# MarketPlace

# THE MARKETPLACE – MATERIALS MODELLING MARKETPLACE FOR INCREASED INDUSTRIAL INNOVATION

4th April 2023

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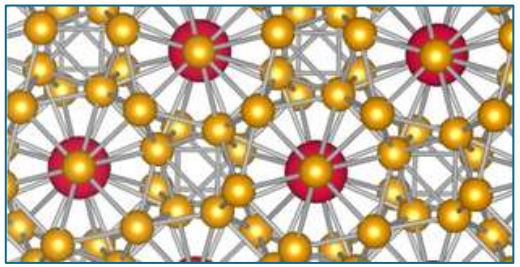
The MARKETPLACE project is funded by Horizon 2020 under H2020-NMBP-25-2017 call with Grant agreement number: 760173

# Introduction and Motivation

# The MarketPlace: introduction and motivation

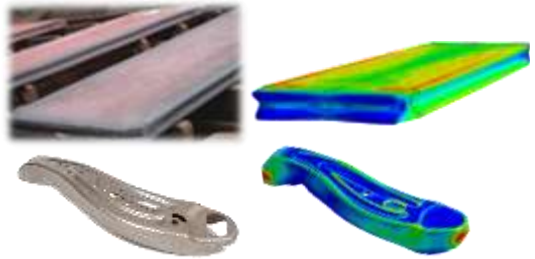
## Needs for modelling and simulation for optimal materials, processes, and products

### Material design



- Virtual material design, e.g. steel development
- Material discovery, e.g. substitution of critical elements
- …

### Process design

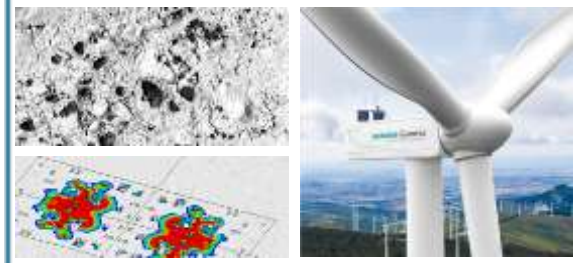


- Virtual design of processes, e.g. steel
- Analysis, evaluation, and optimization of processes & process chains
- …

### Component design


- Component performance
- Computer-aided crash assessment
- Lifetime prediction
- Static design
- …

### Sustainable design



- Simulation assisted sustainability analysis
- Holistic approach by incorporating the whole lifetime of a material
- …





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# The MarketPlace: a short overview

## The user perspective about material modelling and simulation

| Industrial R&D | Researcher | Software Vendor | Consultant |
|---|---|---|---|
| ■ E.g. **SMEs** in the field of additive manufacturing: »I am interested in the properties of additively manufactured microstructures: from the powder composition to the component...« | ■ E.g. **Material modeler.** »I would like to adapt my material models to material data and make them available to users.« | ■ E.g. **SME-Software Vendor.** » …we realized that monolithic software solutions are neither adequate nor capable of tackling the host of phenomena occurring during production and service life of materials and products.« | ■ E.g. **SME-Consultant.** »Successful industrial materials modelling more & more depends on assembling knowledge, software and data from a wide range of fields which can be perplexing for SMEs and challenging even for large enterprises.« |



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# What is the MarketPlace marketplace?

# The MarketPlace: a short overview

## Platform perspective: One-Stop shop for material modelling and simulation

> Search model data, experts, expertise, …

| **EXPLORE**<br>search data and knowledge | **INTERACT**<br>advice and support readily | **CREATE & EXECUTE**<br>develop and deploy |
|---|---|---|
| Material relation data | Training | App Store |
| Software data | Education | Workflow manager |
| Benchmark data | Discussion and user feedback | Integrated Open Simulation Platforms |
| Validation data | Translation Services | HPC integration |

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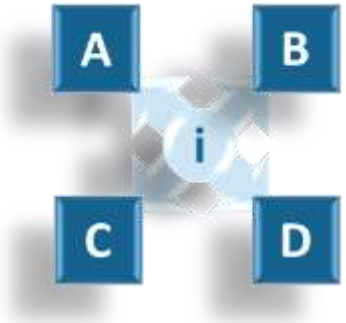
# The MarketPlace: a short overview

## Technological perspective: »The key concepts«

### Interoperability

- Seamless communication between services and tools via semantic technologies
- integrated simulation platforms (e.g. AiiDA, AixViPMaP, SimPhoNy-remote)




### Ontology

- Platform management (experts, software, ...)
- Software & workflow communication (Who am I? What can I do?)

### Variability

- User Registration and User Roles
- Registration of Apps
- Registration of pre-configured workflows
- user-specific content


### Platform design and -ressources

- Web services
- Integrated services via API
- App Store (Marketplace API)
- HPC Services
- safety Web-Services

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# The MarketPlace Platform

## Technological perspective: services based on vocabular, taxonomy, and ontology

- MarketPlace has integrated services based on onlogies: e.g.
  - ontology-based **Knowledge Service**
  - ontology-based **Model Relation** database
- These **services** are **based** on different **ontologies**, partially EMMO compliant, e.g.
  - **Expert** ontology – characterizes  an expert for matching operation
  - Software ontology – taxonomy for software
  - Material ontology – taxonomy for material
  - Manufacturing ontology - taxonomy for manufacturing
  - Application handling ontology
  - European Virtual Marketplace Ontology (EVMPO)  – interoperability VIMMP and MarketPlace





