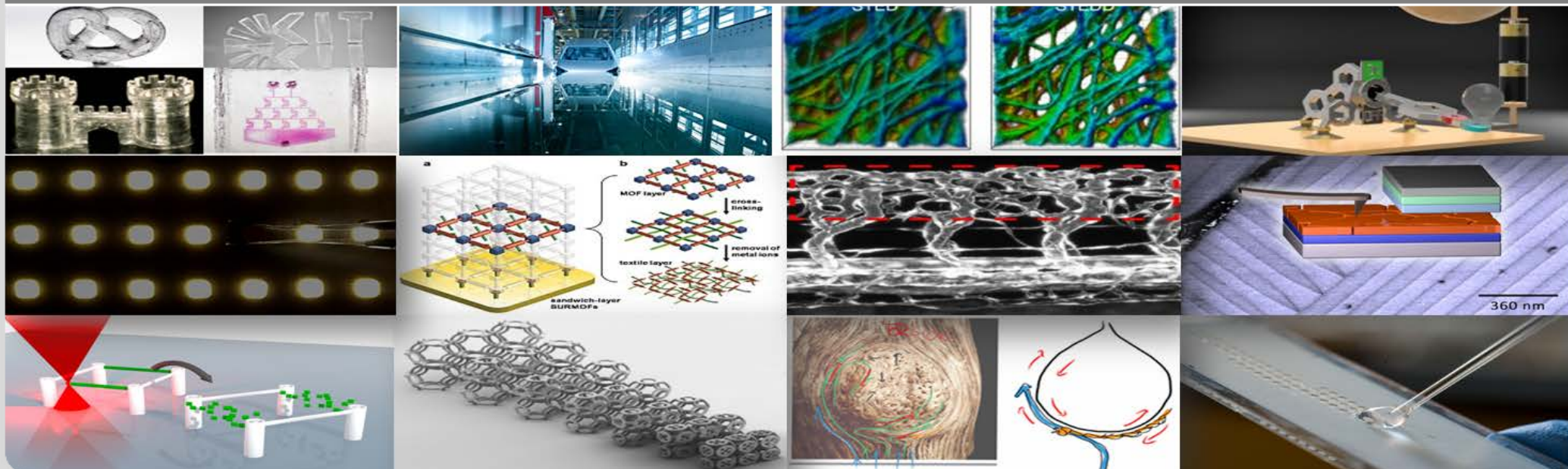


# Ontology Requirements for Software Realization

KIT Center Materials: *Wolfgang Wenzel*

KIT Center Materials, materials in technical and life sciences



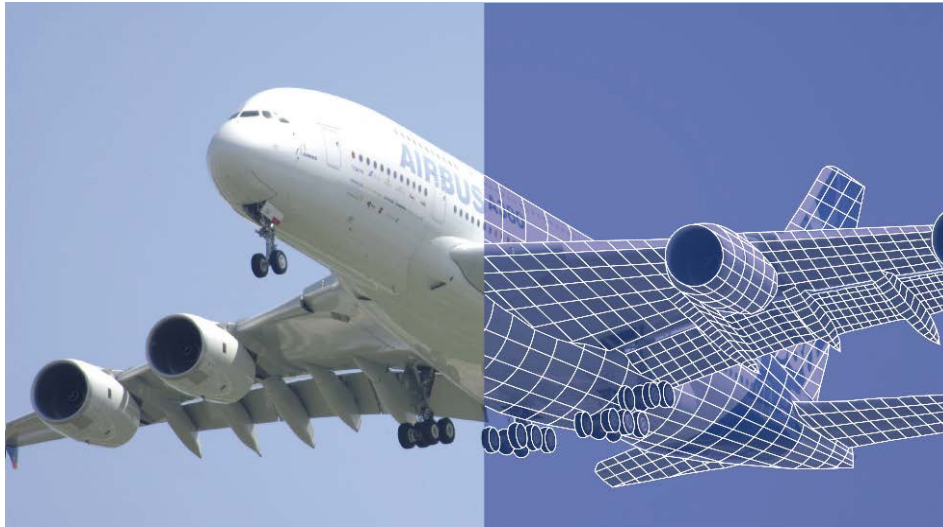


# KIT – The Research University in the Helmholtz Association

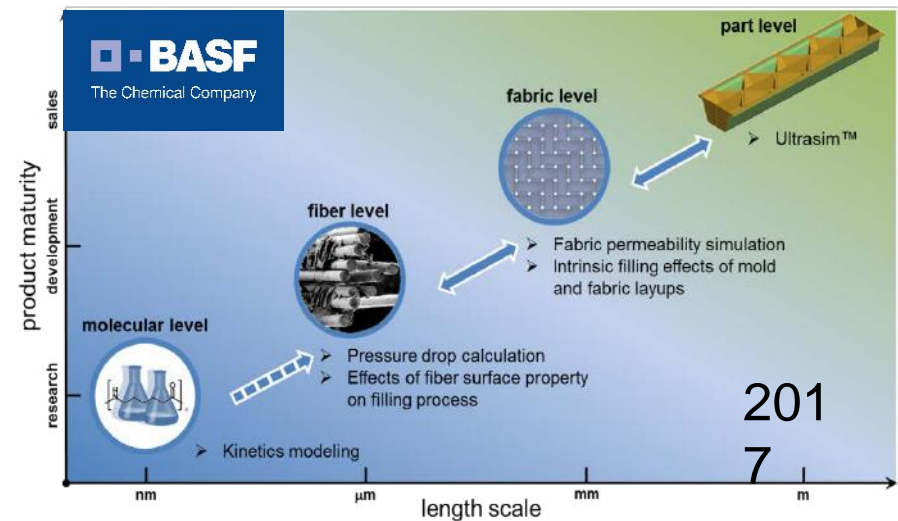




# Computer Aided Product Development



- ❑ Simulations and computer models significantly accelerate R&D in many industrial sectors
- ❑ Digital twin of products and processes enables Industrie 4.0, Internet of Things
- ❑ Challenges for multiscale problems

