Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

13th October 2020
DAMDID 2020
Virtual Materials Marketplace (VIMMP)

- Horizon 2020 project
  - Innovation action, grant agreement no. 760907
  - 4 years project – started on 01.01.2018

http://vimmp.eu/

To support accelerating innovation in manufacturing industries by using materials modelling solutions.
Virtual Materials Marketplace (VIMMP)

- Horizon 2020 project
  - Innovation action, grant agreement no. 760907
  - 4 years project – started on 01.01.2018

http://vimmp.eu/
European digital platforms in materials modelling

- open innovation test beds
- business decision support systems
- repositories and data infrastructures

coordination and support

European Open Science Cloud

materials modelling marketplaces

EMMC
ONTO COMMONS
VIMMP MarketPlace

open innovation platforms
open simulation platforms
open translation environments

DOME 4.0 data marketplace

Funded by the Horizon 2020 Framework Programme of the European Union

Science and Technology Facilities Council

13th October 2020
European Materials Modelling Council (EMMC ASBL)

The non-profit association EMMC ASBL was created in 2019 to ensure the continuity, growth, and sustainability of community activities for modellers, materials data scientists, software owners, materials modelling translators, and manufacturers in Europe. The EMMC regards the integration of materials modelling and digitalization as critical for an advancement of industrial process and product design.

European Materials Modelling Council

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EMMC Focus Area on Digitalization

In computational engineering, digitalization encompasses aspects of representing, managing, accessing, and utilizing digital information about products, components, materials, their behaviour, and their processing.
Knowledge representation in materials modelling

Community-governed development of metadata standards

RoMM VI MODA CWA 17284

Review of Materials Modelling (compendium)
MODA (“Model Data”)
CEN workshop agreement

electronic
atomistic
mesoscopic
continuum
Knowledge representation in materials modelling

Community-governed development of metadata standards

RoMM VI  MODA  CWA 17284  Ontologies

Review of Materials Modelling (compendium)

MODA ("Model Data")

CEN workshop agreement

Domain ontologies
EMMO top-level ontology

electronic
atomistic
mesoscopic
continuum
## Provenance description of simulation results: MODA

<table>
<thead>
<tr>
<th></th>
<th>ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>ASPECT OF THE USER CASE TO BE SIMULATED</td>
</tr>
<tr>
<td></td>
<td>Describe the aspects of the user case textually.</td>
</tr>
<tr>
<td></td>
<td>No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation.</td>
</tr>
<tr>
<td></td>
<td>The information in this chapter can be end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture.</td>
</tr>
<tr>
<td></td>
<td>Simulated input which would have been calculated by another model should not be included (but in chapter 2.4).</td>
</tr>
<tr>
<td></td>
<td>Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities can be documented here.</td>
</tr>
<tr>
<td>1.2</td>
<td>MATERIAL</td>
</tr>
<tr>
<td></td>
<td>Describe the chemical composition... and the values used for properties and from which database these are taken. If pre-processing was needed please specify the methodology.</td>
</tr>
<tr>
<td>1.3</td>
<td>GEOMETRY</td>
</tr>
<tr>
<td></td>
<td>Size, form, picture of the system (if applicable)</td>
</tr>
<tr>
<td></td>
<td>Note that computational choices like simulation boxes are to be documented in chapter 3.</td>
</tr>
<tr>
<td>1.4</td>
<td>TIME LAPSE</td>
</tr>
<tr>
<td></td>
<td>Duration of the case to be simulated. This is the duration of the situation to be simulated. This is not the same as the computational times to be given in chapter 3.</td>
</tr>
<tr>
<td>1.5</td>
<td>MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS</td>
</tr>
<tr>
<td></td>
<td>If relevant, please list the conditions to be simulated (if applicable). These can be boundary, initial and global conditions.</td>
</tr>
<tr>
<td></td>
<td>E.g. heated walls, external pressures and bending forces.</td>
</tr>
<tr>
<td></td>
<td>Please note that these could appear as terms in the FE or as boundary conditions, and this will be documented in the relevant chapters.</td>
</tr>
<tr>
<td></td>
<td>Note: These conditions will be expressed in physics relations in CH 2.4.</td>
</tr>
<tr>
<td></td>
<td>Please specify the values used for parameters and from which database these are taken. If pre-processing was needed please specify the methodology.</td>
</tr>
<tr>
<td>1.6</td>
<td>PUBLICATION ON THIS DATA</td>
</tr>
<tr>
<td></td>
<td>Publication documenting the simulation with this single model (if available and if not already included in the overall publication).</td>
</tr>
</tbody>
</table>