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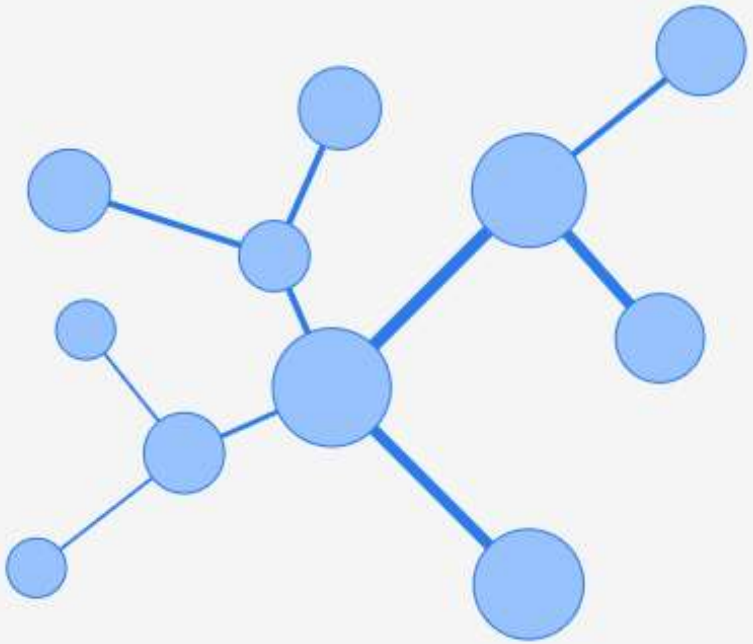

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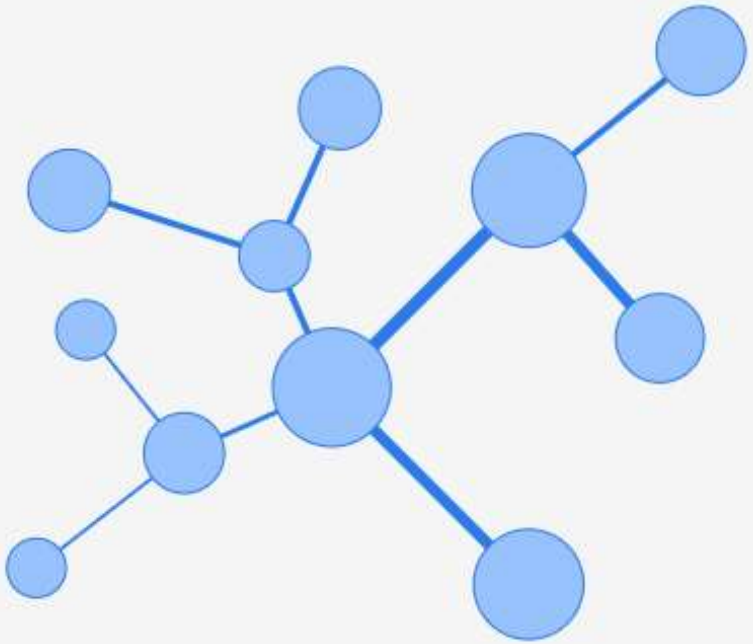
For Increased Innovation in Materials Modelling



