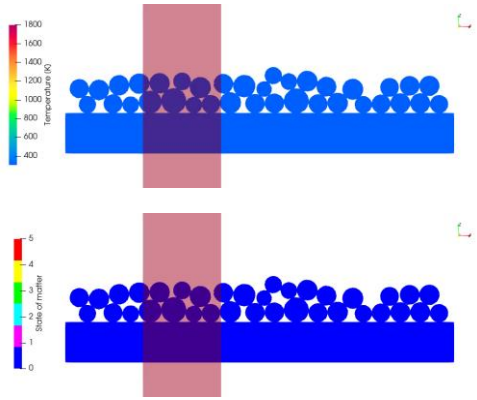
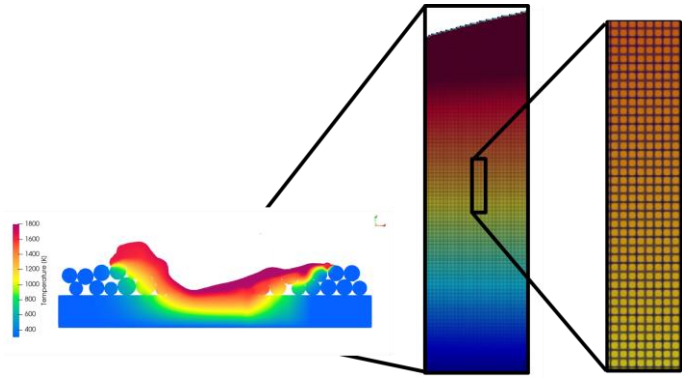
- Platform integration of
  - **SimPARTIX** for melt pool simulation and predicting local temperature and flow fields of the molten super-alloy during the laser-based powder bed fusion process (SPH method)
  - **MICRESS & Thermo-Calc** (solidification and microstructure evolution)
  - **Jupyter-Lab** (orchestration of the workflow)

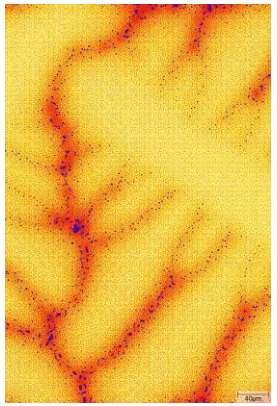
  via **SimPhoNy** remote
- Workflow handling











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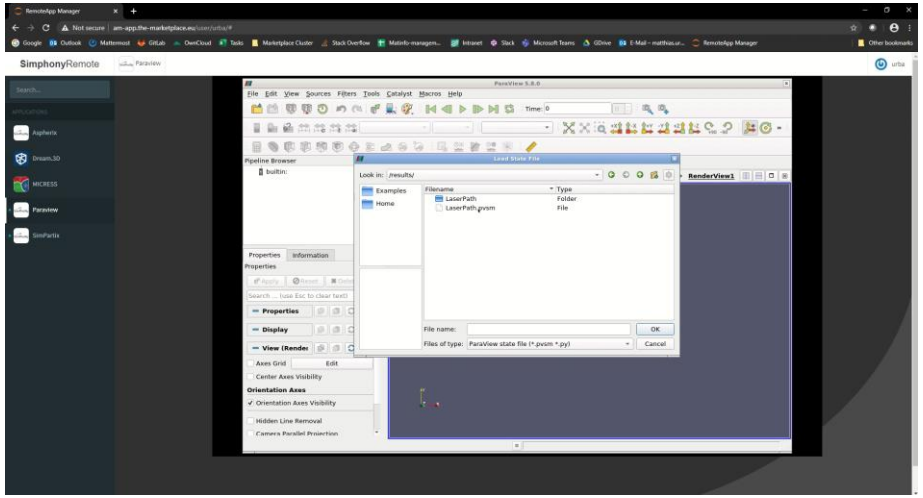

