

# MUSICODE Project

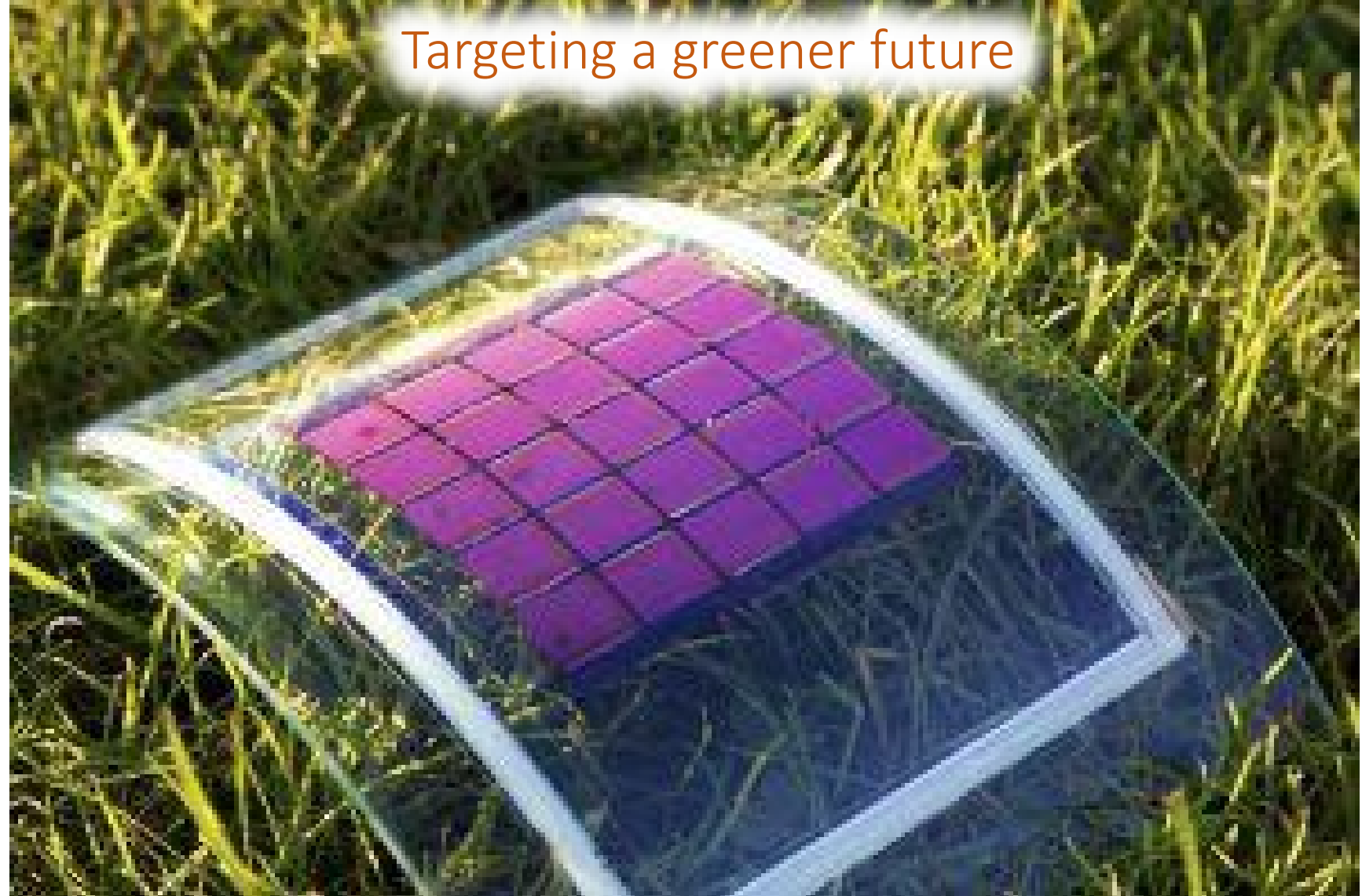
OIP Workshop 2022



This project has received funding from the European Union's HORIZON 2020 Research and Innovation Programme under Grant Agreement No 953187



- Organic Electronics
  - Photovoltaics
  - Light emitters
  - Transistors
- Applied in
  - Buildings & architectures
  - Automotive & transport
  - Wearables & textiles
- Benefits of OE
  - Green technology
  - Renewable energy
  - Environmentally friendly
- But improvements are needed
  - Materials
  - Processing
  - Devices



# Why do we need a modelling platform?

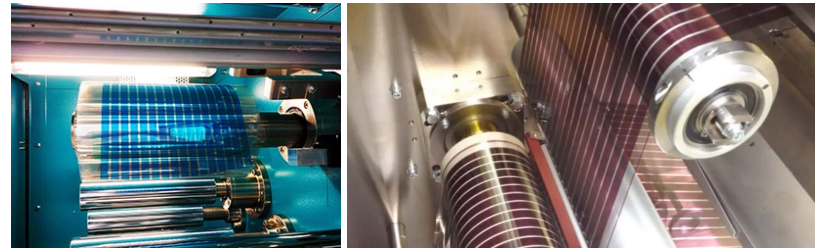
## Target industrial processes: printing and gas transport in Organic Electronics