## MODA workflow description

- **MODA section 1**: use case
- **MODA section 2**: model
- **MODA section 3**: solver
- **MODA section 4**: processor
Provenance description of simulation results: OSMO

OSMO

"sections"

MODA section 1

use case

"aspects"

MODA 1.1

has_use_case_aspect

MODA 1.2

has_use_case_material

MODA 1.3

has_use_case_timespan

MODA 1.4

has_use_case_description

MODA 1.5

has_use_case_material

MODA 1.6

has_use_case_geometry

has_use_case_boundary_condition

has_use_case_literature

OSMO

"graphs"

MODA section 1

use case

"sections"

MODA section 2

model

"aspects"

MODA 1.2

OSMO

Provenance description of simulation results: OSMO

Ontology for Simulation, Modelling, and Optimization

Provenance description of simulation results: OSMO

Ontology for Simulation, Modelling, and Optimization
Provenance description of simulation results: OSMO

OSMO-based provenance description as an extension of the MODA workflow metadata standard:

For all elements of the graph notation, there are corresponding concepts and relations from the ontology OSMO.

Ontology for Simulation, Modelling, and Optimization (OSMO)
Community-governed top-level interoperability layer

Relations covered by the European Materials and Modelling Ontology\(^1\) (EMMO)

1) **Taxonomy:** Conceptual hierarchy (subclass relation)

2) **Semiotics:** Representation of physical entities by signs

3) **Mereotopology:** Spatiotemporal parthood and connectivity

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System of marketplace-level domain ontologies

Ontologies for the Virtual Materials Marketplace

KI – Künstliche Intelligenz 34(3), 423–428, 2020

Release: https://vimmp.eu/?p=349

Ontologies for the Virtual Materials Marketplace

13th October 2020
**Task:** Facilitate the translation of industrial R&D challenges into solutions using scalable and quantitatively reliable materials modelling and simulation.
Translation in materials modelling

- industrial challenge
  - identification of data requirements
  - modelling and simulation outcome
  - actionable decision

TRANSLATION
- DATA EXCHANGE, SOFTWARE & TOOLS
  - Open to all Users & Open APIs
  - Academia & Research
  - Certified Experts & Consultants

TRAINING
- SME & Industry

COLLABORATION
- Business & Software Owners

MATERIALS KNOWLEDGE BASE
- OPEN SIMULATION PLATFORM & HPC

EMMC
Ontologization of EMMC metadata standards

MODA section 1

use case

MODA section 2

model

MODA section 3

solver

MODA section 4

processor

semi-formalized metadata standard (human processable)

formal ontology (machine processable)

1. Aspect of the User Case/System to be Simulated

1.1 Aspect of the User Case to be Simulated

Describe the aspects of the user case textually.

- No modeling information should appear in this box. This case could also be simulated by other means in a benchmarking operation.
- The information in this chapter can be used to provide information on measured data, geometry, etc. It will appear in the pink circle of your workflow picture.
- Simulated input which would have been calculated by another model should not be included (as in chapter 2.4)
- Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the engine can be documented here.

1.2 Material

Describe the chemical composition... and the values used for properties and sources which data these are taken. If post-processing was needed please specify the methodology.

1.3 Geometry

Size, form, picture of the system (if applicable)

Note that computational choices like computer resources are to be documented in chapter 3.

1.4 Time Lapse

Duration of the case to be simulated.

This is the duration of the situation to be simulated. This is not the same as the computational time to be used in chapter 3.

1.5 Manufacturing Process or In-Service Conditions

If relevant, please list the conditions to be simulated (if applicable). These can be boundary, initial, and global conditions.

- E.g., thermal, mechanical, external pressures, and bending forces.
- E.g., these condition in the form of boundary conditions and this will be documented in the relevant chapter.

Note: These conditions will be expressed in physics relations in Ch 2.4

Please specify the values used for parameters and from which database these are taken. If pre-processing was needed please specify the methodology.