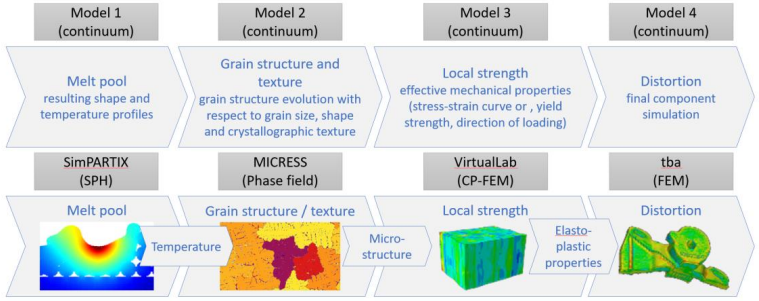

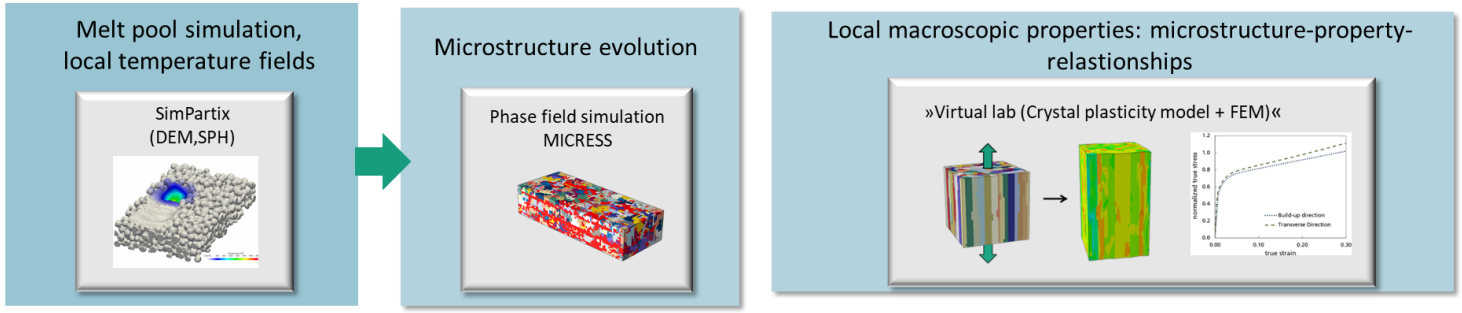

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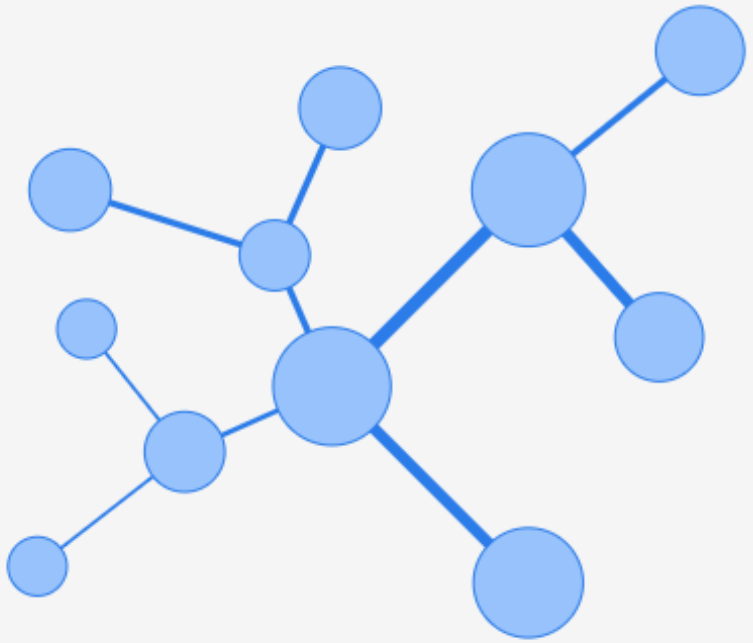

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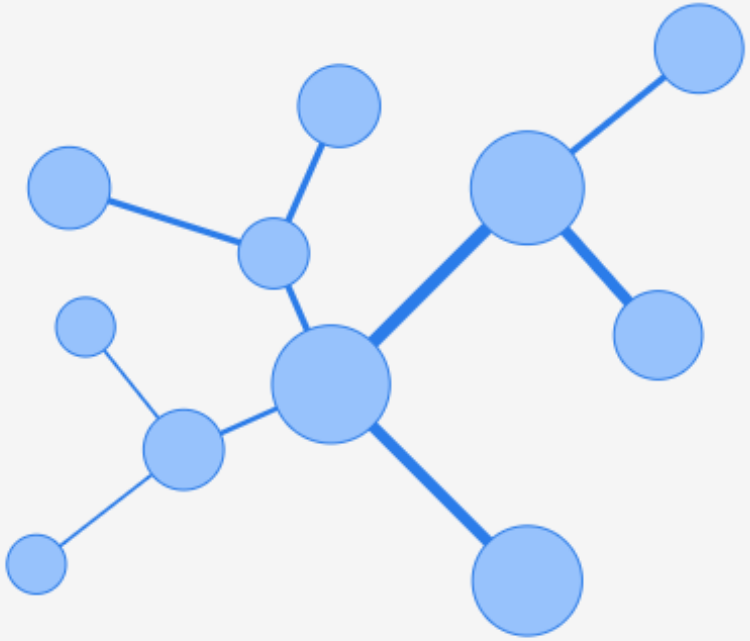
For Increased Innovation in Materials Modelling