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

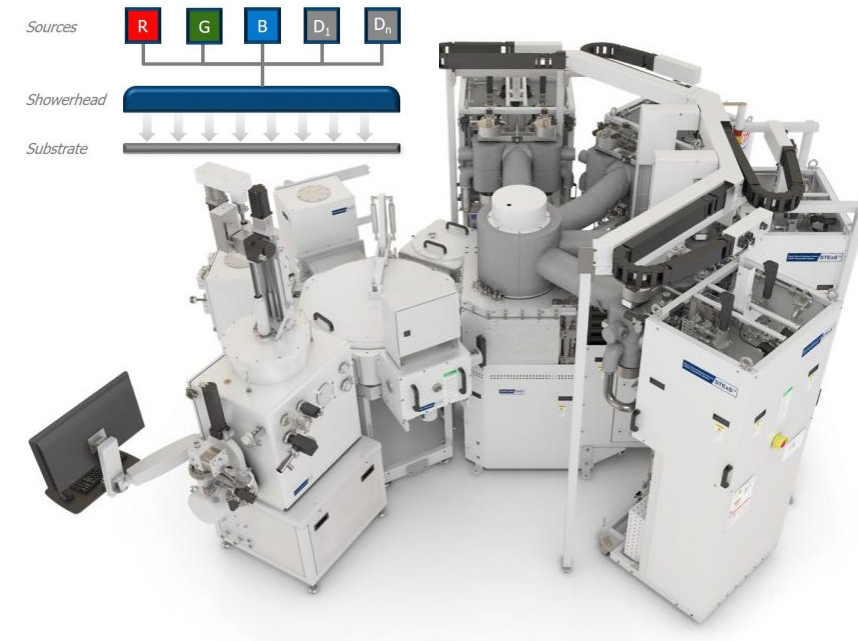
-> enabling virtual R&D

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

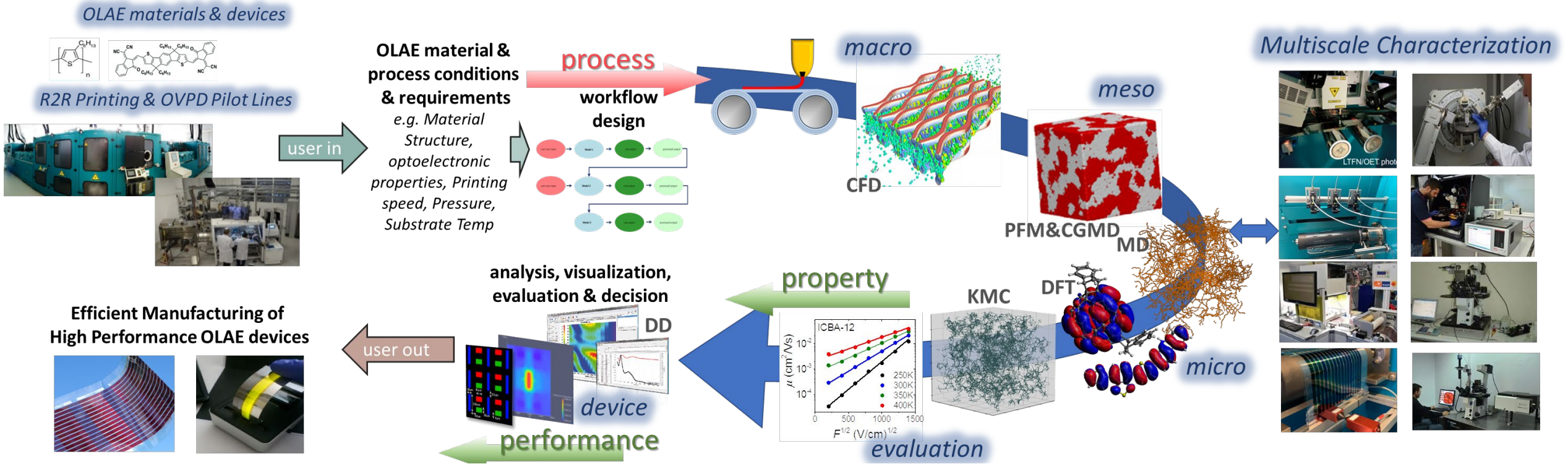
*Roll-to-Roll Printing of OPVs*



*Organic Vapor Phase Deposition of OLEDs*



# The envisioned user experience in the Open Innovation Platform



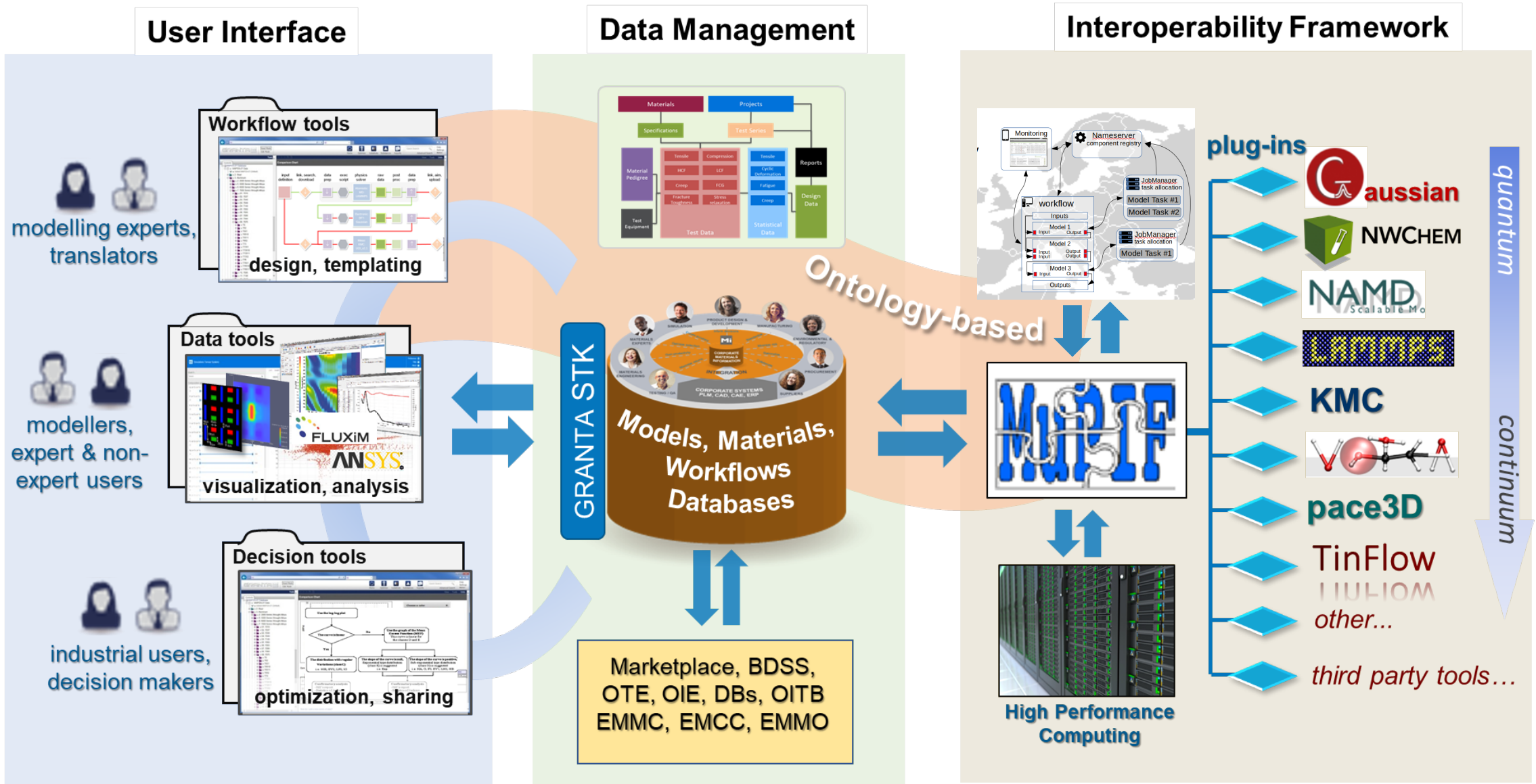
- new material formulations
- solution-based processing
- gas-phase transport

- integrated data management
- workflow design, optimization
- linked to Marketplaces

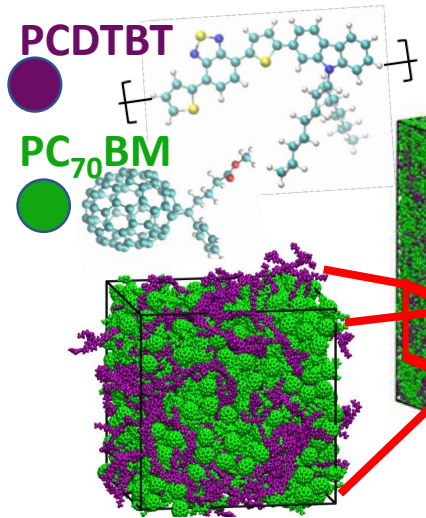
- ontology-based interoperability
- electronic to continuum models
- process-property relations

- 3D multiscale characterization
- material model validation
- industry-accepted protocols