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

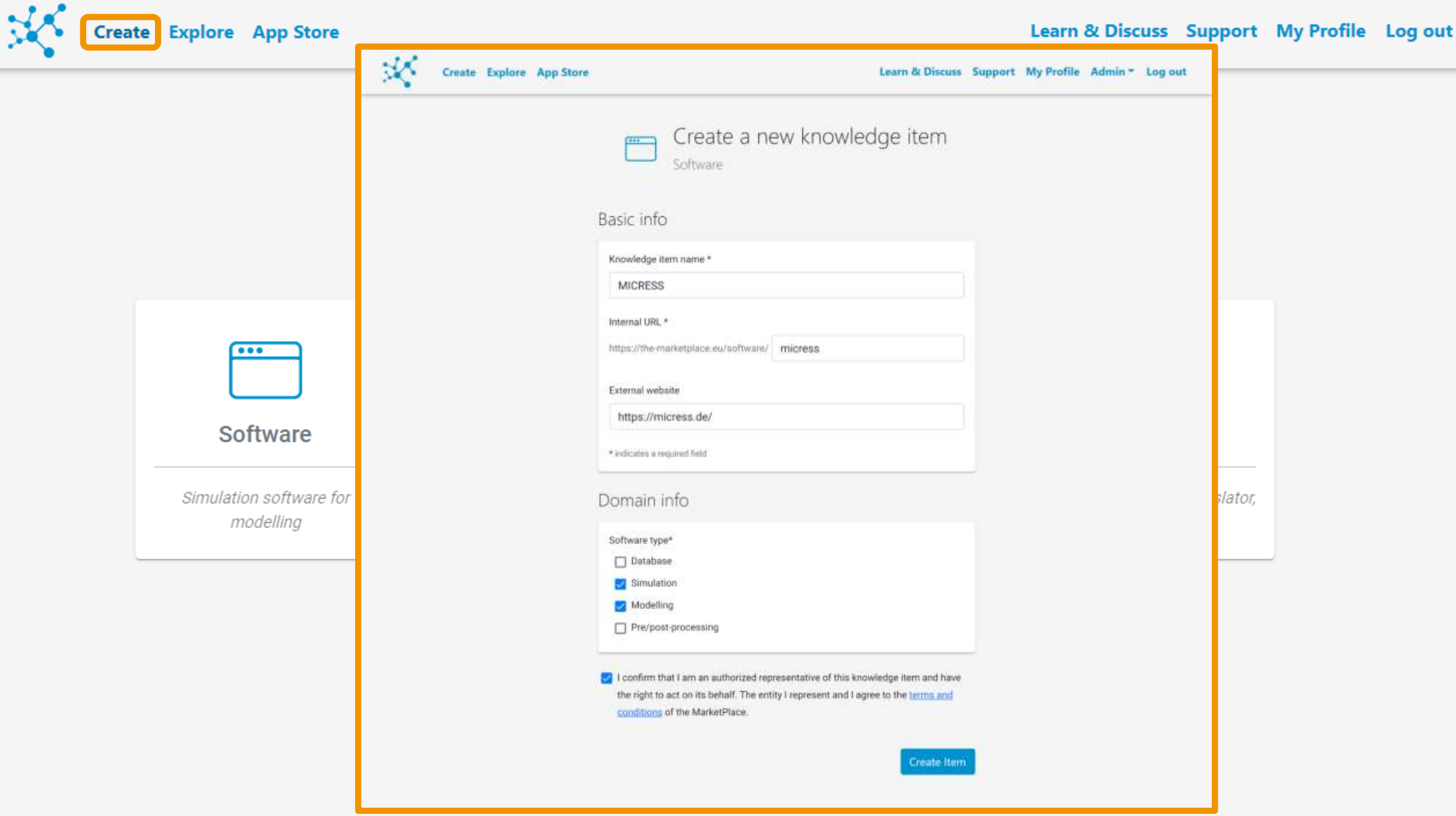
*Simulation software for modelling*

## 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
Software
Simulation software for modelling
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

# Create a knowledge item

## Software

*Simulation software for modelling*

## Organization

*Entities such as teams, labs, companies, etc.*

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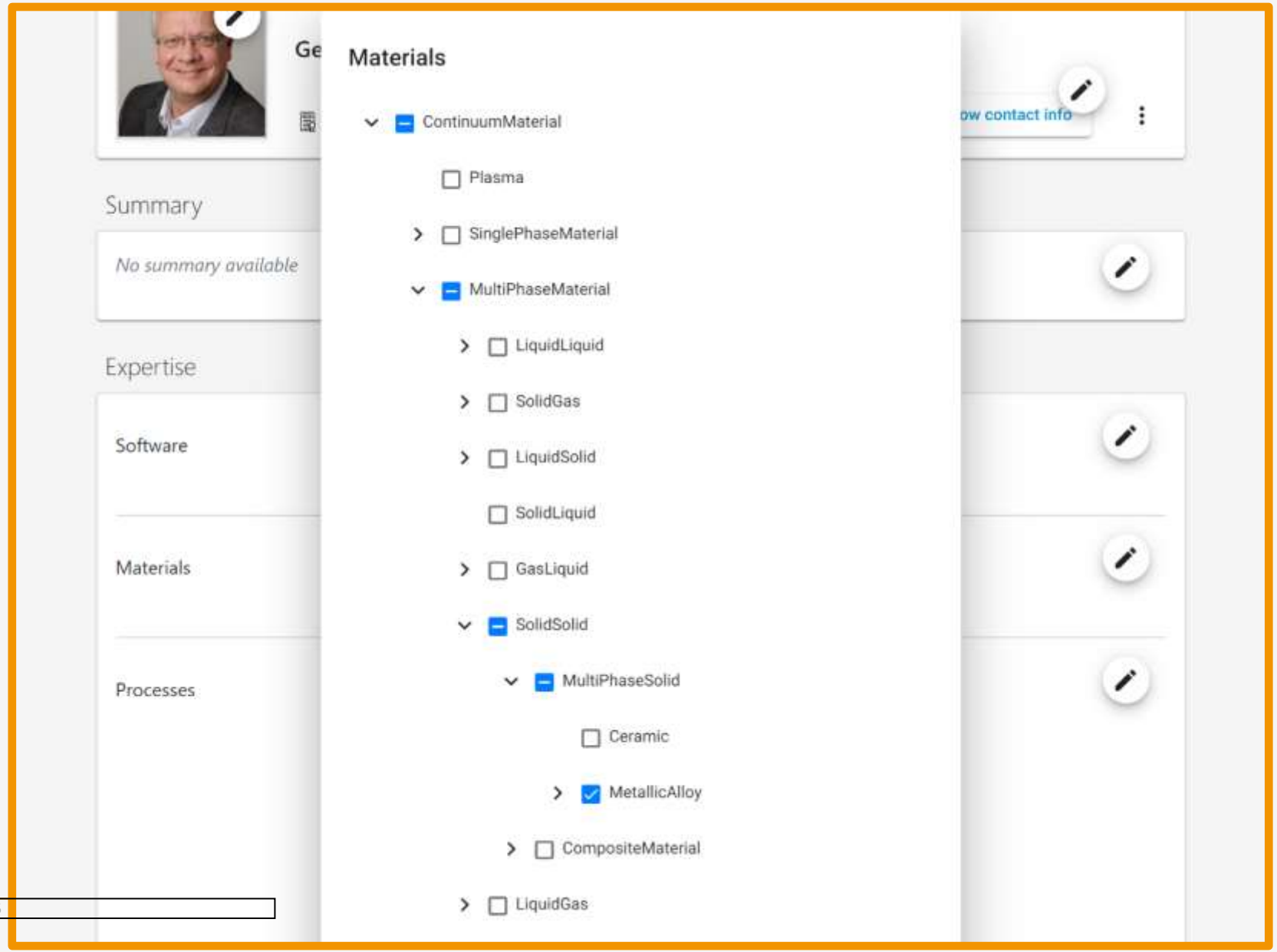
*Examples: AI expert, translator, etc.*