Funded by Horizon 2020 with grant agreement number 760173 (MarketPlace)



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For Increased Innovation in Materials Modelling

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Create a knowledge item

Software

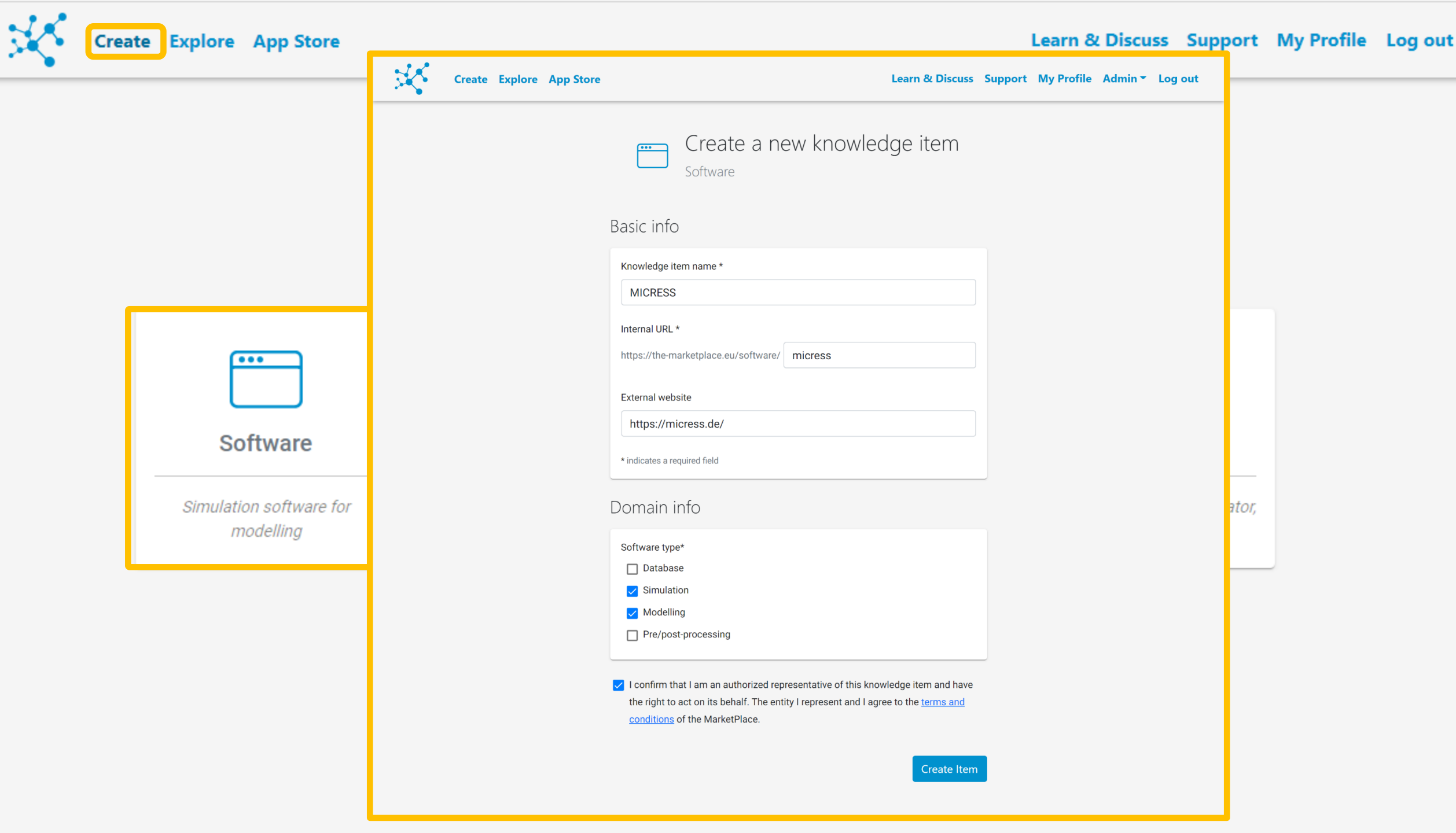
Simulation software for modelling

Organization

Entities such as teams, labs, companies, etc.