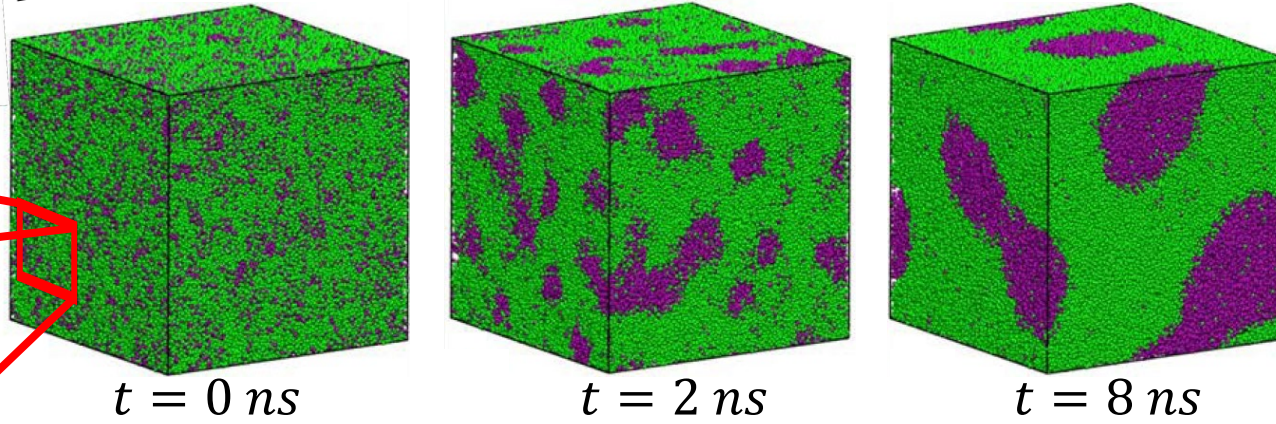
# The concept and structure of the MUSICODE Open Innovation Platform



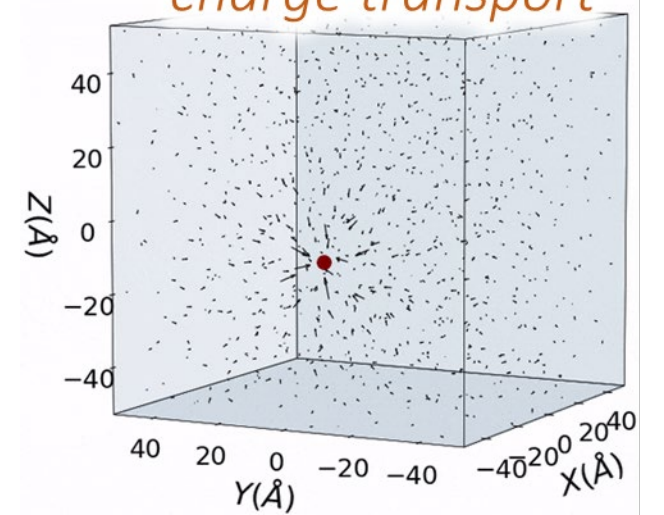
# Integrated multiscale modelling: Workflows, models and data across all scales



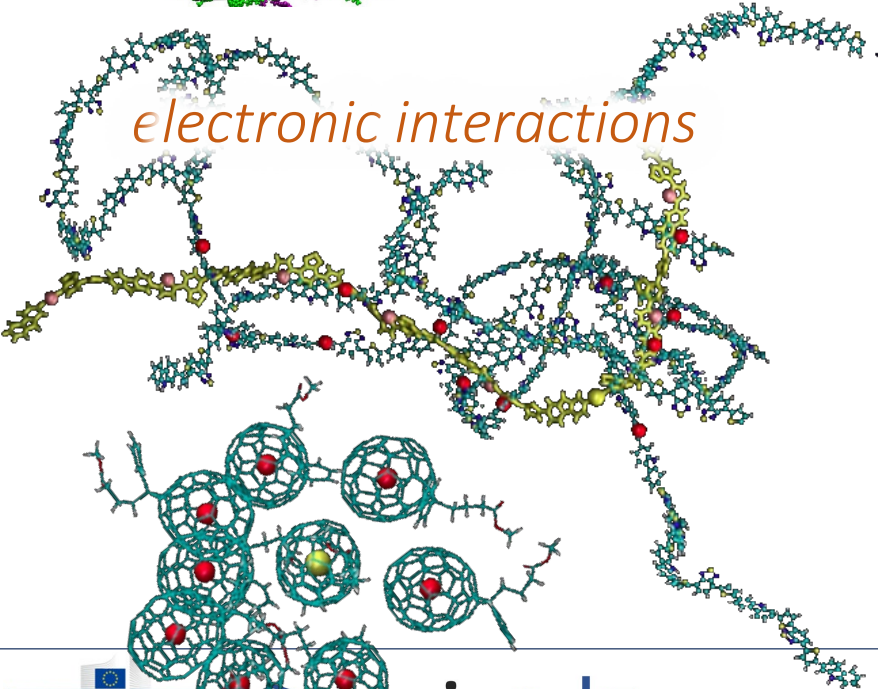
microstructure evolution



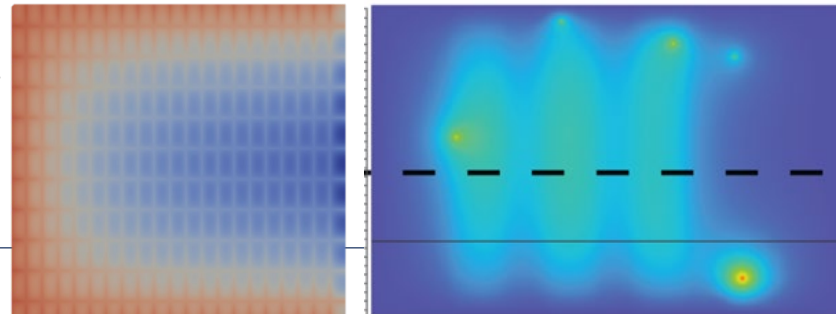
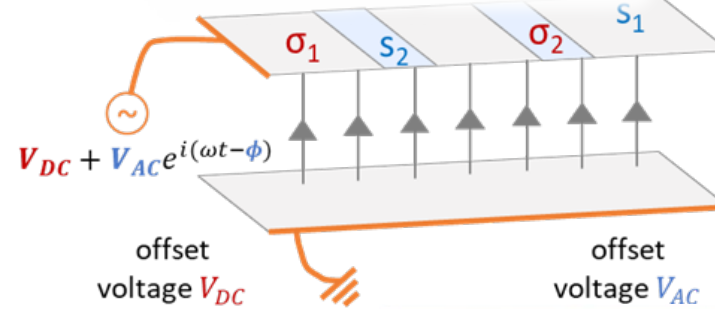
charge transport