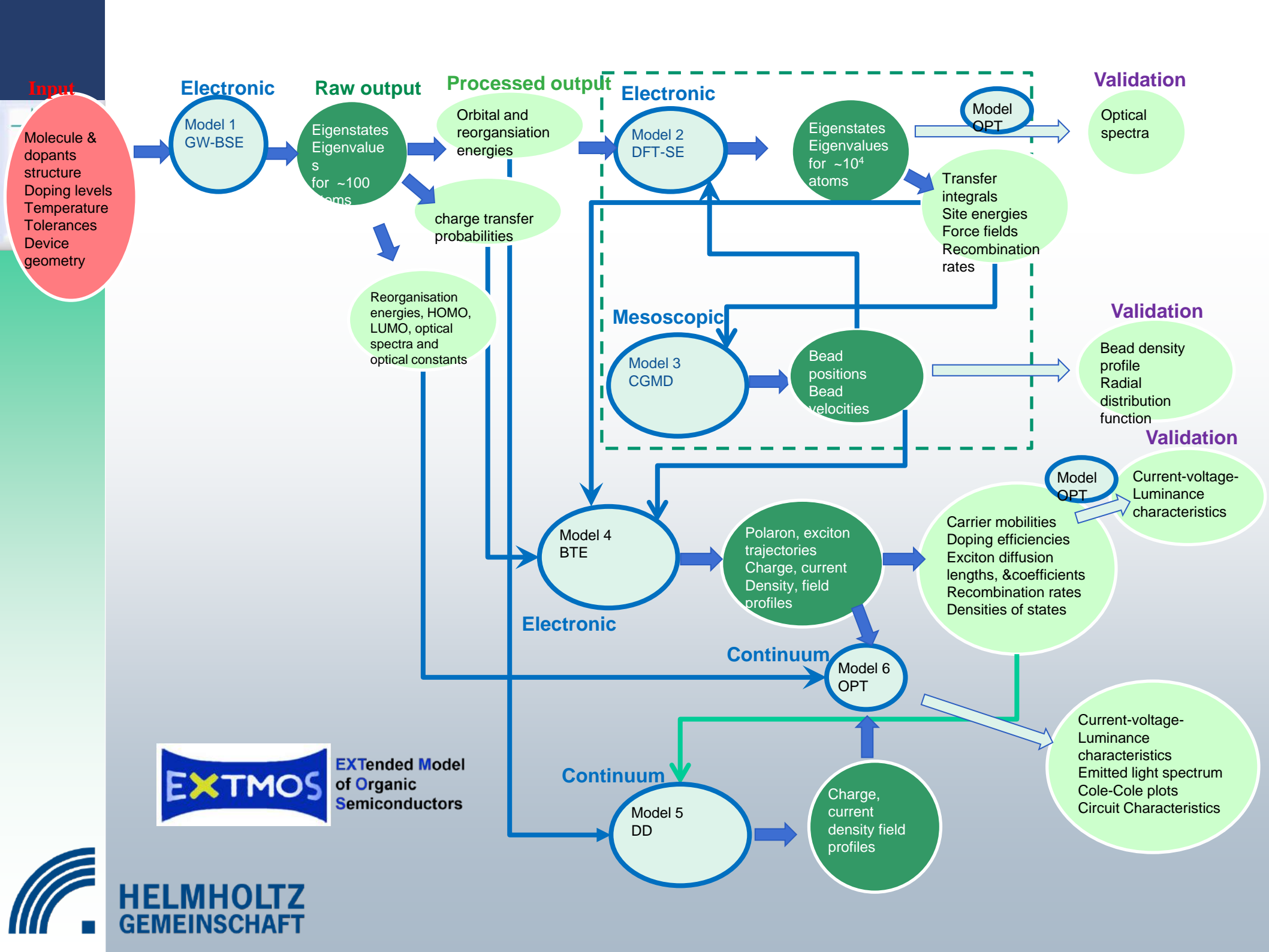


# RoMM / MODA

- ❑ Categorization and definition of simulation tools on a systematic basis
- ❑ 37 EU projects with ....
- ❑ 15 simulation tools per project