Expert

Examples: AI expert, translator, etc.


Create
Explore
App Store
Learn & Discuss
Support
My Profile
Log out
Create
Explore
App Store
Learn & Discuss
Support
My Profile
Admin
Log out
Create a new knowledge item
Software
Basic info
Knowledge item name *
MICRESS
Internal URL *
https://the-marketplace.eu/software/
micress
External website
https://micress.de/
* indicates a required field
Domain info
Software type*
Database
Simulation
Modelling
Pre/post-processing
I confirm that I am an authorized representative of this knowledge item and have the right to act on its behalf. The entity I represent and I agree to the terms and conditions of the MarketPlace.
Create Item
Software
Simulation software for modelling

Create a knowledge item

Software

Simulation software for modelling

Organization

Entities such as teams, labs, companies, etc.

Expert

Examples: AI expert, translator, etc.

Create Explore App Store Learn & Discuss Support My Profile Log out

Summary

No summary available

Expertise

Software

Materials

Processes

Materials

- ContinuumMaterial
  - Plasma
  - SinglePhaseMaterial
  - MultiPhaseMaterial
    - LiquidLiquid
    - SolidGas
    - LiquidSolid
    - SolidLiquid
    - GasLiquid
    - SolidSolid
      - MultiPhaseSolid
        - Ceramic
        - MetallicAlloy
      - CompositeMaterial
    - LiquidGas

Expert

Examples: AI expert, translator, etc.