## Expert

*Examples: AI expert, translator, etc.*

Search

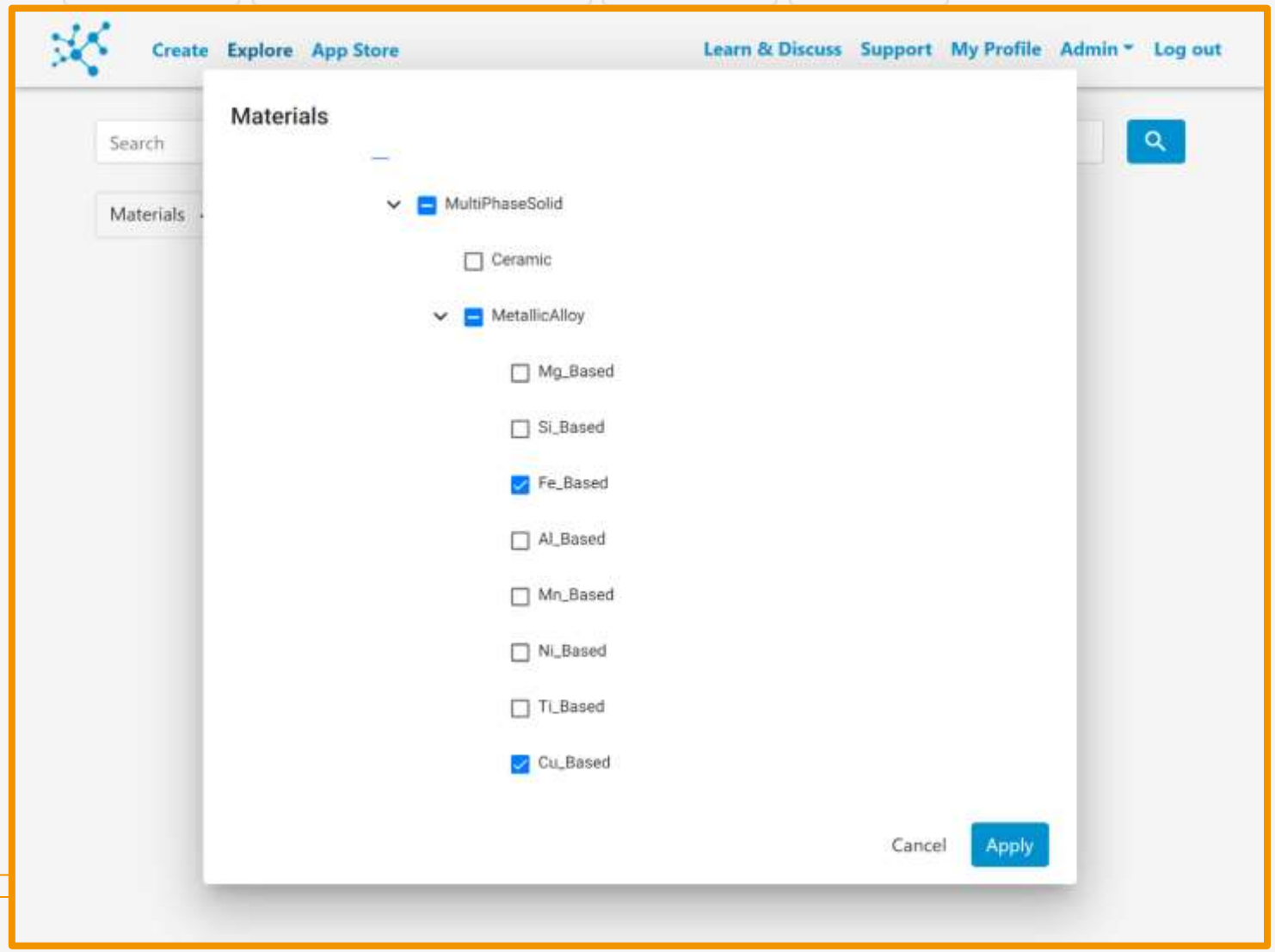
All categories

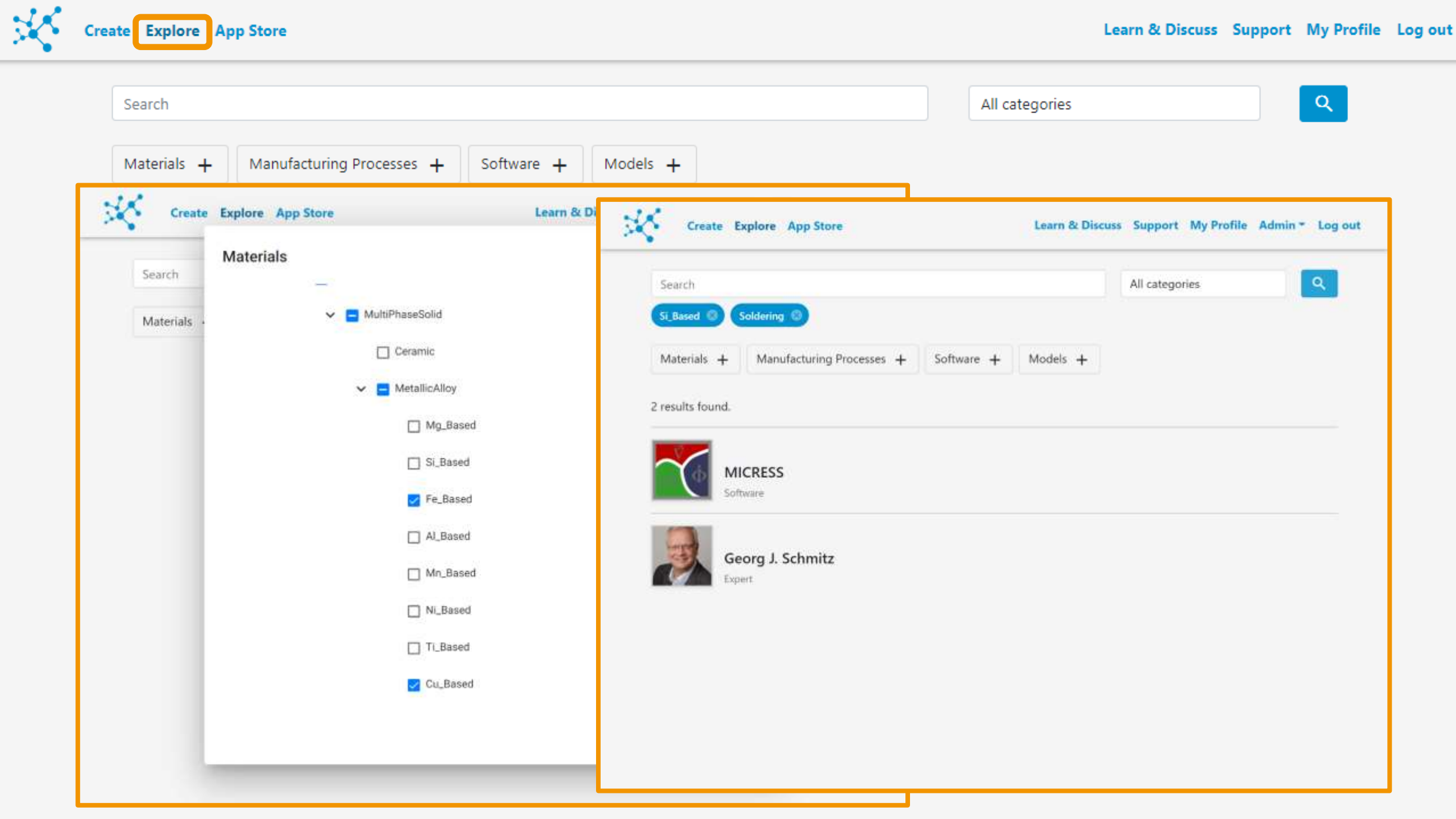
Materials +

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


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

# The MarketPlace: a short overview

## Technological perspective: »The key