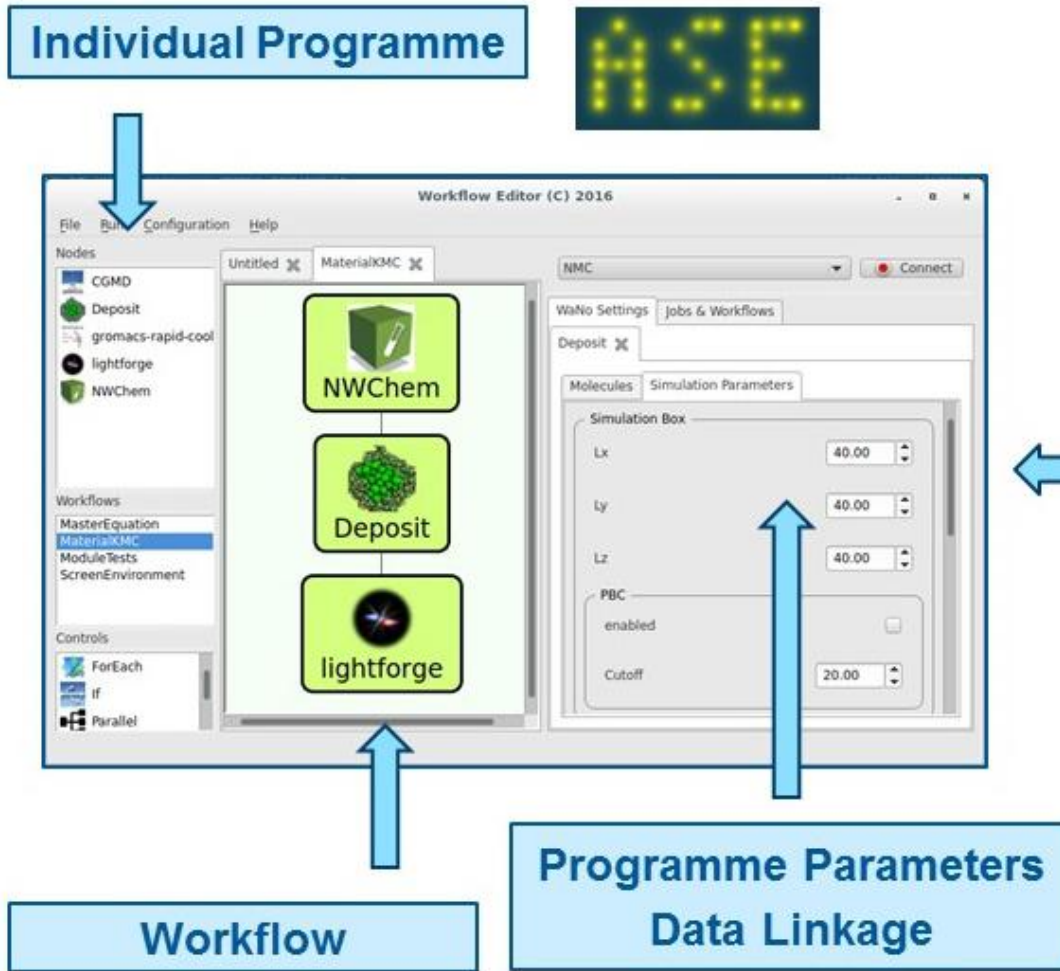
Interoperability  
Challenge







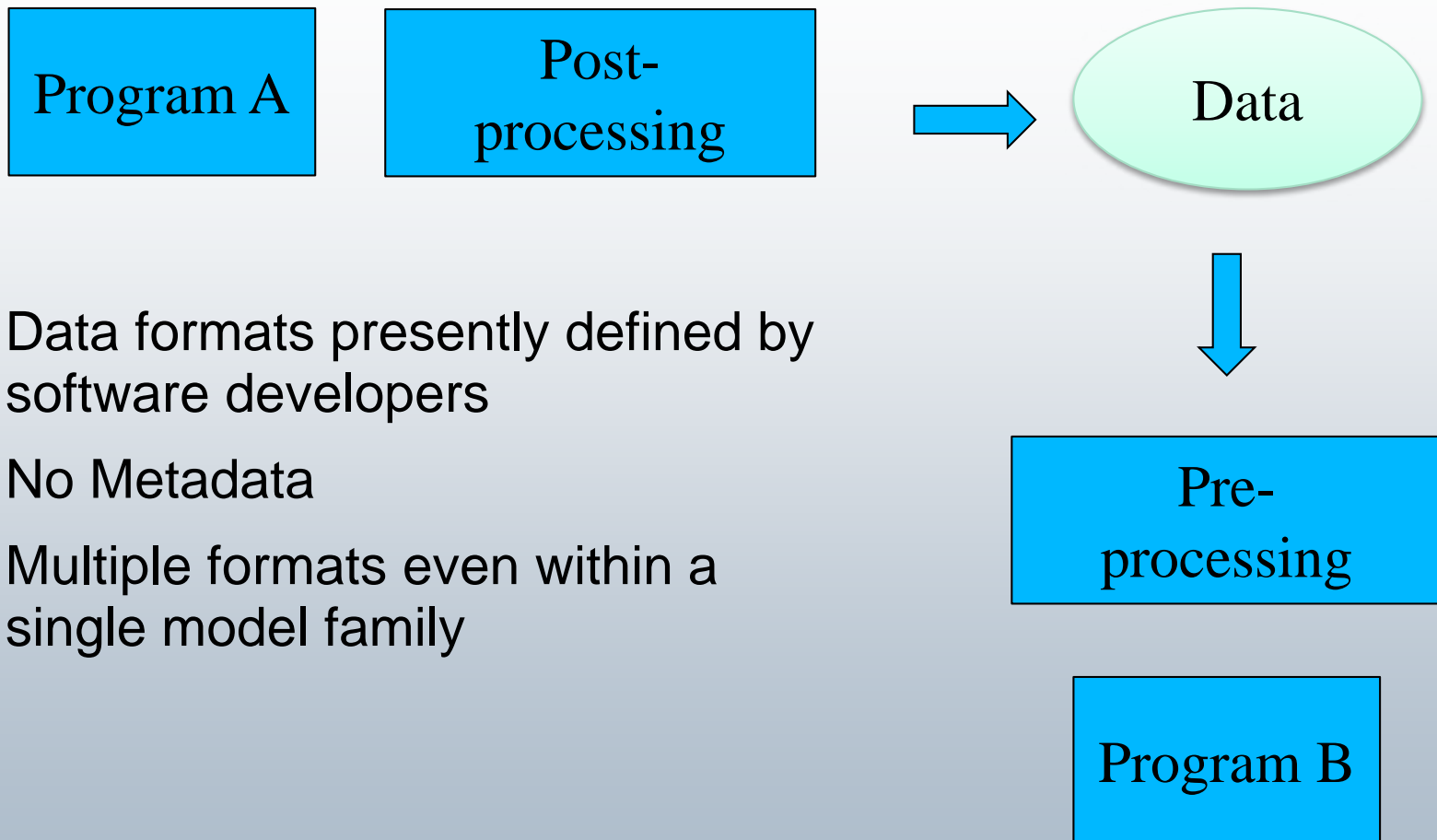
# Simstack Workflow Engine



UNICORE