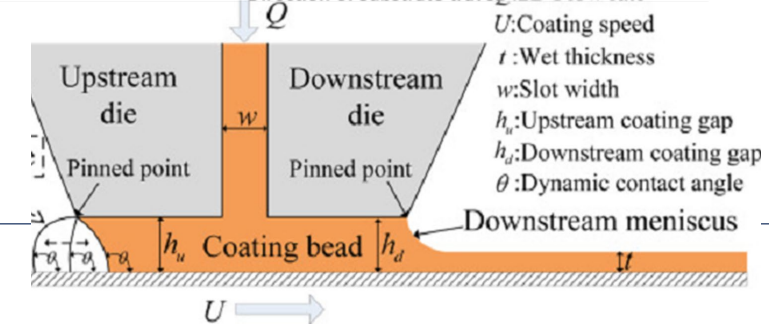
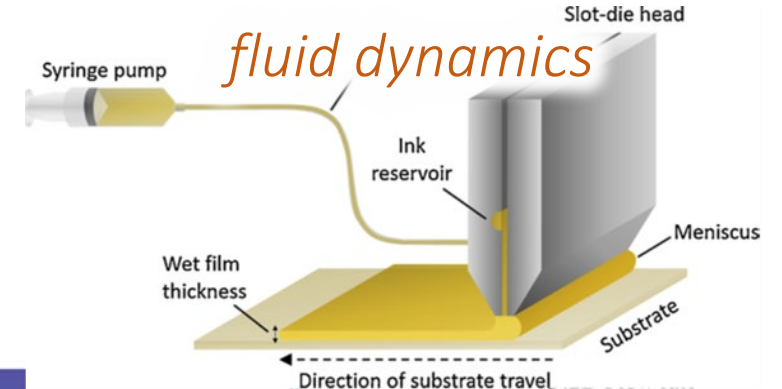
electronic interactions