Search

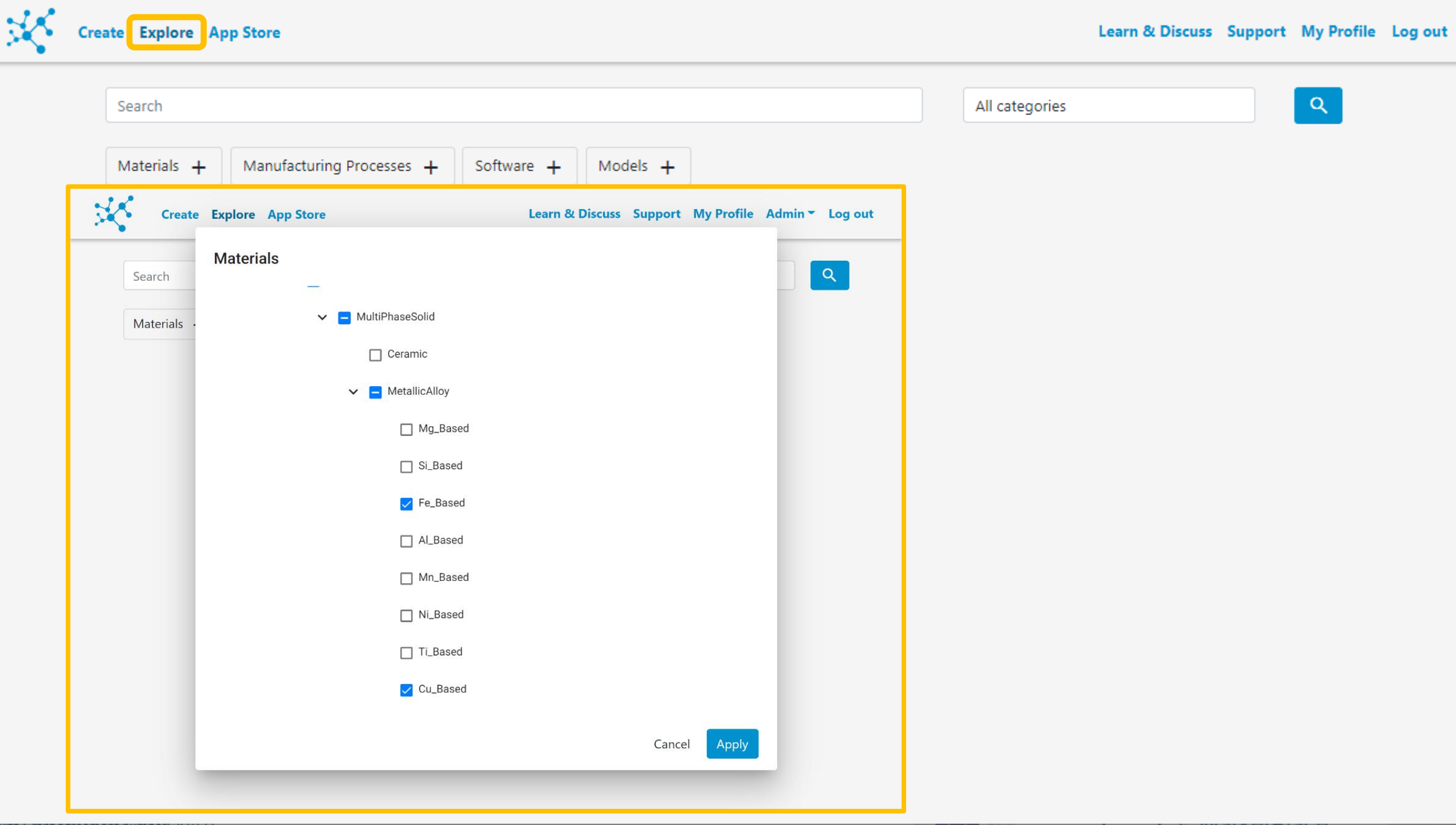
All categories

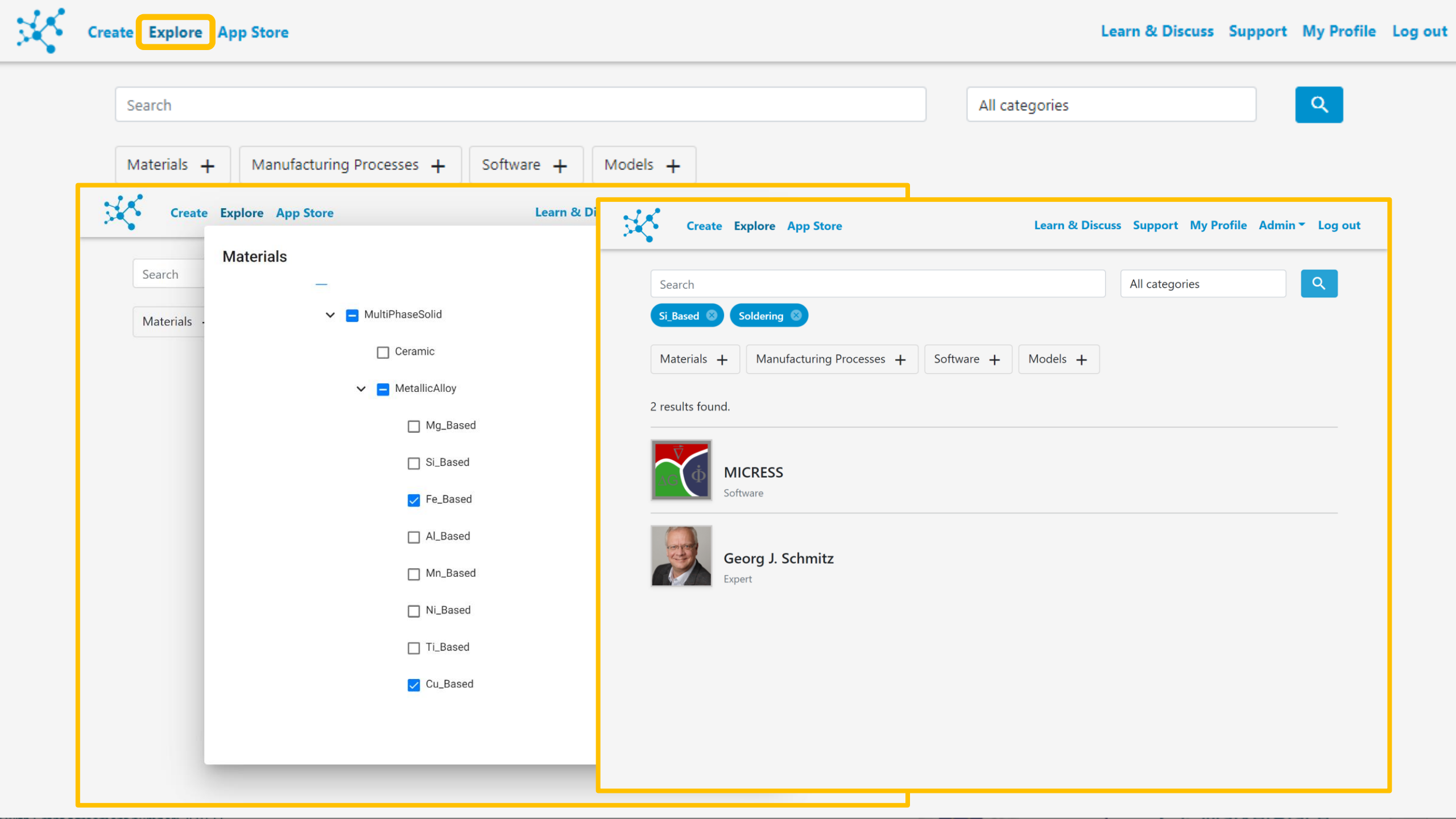
Materials +

Manufacturing Processes +

Software +

Models +


Create
Explore
App Store
Learn & Discuss
Support
My Profile
Log out
Search
All categories
Materials +
Manufacturing Processes +
Software +
Models +
Create
Explore
App Store
Learn & Discuss
Support
My Profile
Admin
Log out
Search
Materials
Materials
MultiPhaseSolid
Ceramic
MetallicAlloy
Mg_Based
Si_Based
Fe_Based
Al_Based
Mn_Based
Ni_Based
Ti_Based
Cu_Based
Cancel
Apply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Log out
Search
All categories
Si_Based
Soldering
Materials +
Manufacturing Processes +
Software +
Models +
2 results found.
MICRESS
Software
Georg J. Schmitz
Expert

