MATERIALS MODELLING **MARKETPLACE** FOR INCREASED INDUSTRIAL INNOVATION

The MarketPlace Consortium

The MarketPlace project
The challenge

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
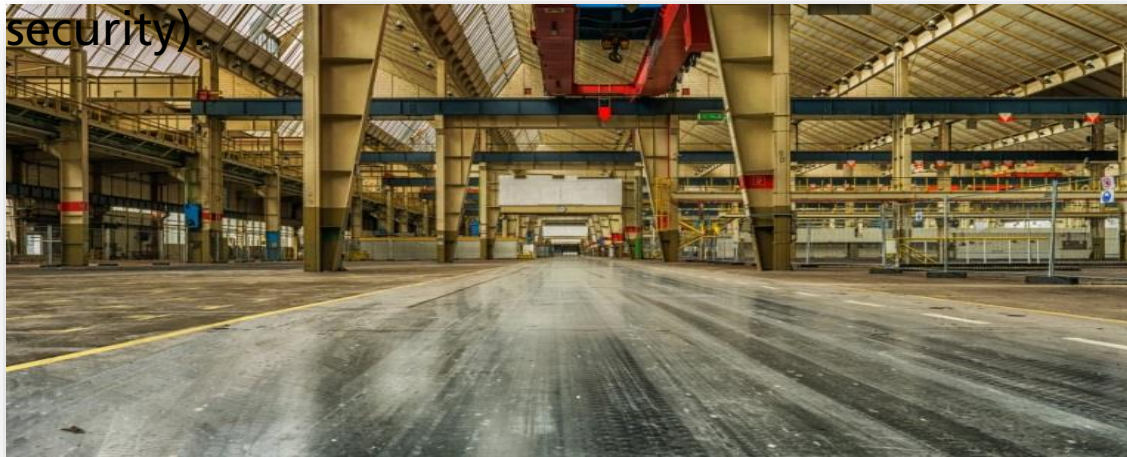
at any time and at any place.

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) security)

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	Interact: Get advice and support readily	Create & Execute: develop & deploy

Materials Models Data

$$\underline{\sigma} = \underline{\sigma}(\underline{\varepsilon})$$
$$\hat{H}\,\Psi = E\,\Psi$$

Software Tools

Benchmarks

Validation Data

Training and Education

Expertise Discussions and User Feedback

Translation Services

Workflows Builders and Executers

AiiDA

M O D A

SimPhoNy

AIXVIPMAP

SuperCap   PV Enhance   SinterAll

Integrated Open Simulation Platforms

Databases of available tools Modelling App Store

PowderFill   Alloy Diffusion   App ...

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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)
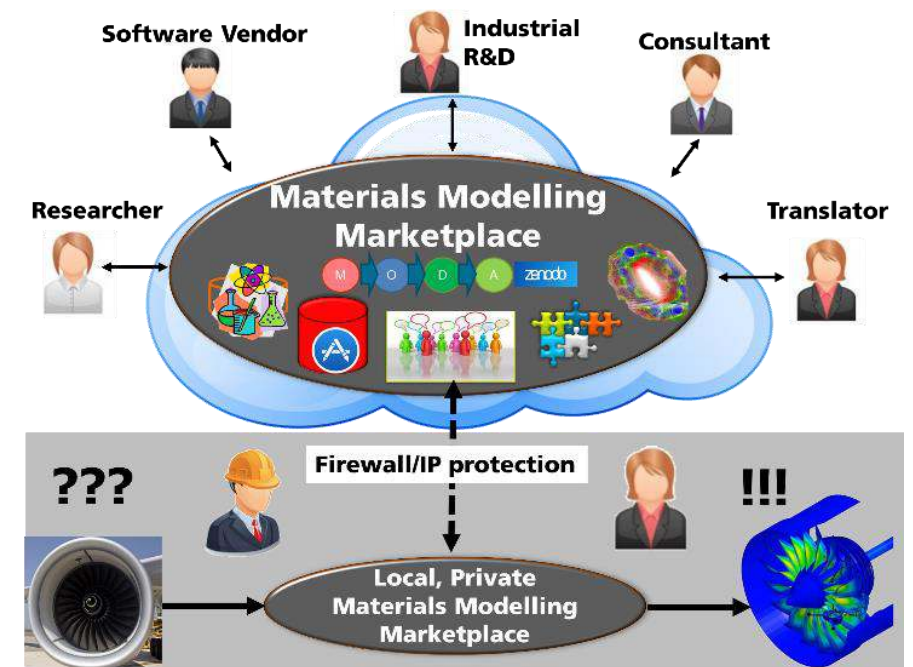
- Integration of existing Platforms

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MarketPlace Platform design

- decentralized access to applications and disparate databases

- control and management of the extensive materials information

- data and knowledge scattered across Europe and beyond

MarketPlace @Fraunhofer

MarketPlace

MarketPlace

MarketPlace @YourOrganisation

Service Provider | End User

MarketPlace Front End

MarketPlace back-End

RESTful API Plug-in System containerization

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

Software Vendor

Industrial R&D

Consultant

Researcher

Materials Modelling Marketplace

M O D A zenodo

Translator

???