devices & modules

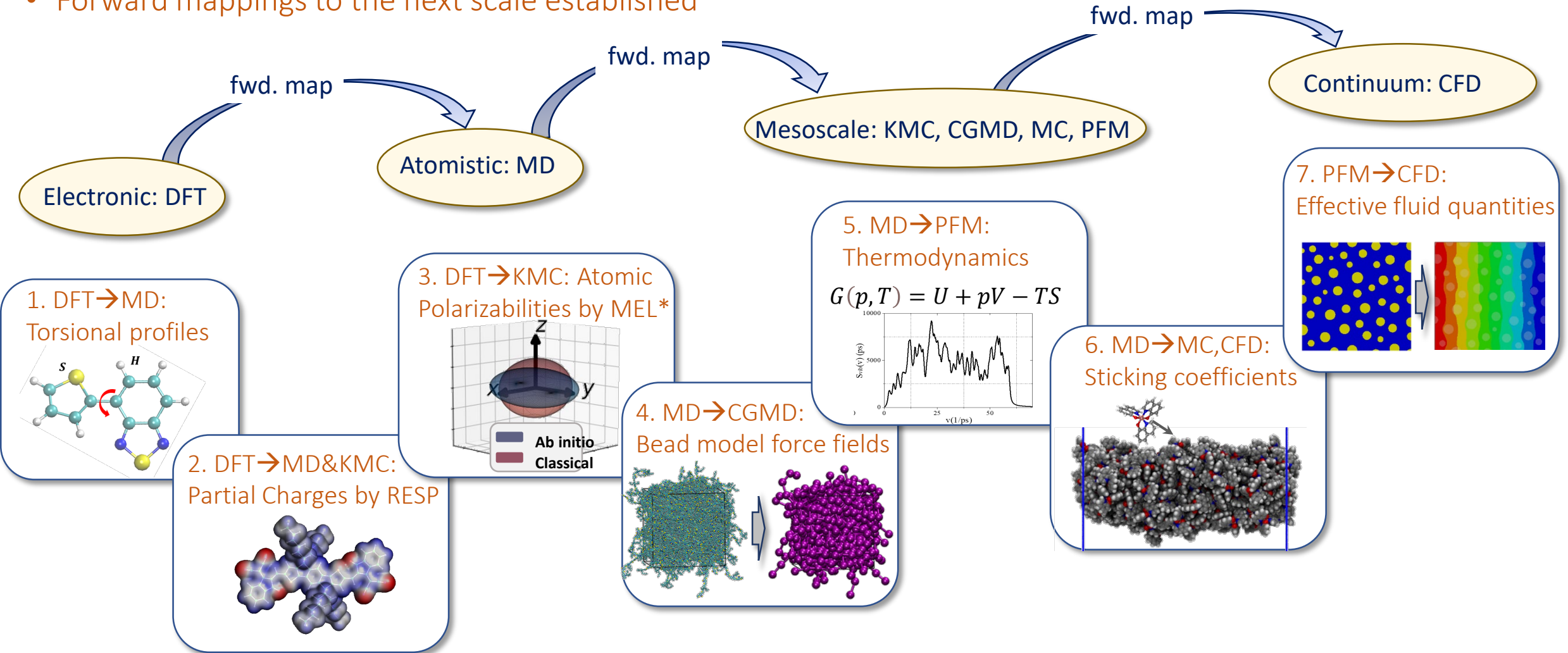


fluid dynamics

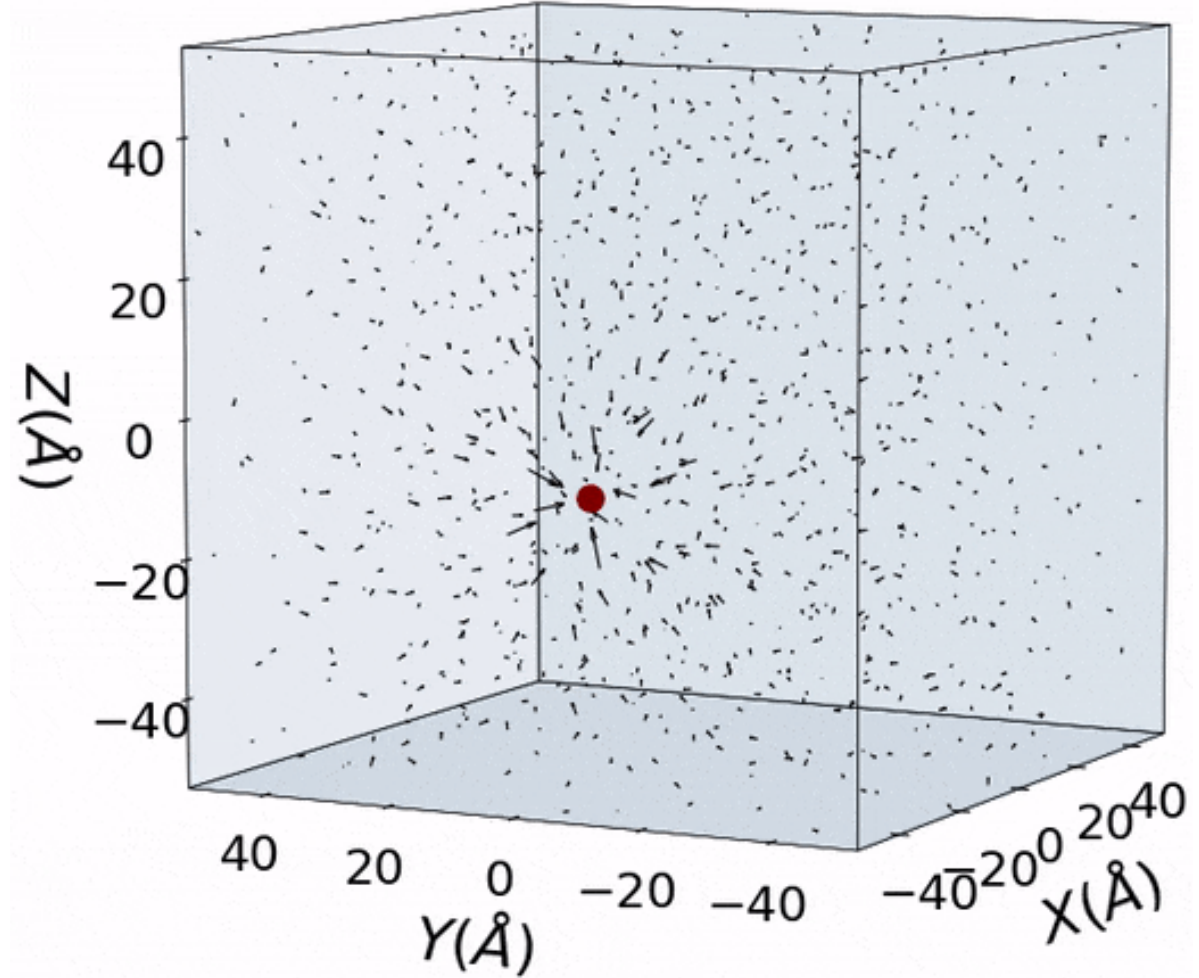
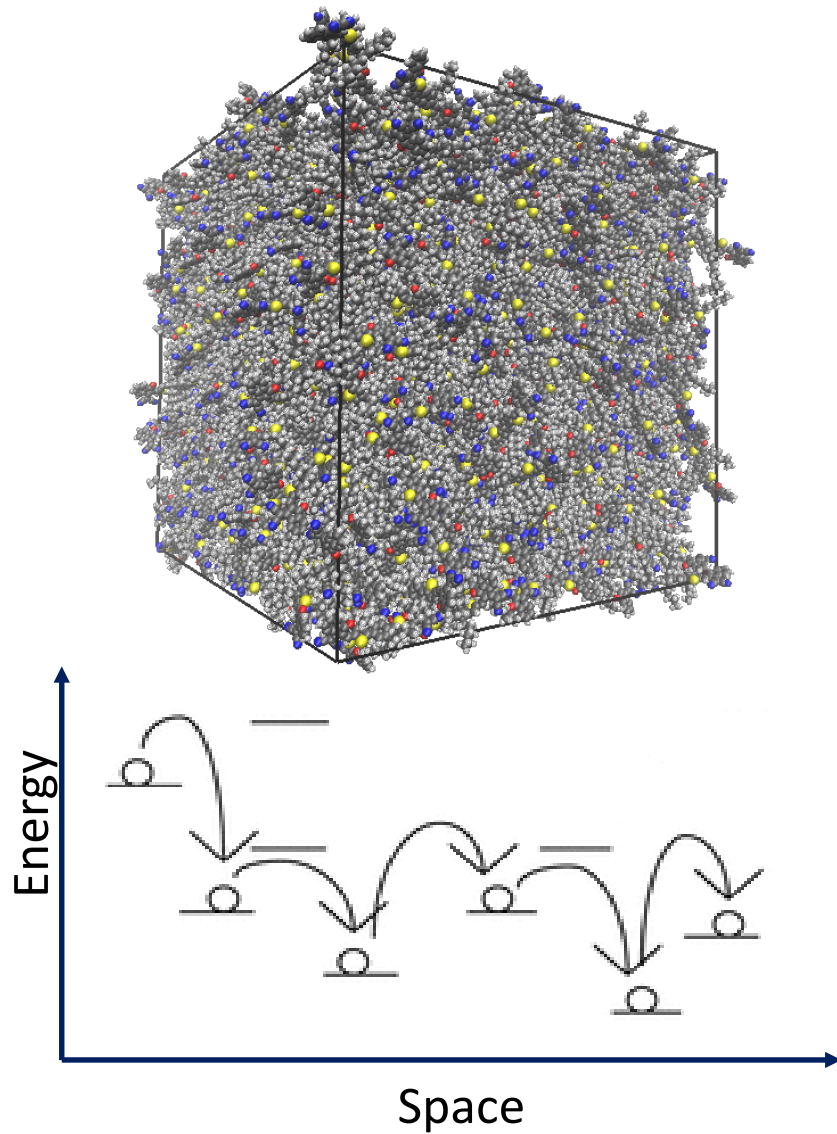


# Development of multiscale Modelling tools

- Forward mappings to the next scale established

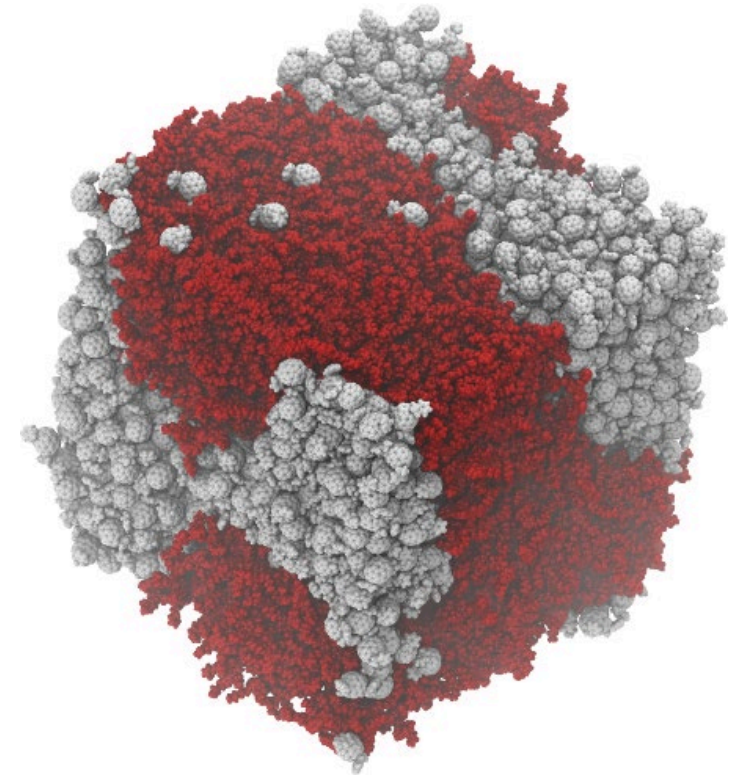
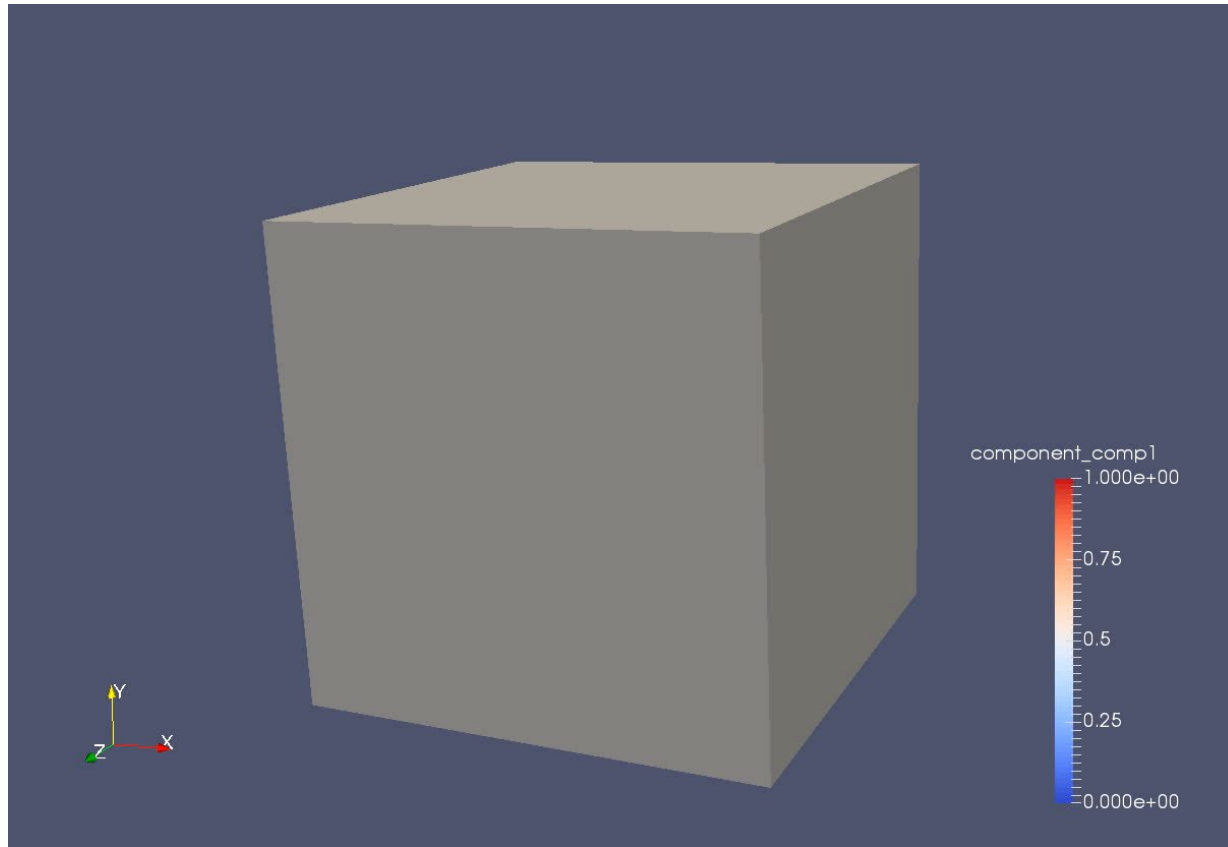