concepts«

### Interoperability

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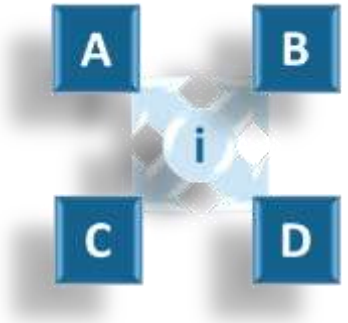
- integrated simulation platforms (e.g. AiiDA, AixViPMaP, SimPhoNy-remote)

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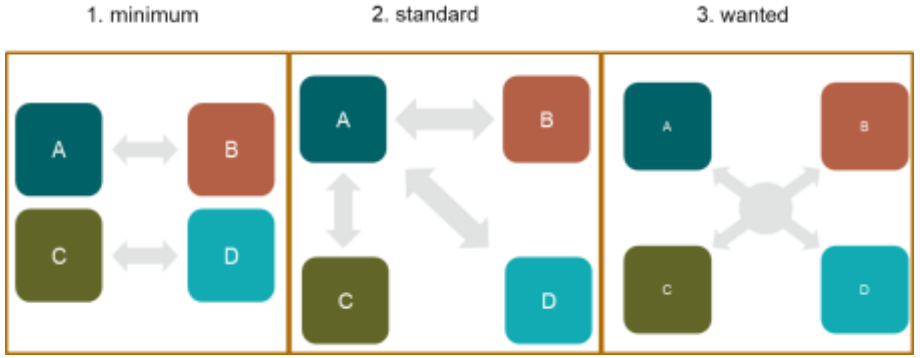
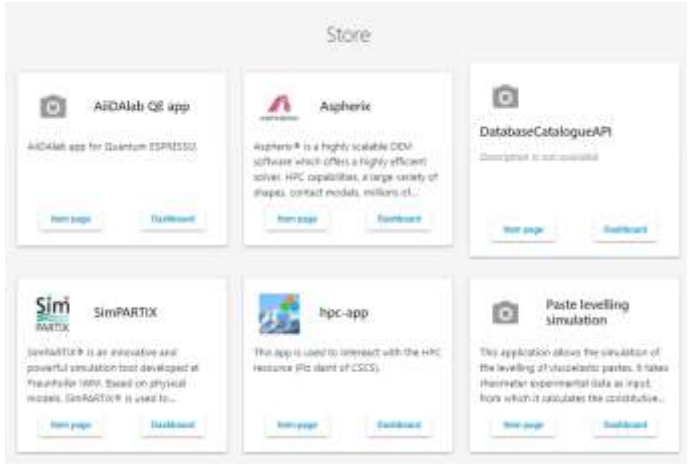
# The MarketPlace Platform