1.6 Publication on This Data

Publication documenting the simulation of this single model (if available and if not already included in the overall publication).
Materials Modelling Translation Ontology

Input from FORCE

business case

Input from FORCE

industrial case

EMMC translation case template

application case

MODA section 1

use case

OSMO

MODA section 2

model

MODA section 3

solver

MODA section 4

processor

semi-formalized metadata standard (human processable)

VIMMP VIRTUAL MATERIALS MARKETPLACE

formal ontology (machine processable)
Materials Modelling Translation Ontology

EMMC Translators’ Guide
https://emmc.info/translators-guide-2/

from EMMC Translation Case Template (ETCT)

from EMMC Translators’ Guide (ETG)
VIMMP ontology-based translation router

**mm_topic_basic** (codes 1XXX and 2XXX):
Basic prerequisites for materials modelling.

**mm_topic_computational** (codes 3XXX):
Computational and numerical aspects of materials modelling.

**mm_topic_data** (codes 4XXX):
Data science and technology aspects.

**mm_topic_materials** (codes 5XXX):
Topics related to fluid and solid materials.

**mm_topic_social** (codes 6XXX):
Social, economic, and community aspects.

**mm_topic_theoretical** (codes 7XXX):
Theory (non-computational aspects).

**mm_topic_interdisciplinary** (codes 8XXX)

**mm_topic_side** (codes 9XXX):
Topics from other disciplines.

3100, 7100 electronic
– 3120, 7120 physical equation EL.1
– 3130, 7130 physical equation EL.2
– etc.

3200, 7200 atomistic and mesoscopic
– 3220, 7220 equations A.1 and M.1
– 3222, 7222 physical equation A.1
– 3225, 7225 physical equation M.1
– 3230, 7230 equations A.2 and M.2
– etc.
– etc.

3300, 7300 continuum
– 3320, 7320 physical equation CO.1
– 3330, 7330 physical equation CO.2
– etc.
VIMMP ontology-based translation router

**mm_topic_basic** (codes 1XXX and 2XXX):
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Topics from other disciplines.

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Under 61XX: industrial

- 6120 chemical
- 6130 petrochemical
- 6140 transport
  - 6142 aerospace
  - 6144 automotive
  - 6148 railway
- 6150 biotechnology
- 6155 food
- 6160 medicine
- 6165 paper
- 6170 electrical
- 6175 machinery
- 6180 metal (basic and fabricated)
- 6190 special topics
VIMMP ontology-based translation router

**mm_topic_basic** (codes 1XXX and 2XXX):
Basic prerequisites for materials modelling.

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**mm_topic_side** (codes 9XXX):
Topics from other disciplines.

| 5100 general |
| 5200 fluid |
| 5300 bio |
| 5350 ceramic |
| 5400 composite |
| 5450 electrolyte |
| 5500 metal |
| 5550 mineral |
| 5600 nano |
| 5650 organic |
| 5700 polymer |
| 5750 semiconductor |
| 5800 ultracold |
| 5850 unstable |
| 5900 special topics |

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Speak to our experts at no cost

Which class of model?

- Electronic
- Allopathic
- Monocropic
- Continuus

I don't know

Which business area are you from?

- Automanufacturing
- Aerospace
- Chemical Industry
- Life Science
- Medical
- Manufacturing
- Other

Which material class are you interested in?

- Metal
- Polymer
- Composites
- Ceramic
- Other

Continue

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Science and Technology Facilities Council

21 | 13th October 2020
Data management on the VIMMP back end
The present work is a collaboration of UKRI STFC Daresbury Laboratory with:

Geesthacht – Natalia A. Konchakova
Kaiserslautern – Peter Klein
Stuttgart – Björn Schembera

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement no. 760907.

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Kaiserslautern – Peter Klein
Stuttgart – Björn Schembera

Formulations and Computational Engineering (FORCE)
H2020 GA no. 721027
http://www.the-force-project.eu/

EMMC Coordination and Support Action
H2020 GA no. 723867
http://emmc.info/

Virtual Materials Marketplace (VIMMP)
H2020 GA no. 760907
http://vimmp.eu/

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(M. T. Horsch, S. Chiacchiera, M. A. Seaton, I. T. Todorov)