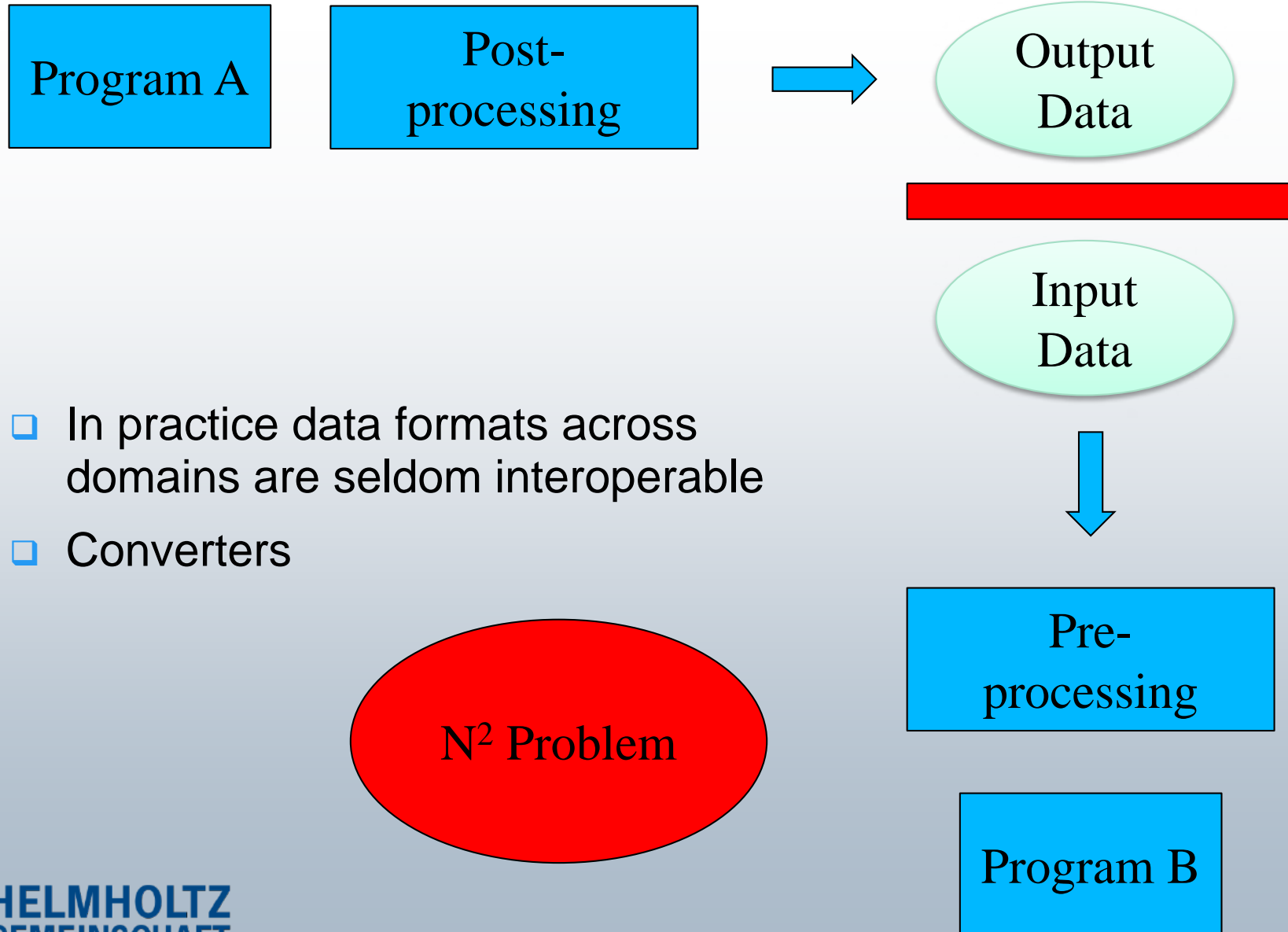


# Interoperability Challenge in Software



- ❑ Data formats presently defined by software developers
- ❑ No Metadata
- ❑ Multiple formats even within a single model family

# Interoperability Challenge in Software





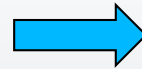
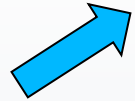
# Data Adapters