# Some highlights: charge transport and mobility

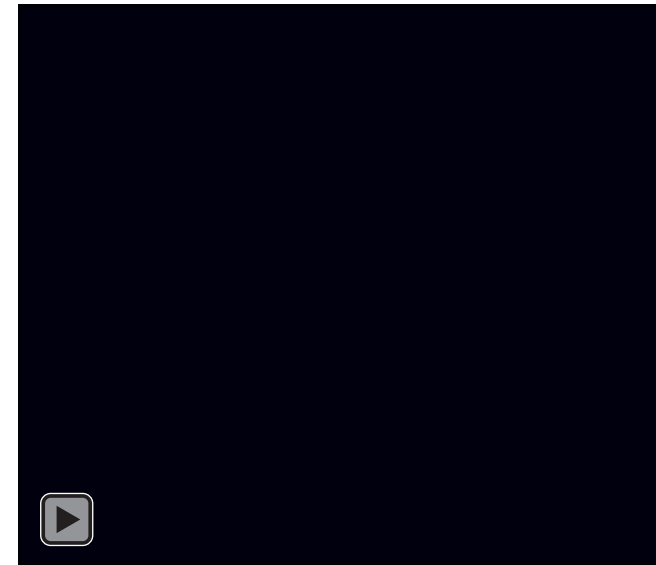
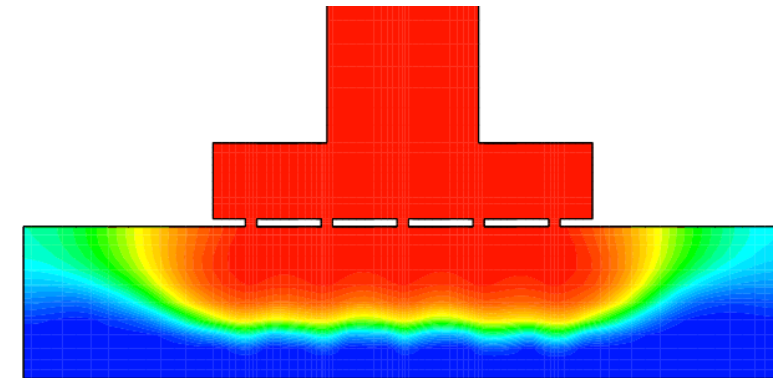
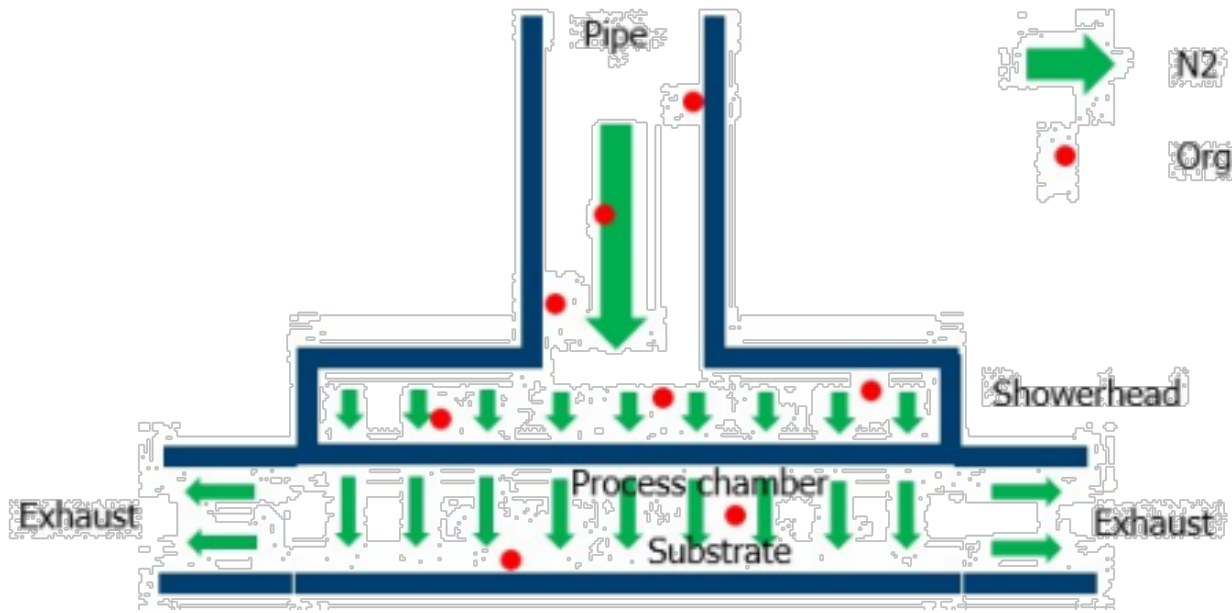