Firewall/IP protection

!!!

Local, Private Materials Modelling Marketplace

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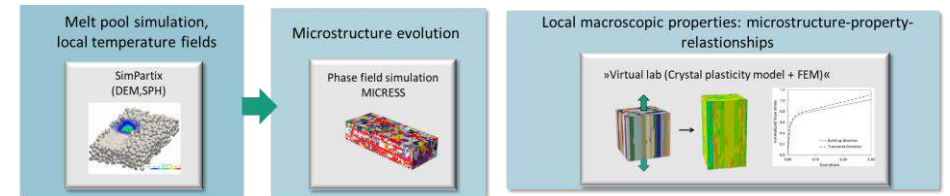
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Use Cases in the MarketPlace context

- 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!

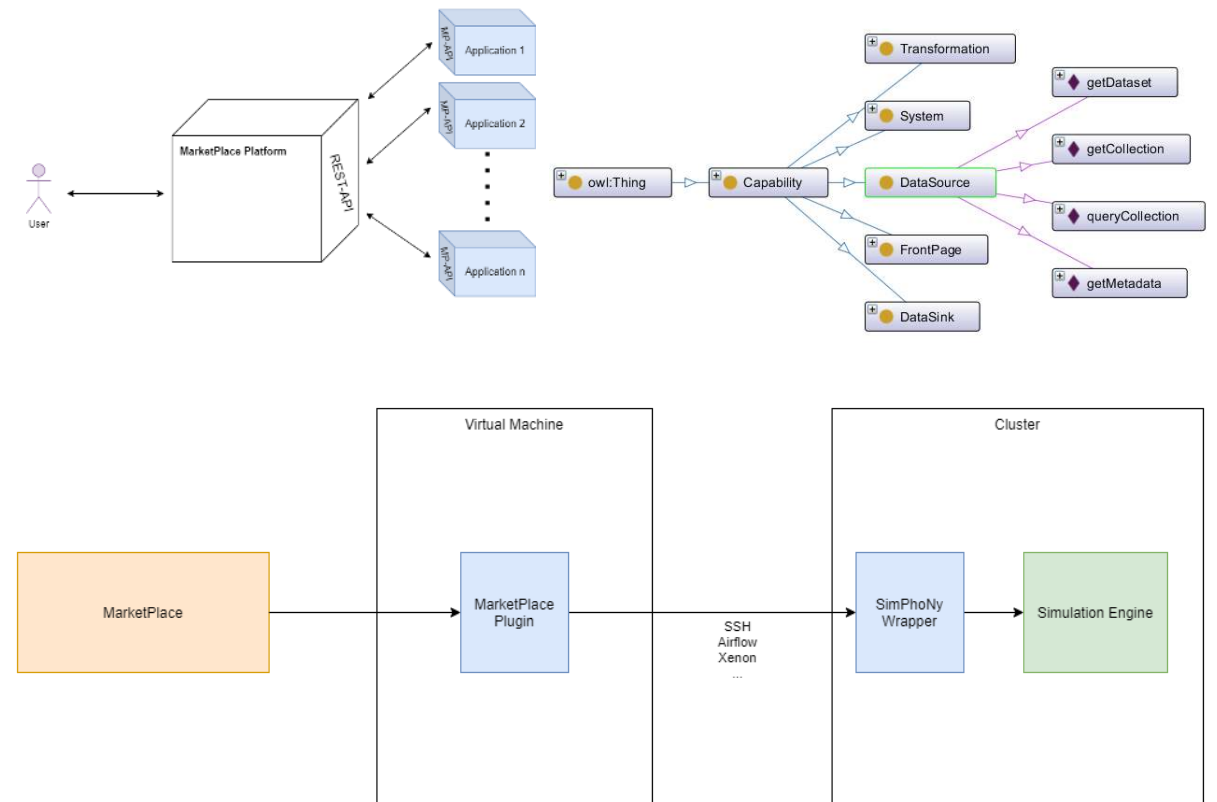- **User Case 1:** Additive manufacturing of superalloys

Melt pool simulation, local temperature fields	Microstructure evolution	Local macroscopic properties: microstructure-property-relastionships
SimPartix (DEM,SPH)	Phase field simulation MICRESS	»Virtual lab (Crystal plasticity model + FEM)«

- **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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MarketPlace API

- The MarketPlace distinguishes between several types of applications:

  - Data Source

  - Data Sink

  - Transformation

  - (Workflow)

- From those types, as set of capabilities is derived

- An application may choose to implement a subset of capabilities which are recognized by the platform

- As a result:

  - The user is informed about what an application can do

  - Workflow can be automatically validated

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Demonstration: Data exchange in the MarketPlace

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Demonstration: Application registration

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