RoMM



Program A

Post-processing

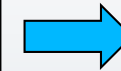


Data Adapter



URL

Data Adapter



URL

Data Adapter



URL



Data Ontology

- ❑ Data Adapters convert proprietary to standard formats
- ❑ Metadata include
- ❑ URL deposition includes validation

# Data Ontology

Data  
Ontology

- should be based on model ontology
- should define standard data types for each equation
- define model specific instantiations of generic data

Generic Data  
Type

Geometry



Validator

Specific Data  
Type

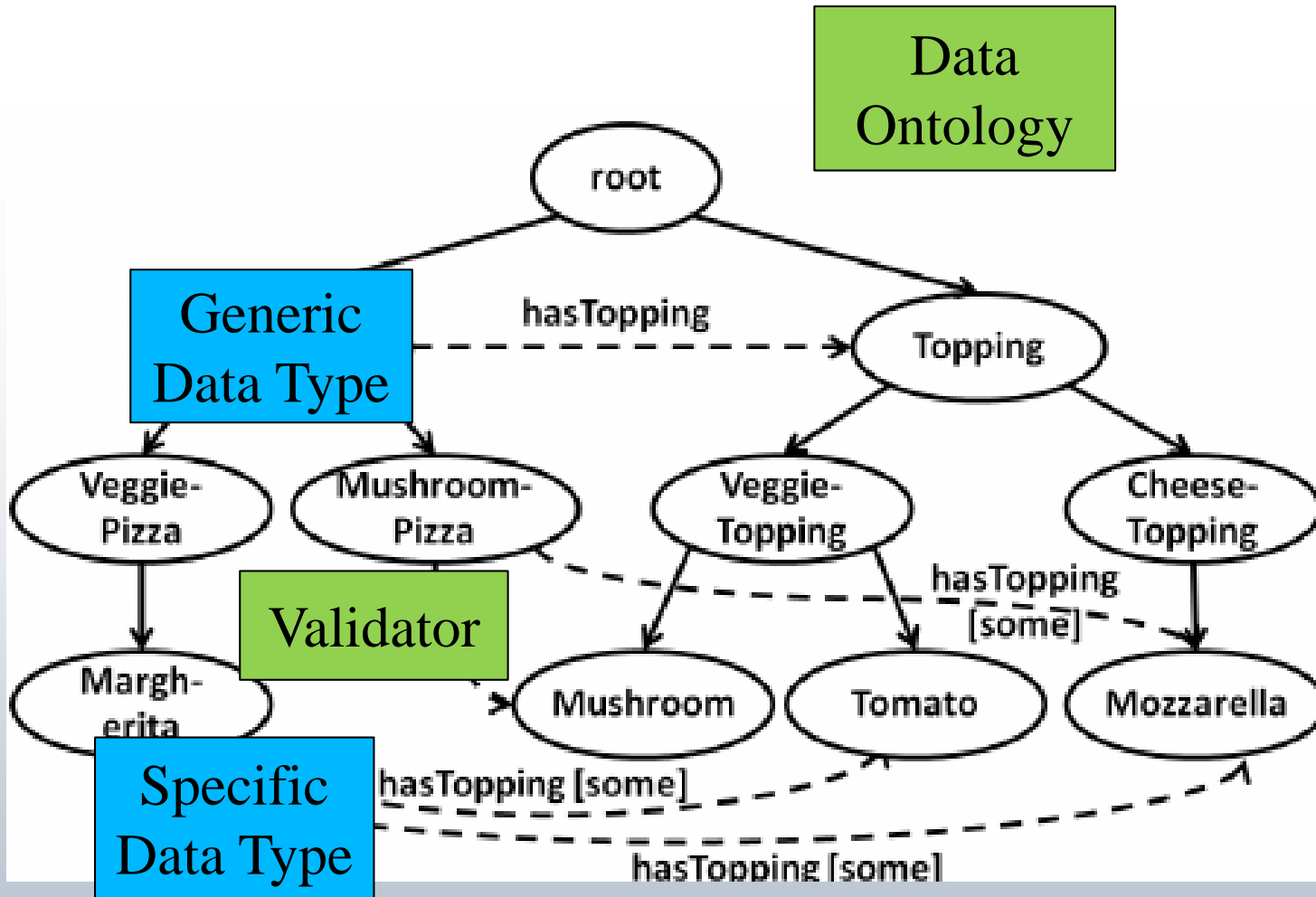
Molecular Dynamics  