Register Hydra

Callback URL

Authorization Flow / Grant Type

○PKCE

◉Authorization Code Flow

Scopes

- ☐ Email
- ☐ Profile
- ☑ OpenId
- ☐ Offline

Register Hydra

Register Application

Application ID

Application Name

Application Description

Version

HomePage URL

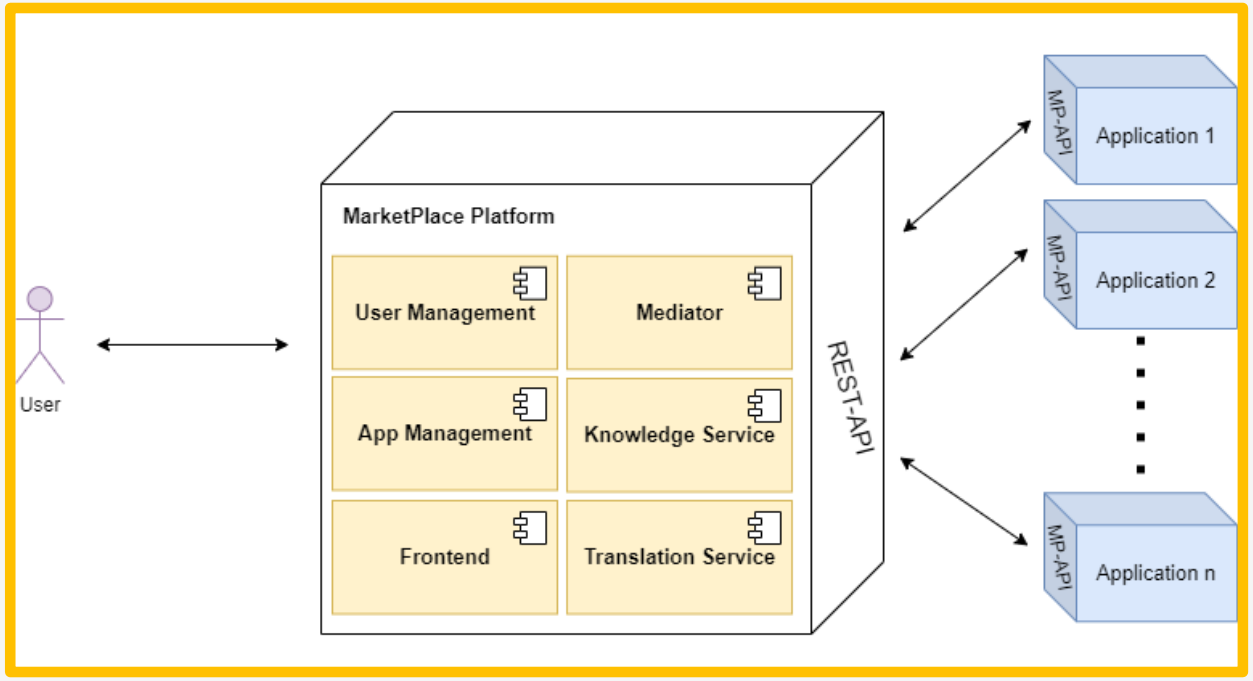
Application logo URL

Product Name

Product ID

OpenAPI Datei auswählen Keine Datei ausgewählt

Clear Register Application



App Store

Actions:

- Register an new app
- Learn more about app registration
- Ask for support

Granta_Localhost_Insecure_Public_Client

Granta_Public

Read more

Web application | API | Purchase

Knowledge App

Knowledge App

Read more

Web application | API | Purchase

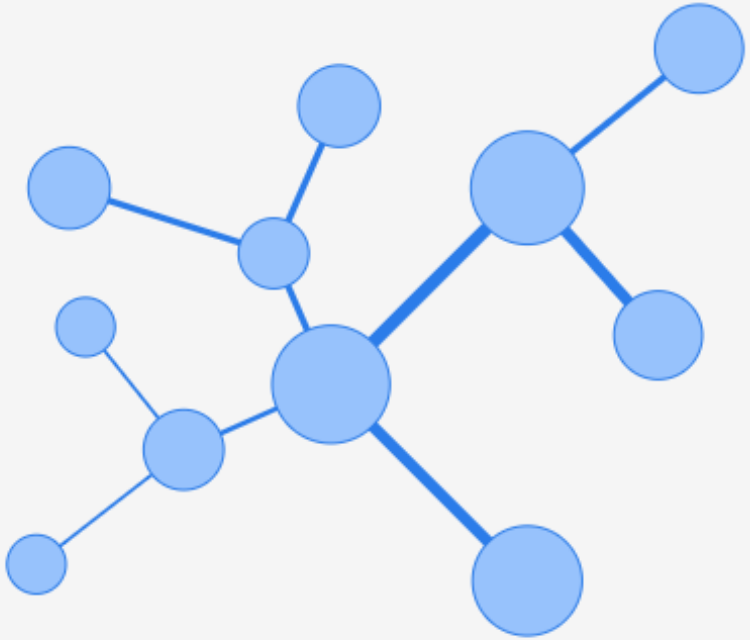
OPTIMADE Gateway App

OPTIMADE Gateway Structures

Read more

Web application | API | Purchase

dev-Discourse



MarketPlace

For Increased Innovation in Materials Modelling

Funded by Horizon 2020 with grant agreement number 760173 (MarketPlace)

MarketPlace

all categories | Categories | Latest | Top

Education/Training

This category accumulates education and training material for all MarketPlace users.

Translation of Real Use Cases

SimPhoNy Educational

MICRESS AiiDA

Translation Services

Dissemination Material

Software BLOG

Uncategorized

Topics that don't need a category, or don't fit into any other existing category.

Query for New Potential Projects

Here Customers can describe their problem in accordance with the provided template.

Running projects (WT)

Use Case 3

+

MarketPlace

all categories | Categories | Latest | Top

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Software BLOG

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Topics that don't need a category, or don't fit into any other existing category.

Query for New Potential Projects
Here Customers can describe their problem in accordance with the provided template.