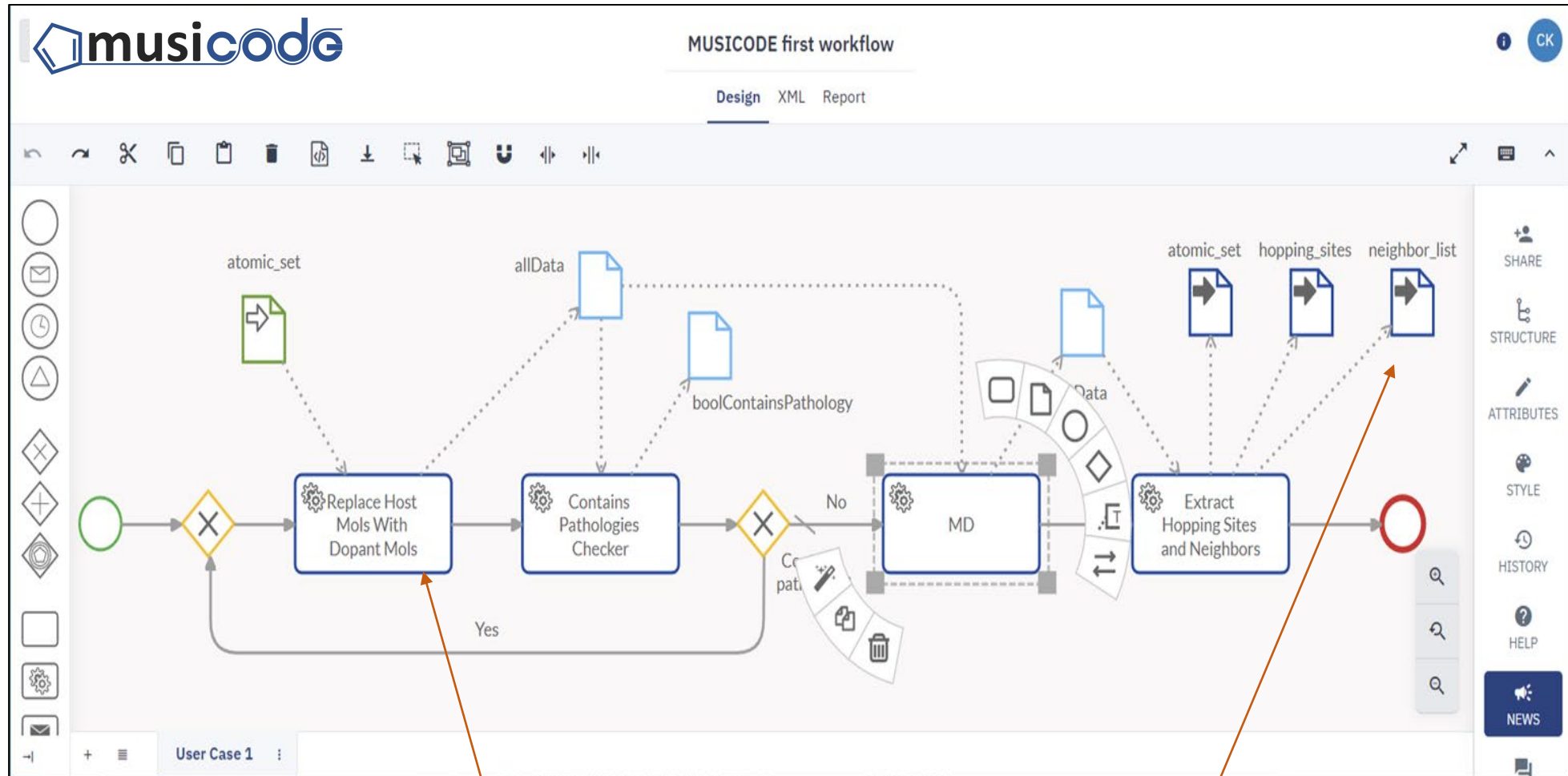
# Some highlights: microstructure evolution



# Some highlights: growth by vapor phase deposition



# Standard workflow representation based on BPMN



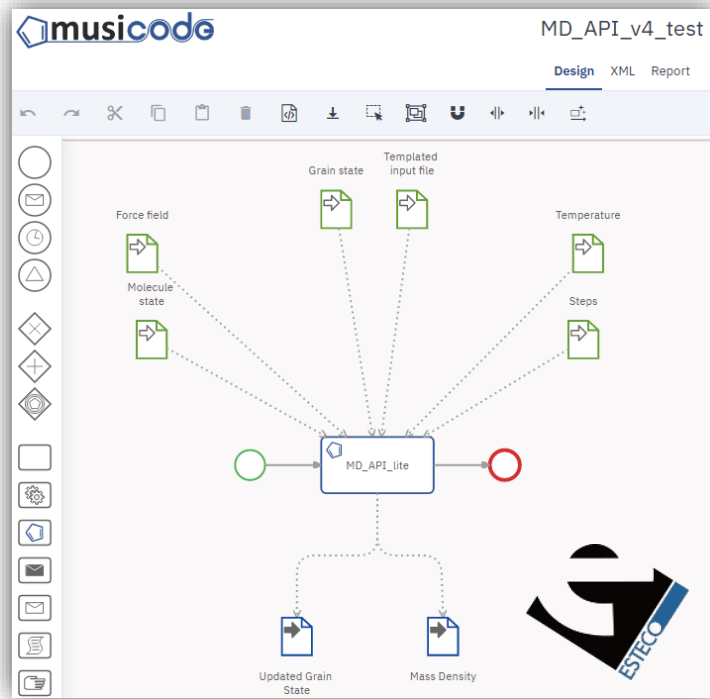
*model nodes*

*data nodes*

# Workflow scenarios

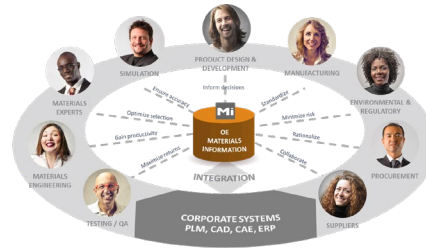
## Expert User

### 1. Designs the Workflow on the editor



### 2. Publishes the Workflow on the DMS

Molecular-Relaxation (2022-06-28 14-19-11)	
<b>General Info</b>	
Status	Released
Create execution	<a href="https://musiccode.grantami.com/musiccode/Ui/templates/a2db2905-02d4-4d50-9dbf-652d2ec4f4ad">https://musiccode.grantami.com/musiccode/Ui/templates/a2db2905-02d4-4d50-9dbf-652d2ec4f4ad</a>
Author	DarioCampagna
<b>Definition</b>	



## Non-Expert User

### 1. Selects a simulation template

### 2. Picks up a Grain and a Molecule record from the MUSICODE DB

### 3. Modifies Parameters

### 4. Executes the Simulation Template to retrieve Desired quantities

2 Inputs configuration

**Molecule (From ML\_Musicode > Molecules)**

Pick a record \*  
Propene M18 Demo

Record details

**Grain (From ML\_Musicode > Grains)**

Pick a record \*  
20 Propene grain M1...

