THE MARKETPLACE – MATERIALS MODELLING MARKETPLACE FOR INCREASED INDUSTRIAL INNOVATION

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Introduction and Motivation
# The MarketPlace: introduction and motivation

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

<table>
<thead>
<tr>
<th>Material design</th>
<th>Process design</th>
<th>Component design</th>
<th>Sustainable design</th>
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</thead>
<tbody>
<tr>
<td>Virtual material design, e.g. steel development</td>
<td>Virtual design of processes, e.g. steel, Analysis, evaluation, and optimization of processes &amp; process chains</td>
<td>Component performance, Computer-aided crash assessment, Lifetime prediction, Static design</td>
<td>Simulation assisted sustainability analysis, Holistic approach by incorporating the whole lifetime of a material</td>
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<td>Material discovery, e.g. substitution of critical elements</td>
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# The MarketPlace: a short overview
## The user perspective about material modelling and simulation

<table>
<thead>
<tr>
<th>Industrial R&amp;D</th>
<th>Researcher</th>
<th>Software Vendor</th>
<th>Consultant</th>
</tr>
</thead>
<tbody>
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<td>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...«</td>
<td>E.g. Material modeler. »I would like to adapt my material models to material data and make them available to users.«</td>
<td>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.«</td>
<td>E.g. SME-Consultant. »Successful industrial materials modelling more &amp; 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.«</td>
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What is the MarketPlace marketplace?
The MarketPlace: a short overview
Platform perspective: One-Stop shop for material modelling and simulation

EXPLORE
search data and knowledge
Material relation data
Software data
Benchmark data
Validation data

INTERACT
advice and support readily
Training
Education
Discussion and user feedback
Translation Services

CREATE & EXECUTE
develop and deploy
App Store
Workflow manager
Integrated Open Simulation Platforms
HPC integration

> Search model data, experts, expertise, ...

Material relation data
Software data
Benchmark data
Validation data

\[ \rho \nu = \text{div}(T) + \rho \]

\[ T = \frac{\partial}{\partial \tau} T + \frac{\partial}{\partial x} T \]

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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 -resources
- Web services
- Integrated services via API
- App Store (Marketplace API)
- HPC Services
- Safety Web-Services
The MarketPlace Platform

Technological perspective: services based on vocabulary, taxonomy, and ontology

- MarketPlace has integrated services based on ontologies: 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
MarketPlace

For Increased Innovation in Materials Modelling
MarketPlace
For Increased Innovation in Materials 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 a knowledge item

Software
Simulation software for modelling

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

Expert
Examples: AI expert, translator, etc.
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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.

![Diagram showing Level 1 and Level 2 integration]

App Store
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
**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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Use Case 1: Data documentation via MODA for the use cases

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Summary of the experiences?
# The MarketPlace

## Digital Marketplaces Status and Experience

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<tr>
<th>Ontology development: challenges</th>
<th>Ontology: added value</th>
<th>Standards</th>
<th>Ontology update and extension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaching cross discipline acceptance</td>
<td>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</td>
<td>EMMO is used</td>
<td>Taxonomies for the annotation of knowledge items could easily be updated</td>
</tr>
<tr>
<td>Large variety of domain ontologies are required</td>
<td>Helpful for data exchange: e.g. between Apps in the level 2 integration</td>
<td>Ontologies for the use cases and the material relation database are EMMO-based</td>
<td>Ontologies for &quot;level 2&quot; integration could also be easily updated as long as mappings to shared concepts are provided as well.</td>
</tr>
<tr>
<td>Dealing with missing concepts in the ontology</td>
<td></td>
<td>Partially, taxonomies like for the annotation of knowledge items were done independently</td>
<td></td>
</tr>
<tr>
<td>No established collaborative development environment</td>
<td></td>
<td></td>
<td>Missing ontology terms: still unresolved</td>
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<tr>
<td>Using ontologies for interacting with other platforms</td>
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### The MarketPlace

#### Digital Marketplaces Status and Experience

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

Thanks a lot for your attention!

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http://the-marketplace-project.eu