Create a new Topic

Type title, or paste a link here

Query for New Potential Projects

:boom: **Project title:**

:large_blue_circle: **Material:**

:old_key: **KPI:**

:microscope: **Method:**

:pill: **Granularity:**

💥 **Project title:**

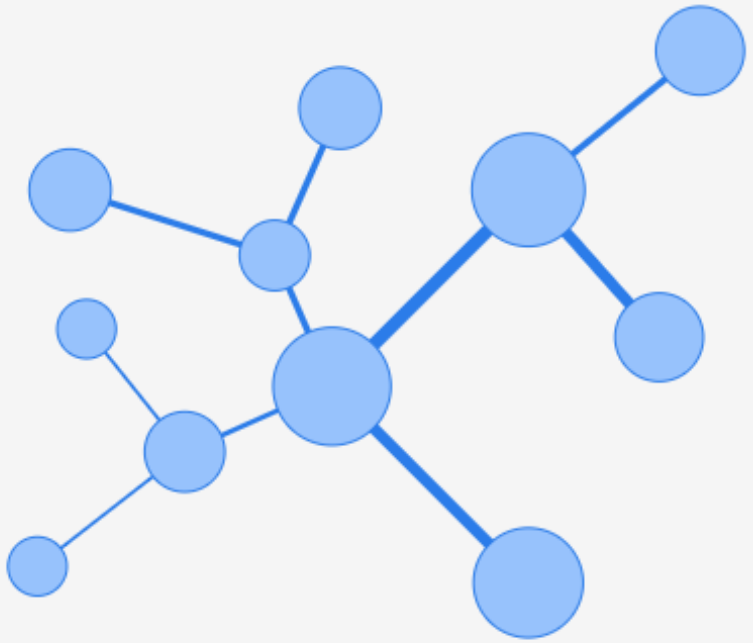
🔵 **Material:**

🗝️ **KPI:**

🔬 **Method:**

💊 **Granularity:**

Create Topic cancel



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See you soon on

The Materials Modelling MarketPlace

explore – interact – create and execute – improve your materials, processes, and products

A sustainable **MarketPlace for materials modelling** with coherent services on

- **explore** data and knowledge by searching in databases of material models and material data, software tools, benchmarks, as well as validation data,
- **interact** by getting advice and support readily for training and education, expertise discussions and user feedback, as well as translation services,
- **create and execute** simulations by using workflow builders and integrated open simulation platforms.

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Onto Commons Workshop: Industry Commons Marketplaces

1. **Marketplace Knowledge graph**
   - What could be the scope of such a Knowledge graph?
   - What can we learn from the existing Knowledge Graphs (e.g. from the life sciences)?
   - How can we create such a knowledge graph?
2. **Marketplaces Ontology framework**
   - Which ontologies are already in use by the marketplaces?
   - Could the used top-level ontologies be aligned in the course of OntoCommons?
   - What could be the added value for a global ontology framework?
3. **Common API for Marketplaces**
   - What could be achieved with a global API? Global search, … ?
   - How can marketplace users benefit from interaction between marketplaces?
   - What could be potential technical and legal hurdles?
4. **Demonstrators**
   - Do the demonstrators use the Ontologies?
   - If yes, how and which tools do they use?

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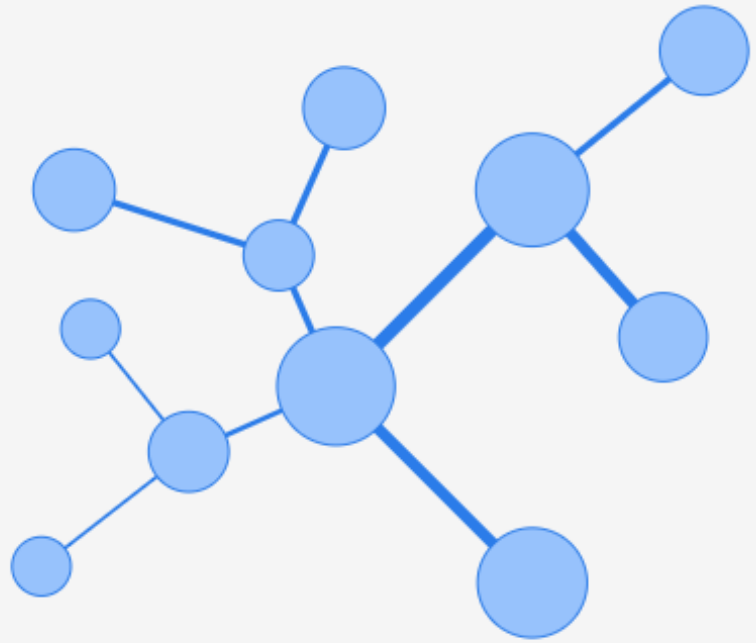

MarketPlace

For Increased Innovation in Materials Modelling

Thanks a lot for your attention!

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http://the-marketplace-project.eu

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