## Technological perspective: Cross domain interoperability via standards & ontologies

- **MarketPlace** employs **multi-level model** of **software integration**
  - **Level 0**: Frontend link only
  - **Level 1**: API via MarketPlace specs. Data payload is opaque to the system.
  - **Level 2**: Semantic integration. Data is described via ontologies and is transparent to the system.
- In MarketPlace, **ontologies are used for level 2 integration** of apps as well as for annotation of knowledge item to increase their discoverability
- **Software integration** procedure is used in the **App Store**
- **Semantic tools**: Uniform API, ontology for data discoverability




**App Store**





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# The MarketPlace

## Our use cases for platform development & demonstration

**Use Case 1: Additive manufacturing of superalloys**

**Use 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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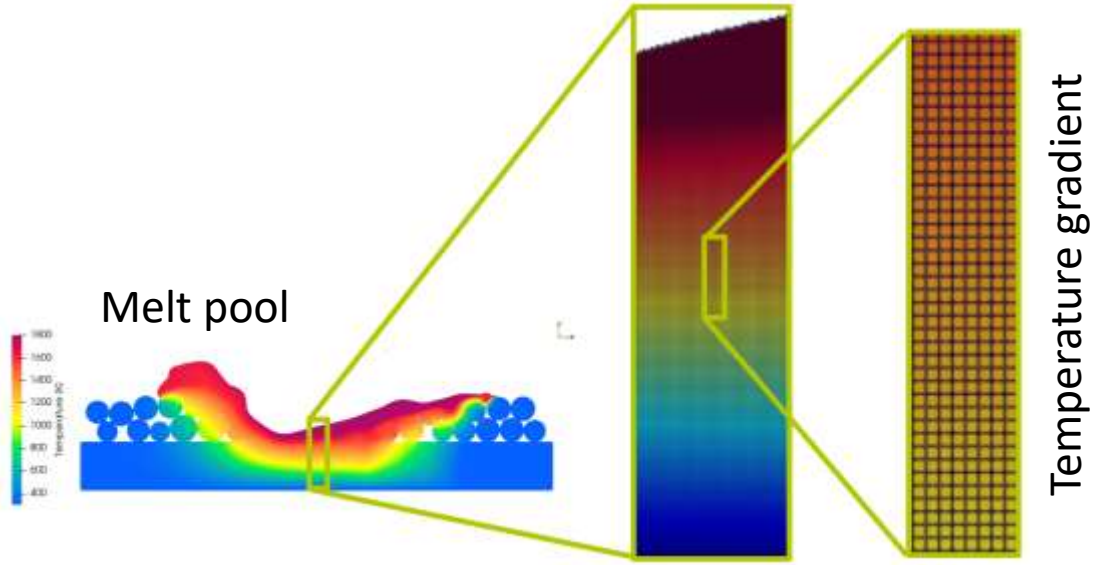
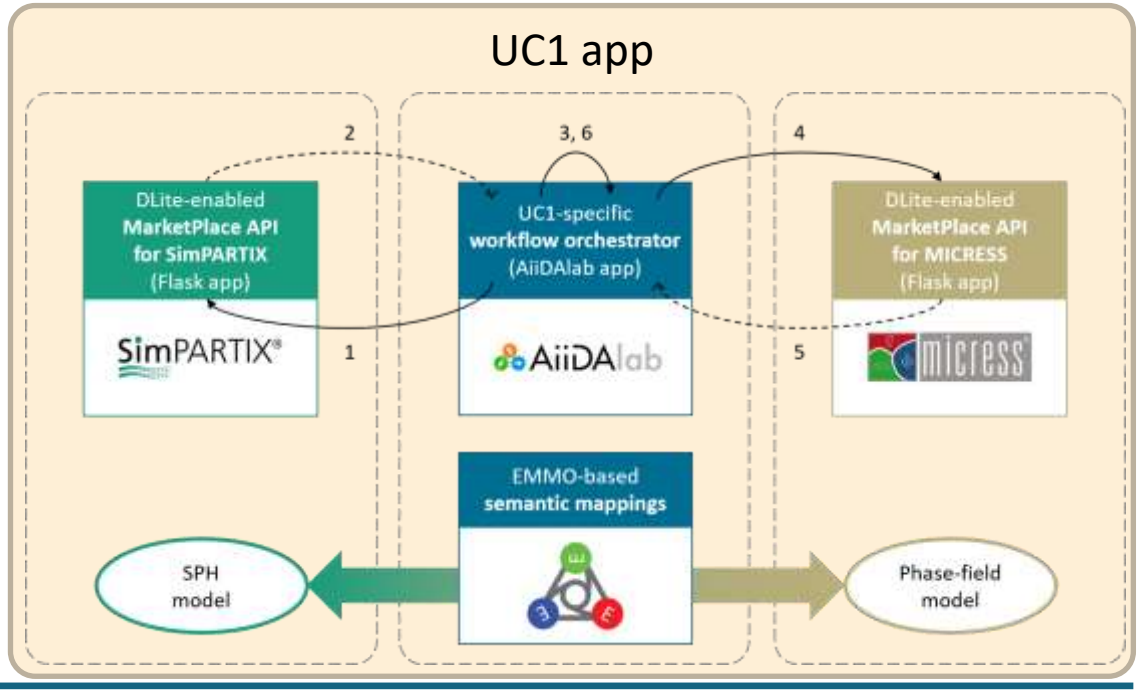
# The MarketPlace