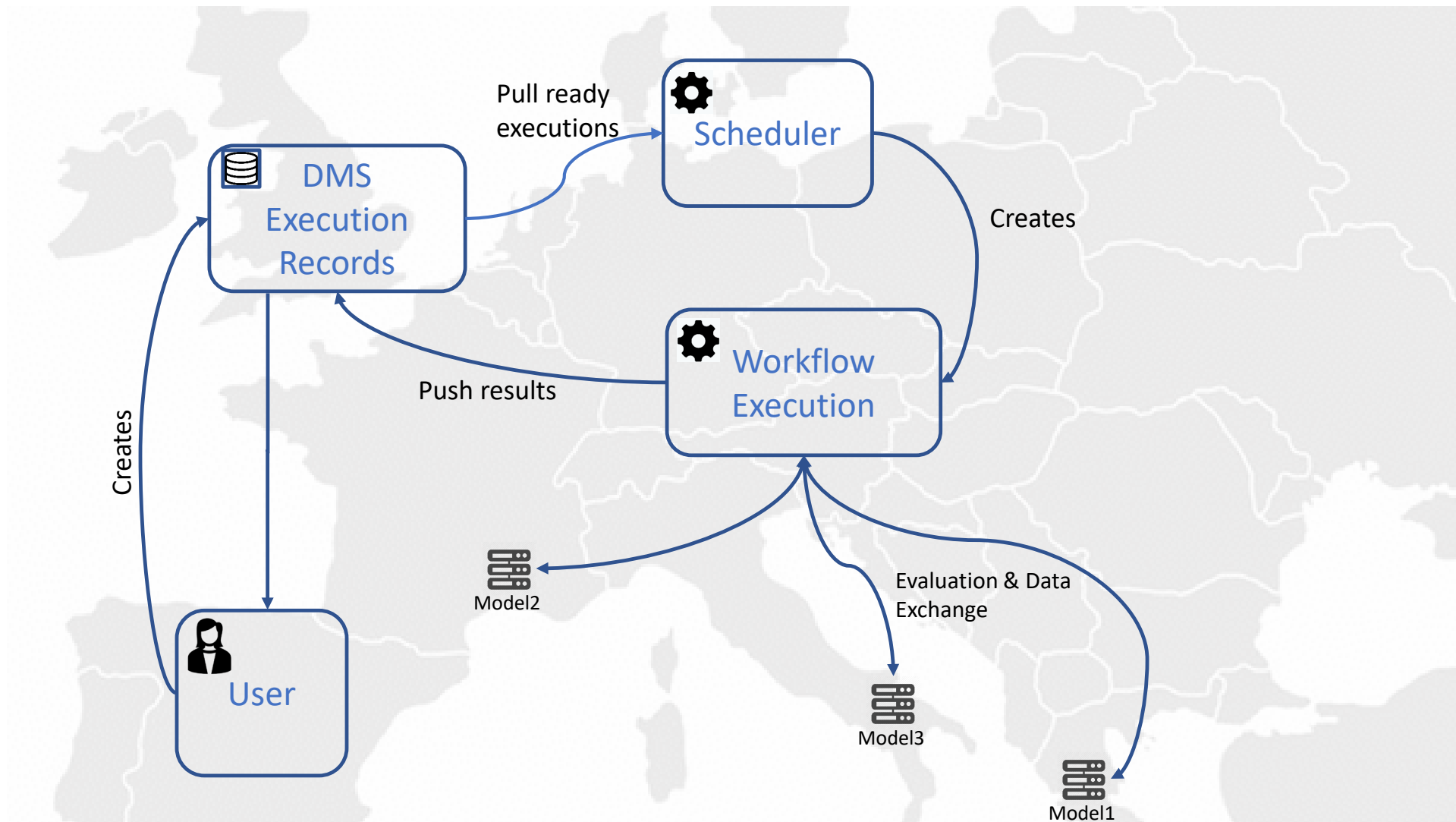
Record details

3 Parameters

Temperature [ ] \*  
300

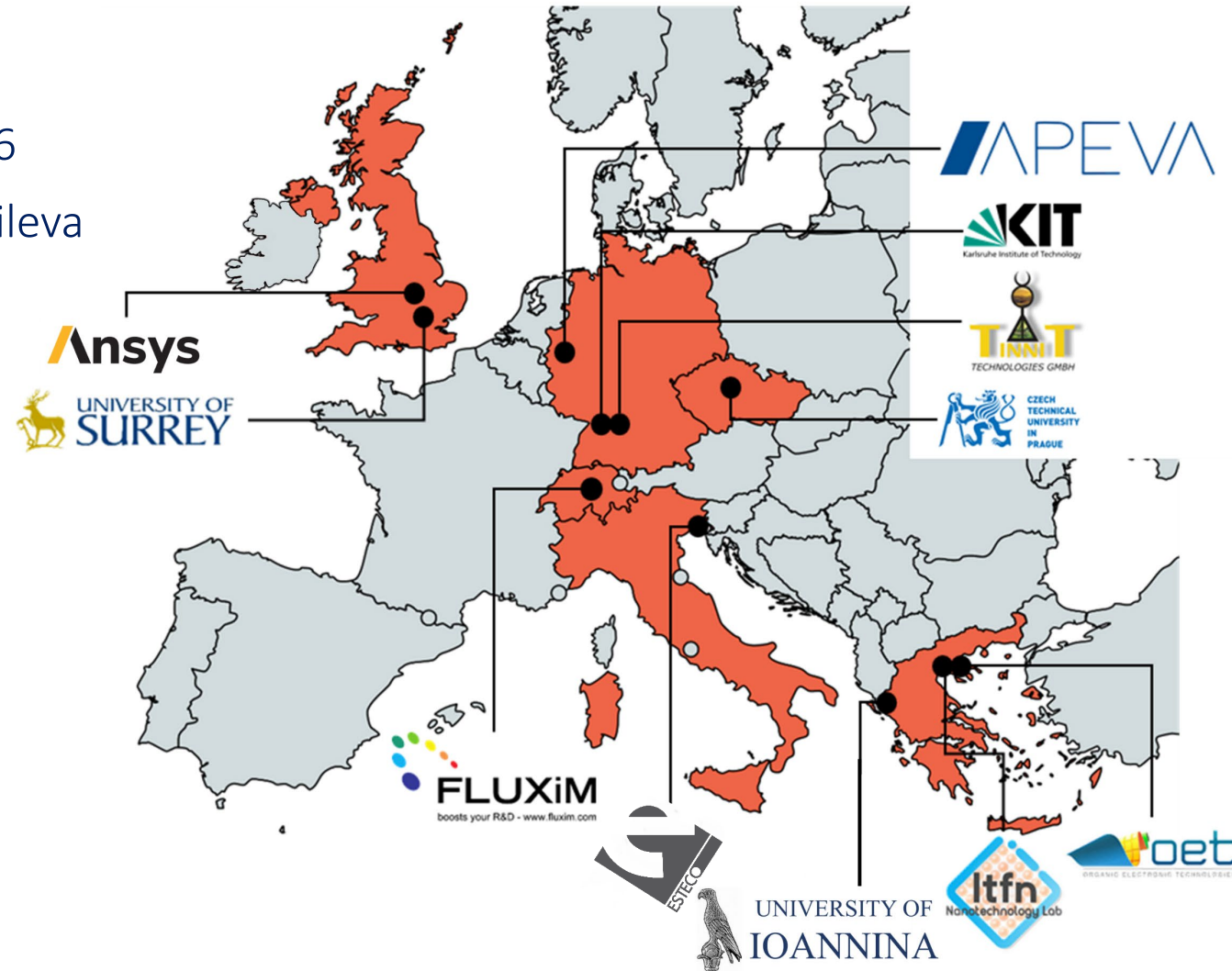
Steps [ ] \*  
200

# Workflow execution on Simulation platform



# The MUSICODE project consortium

- **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:**
  - University of Ioannina, Greece (Coordinator)
  - Karlsruhe Institute of Technology, Germany
  - University of Surrey, UK
  - Nanotechnology Lab LTFN, Aristotle University of Thessaloniki, Greece
  - Czech Technical University in Prague, Czech Republic
  - Fluxim AG, Switzerland
  - TinniT Technologies GmbH, Germany
  - Ansys, UK
  - ESTECO SPA, Italy
  - Organic Electronic Technologies, Greece
  - APEVA SE, Germany





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