System

# Approach

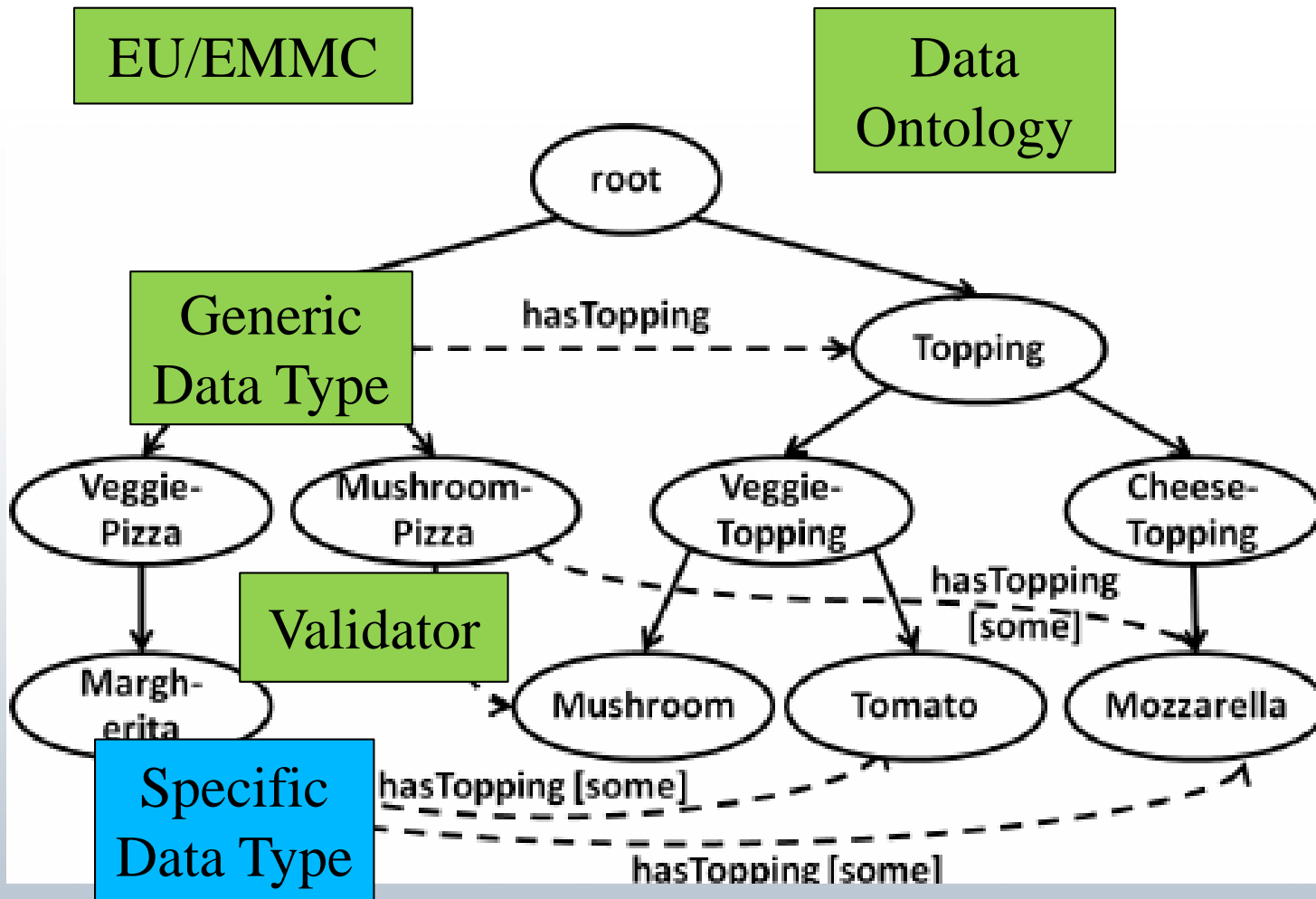
- ❑ Data Ontology based on Model Ontology can improve/solve the interoperability challenge
- ❑ Data Adapters for software based on model specific data types derived from generic data types
  - ❑ Solve the  $O(N^2)$  problem
  - ❑ Permit validation and meta-data
- ❑ Data Ontologies need to specify only the generic data types and provide validators
- ❑ Interoperability is ensured by inheritance



# What Do We Need



# Who Does What



# Thank you for your attention



<http://www.int.kit.edu/nanosim>