## Use Case 1: Additive manufacturing of superalloys




- UC1 models the **laser powder bed fusion process of super-alloys**.
  - The **SimPARTIX app** is used for the melt pool simulation which generates a temporally and spatially resolved **temperature field** which is then used by the …
  - … **MICRESS app** which **calculates the microstructure** formation simulation based on derived temperature gradient.
- "Level 2" integration of the UC1 app has been achieved. This is realized by **semantic mapping of the data** transferred between the simulation codes using **DLite containers referring to EMMO entities**.





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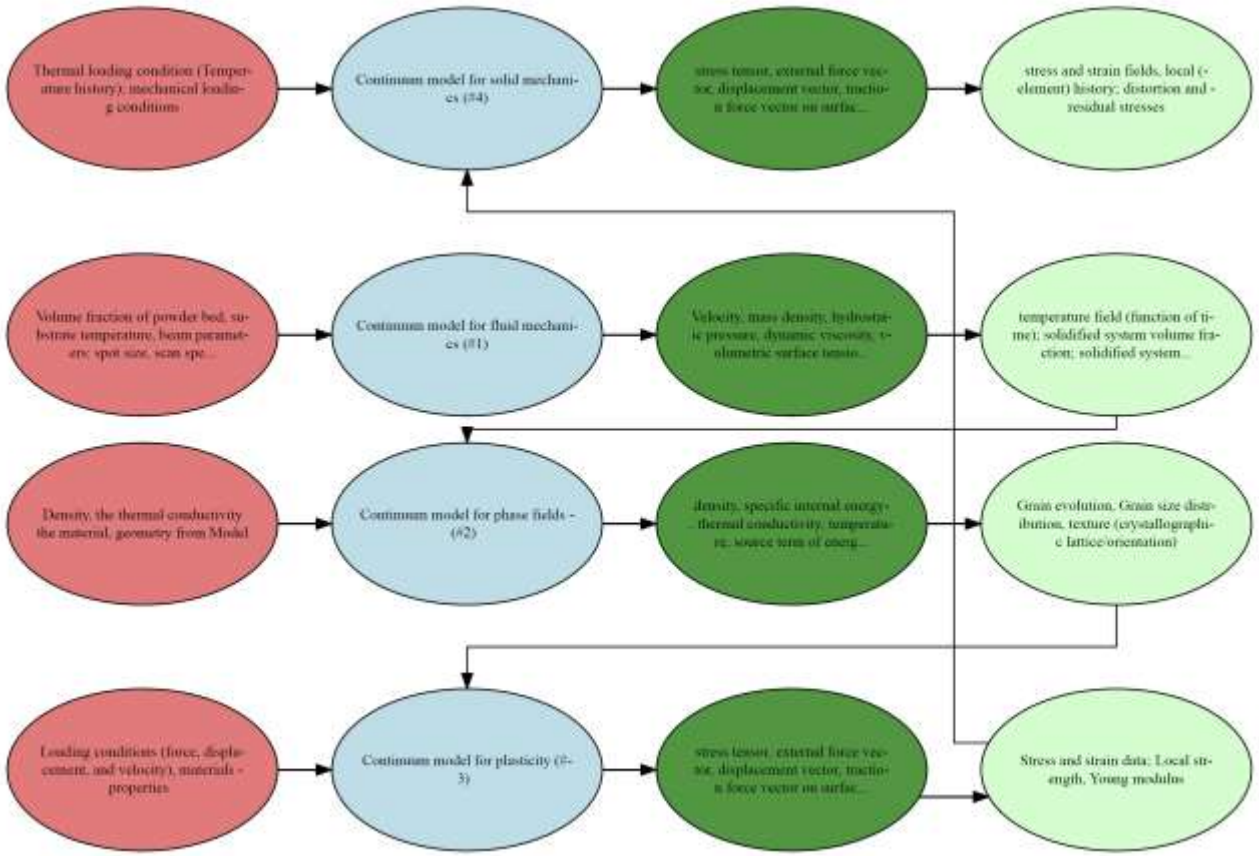
# The MarketPlace

## Use Case 1: Data documentation via MODA for the use cases




EMMC MODA Portal

| | |
|---|---|
| **SUBTYPE 1:** | Fluid Mechanics |
| **ENTITY:** | Continuum Volume |
| **MODEL (EQUATION SET) NAME:** | Navier Stokes equation |
| **MODEL (EQUATION SET) DESCRIPTION:** | The transport equations for the melt pool dynamics process solving Continuity, momentum, Energy and Adsorption Equation |

**EQUATIONS:**

**EQUATION 1**

**EQUATION PREVIEW:** $\nabla \cdot \boldsymbol{u} = 0$

**PHYSICS QUANTITIES**

| | | |
|---|---|---|
| **QUANTITY 1** | **NAME:** | Velocity |
| | **SYMBOL:** | $u$ – velocity |
| | **DESCRIPTION:** | |

**EQUATION 2**

**EQUATION PREVIEW:** $\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \mu \nabla^2 \boldsymbol{u} + \boldsymbol{f}_S + \rho \boldsymbol{g}$

**PHYSICS QUANTITIES**

| | | |
|---|---|---|
| **QUANTITY 1** | **NAME:** | mass density |
| | **SYMBOL:** | $\rho$ |
| | **DESCRIPTION:** | |
| **QUANTITY 2** | **NAME:** | hydrostatic pressure |
| | **SYMBOL:** | $p$ |
| | **DESCRIPTION:** | |
| **QUANTITY 3** | **NAME:** | dynamic viscosity |
| | **SYMBOL:** | $\mu$ |
| | **DESCRIPTION:** | |
| **QUANTITY 4** | **NAME:** | volumetric surface tension force |





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# Summary of the experiences?

# The MarketPlace

## Digital Marketplaces Status and Experience

| Ontology development: challenges | Ontology: added value | Standards | Ontology update and extension |
|---|---|---|---|
| ■ Reaching cross discipline acceptance<br>■ Large variety of domain ontologies are required<br>■ Dealing with missing concepts in the ontology<br>■ No established collabo-rative development environment<br>■ Using ontologies for interacting with other platforms | ■ Ontologies enable key services: e.g. to find an expert in the field of metal plasticity with knowledge in modelling and simulation of a forming process is possible<br>■ Helpful for data exchange: e.g. between Apps in the level 2 integration | ■ EMMO is used<br>■ Ontologies for the use cases and the material relation database are EMMO-based<br>■ Partially, taxonomies like for the annotation of knowledge items were done independently | ■ Taxonomies for the annotation of knowledge items could easily be updated<br>■ Ontologies for "level 2" integration could also be easily updated as long as mappings to shared concepts are provided as well.<br>■ Missing ontology terms: still unresolved |



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# The MarketPlace

## Digital Marketplaces Status and Experience

| FAIR-principles | Relation to data spaces | Platform access and sustainability | Support by funding bodies |
|---|---|---|---|
| ■ Some ontologies are available on the EMMO GitHub repository<br>■ Documentation is limitedly available<br>■ Github/gitlab is used<br>■ Users are not necessarily aware of ontology use, but data items could still be found, accessed and reused | ■ The MarketPlace do not contain a data space<br>■ Data storage is possible in relational data bases for benchmarking & validation<br>■ Users are required to use a data sink/source app | ■ Access to external users will be possible soon<br>■ A new MarketPlace association should be formed to assure the sustainability of the platform | ■ Overall support is already great<br>■ Legal resources for specific council and guidance could be very beneficial<br>■ Programs to support setting up a business with European partners |



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# The MarketPlace
## Digital Marketplaces Status and Experience

- Name one **concept that works** well in your platform and **another** that poses a **major challenge**.
  - Knowledge app provides a layer of abstraction that makes it easy to connect different items in the system.
  - To address a wide range of domains via ontology is challenging. The effort with complex T-boxes is quite high.
- List **five lessons learned** during the course of the platform development in these project?
  - Using REST API provides a good realization of the "separation of concerns" principle
  - Ontologies are not the only way to achieve interoperability – For example, REST API and standard file format can also achieve this goal
  - Supporting different levels of integration is useful for an easy on boarding process
  - Light-weight apps could be more beneficial to demonstrate the technology than complex use cases
  - Software licenses and other legal issues pose significant challenges



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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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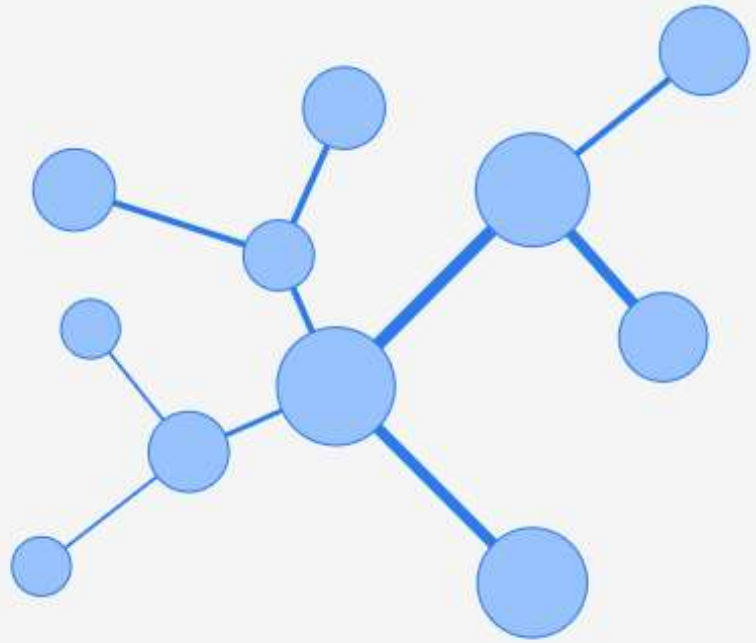
Create Explore App Store

Learn & Discuss Support My Profile Log out



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Thanks a lot for your attention!

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http://the-marketplace-project.eu



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