Interoperability and metadata - major outcomes from recent workshops: IntOp and ICMEg

Adham Hashibon
Georg Schmitz
Workshop on

Metadata and Interoperability in Integrated Computational Materials Engineering (ICME) and Multiscale Materials Modelling (MMM)

Thursday 10 March 2016, 09:20 - 17:00 h
Covent Garden Brussels

Organised by

The Integrated Computational Materials Engineering expert group (ICMEg)
The EU Multiscale Modelling Cluster (EU-MMC)
The Interoperability (IntOP) and Open Software Platform (OSP) working groups of the
European Materials Modelling Council EMMC

Where is the physics?
EU Multiscale Projects Cluster

Anne de Baas, Rene Martins (POs)
Gerhard Goldbeck (PTA)

Integrated Computational Materials Engineering expert group
www.icmeg.eu/

From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures
http://www.nmp-deepen.eu/

Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies
http://www.mmp-project.eu/

Modelling of morphology Development of micro- and Nanostructures
http://modena.units.it/

A Multi-scale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials
http://www.sintef.no/Projectweb/NanoSim/

Simulation framework for multi-scale phenomena in micro- and nanosystems
http://www.simphony-project.eu/
### Agenda - Topics

<table>
<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:30 – 10:10</td>
<td>Classification of materials models, vocabulary, workflows and modelling elements MODA (user case, models, computation, post-processing)</td>
<td>P. Asinari</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Topic</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Implementation, benefits and handling of formal metadata schemata as enablers of Platform interoperability – From Data Structures to Modelling Platforms</td>
<td>T. Hagelien (with input from EU-MMC cluster)</td>
</tr>
<tr>
<td>Proposal for metadata keywords for the description of a microstructure</td>
<td>G.J. Schmitz</td>
</tr>
<tr>
<td>The hierarchical data format HDF5 – a pragmatic basis and viable approach for linking of models in a file based interoperability approach</td>
<td>F. Sacconi, G.J. Schmitz, B. Patzak</td>
</tr>
</tbody>
</table>

### + Concluding Panel discussion:

1. **Discrete electronic SWOs**: Nicola Marzari (psi-K)

...
Discussed a holistic view on materials modelling data: MODA
  – Recognises the universal structure of all models.

Metadata for the representation of knowledge
  – not just a collection of raw data.

Demonstrated the route from MODA to metadata extraction

Metadata for establishing interoperability between different types of models and between models and data.

Interoperability achieved by a fundamental open metadata schema that is based on the elements of material modelling.

Proposed modelling element structures and metadata schema that
  – Are neutral to any implementation.
  – Represent computational metadata of all models, including electronic, atomistic, mesoscopic and continuum models.
Each model in the chain is described in four chapters

Chapter 1: Part of the User Case
Chapter 2: Model
Chapter 3: Computational
Chapter 4: Postprocessing

→ A **vocabulary** across the materials modelling world
→ Basis for Metadata definition and development
Beyond the MODA: Towards a Computational Material Modelling Metadata

- A European Common Unified Data Structure: e-CUDS
  - provide a schema for semantic interoperability
- A European Common Unified Basic Attributes: e-CUBA
  - provide reference agreed upon keywords for syntactic interoperability

MODA

USER CASE/System

GE (PE, MR)

Pre/Post

Computational details

Translation

Computational representation based on (open) metadata schema

e-CUDS computational Model

Model Equations (ME=PE+MR)

Solver & Parameters (SP)

Boundary (B) & Conditions (C)

State Data (SD= {DS})
- **Conceptual** model based on taxonomy and high level ontology of different models covering all scales
- Logical models can vary, but all are interoperable!
- Entity Attribute Value Model

**e-CUDS computational Model**

- **Boundary (B) & Conditions (C)**
- **Model Equations (ME=PE+MR)**
- **State Data (SD= {DS})**
- **Solver & Parameters (SP)**

**Cross domain data structure**

**Interoperability**

**e-CUDS**

- **PE**
- **M₁₋N**
- **MR₁₋N**
- **DSᵀ₁₋N**

**Conceptual**

- **Basic Logical Data Model**
  - **B**
  - **C**
  - **Solver Parameter**

**Material declaration**

**Material relations**

**Data Sets**

**Geometry and application data**
**Properties of the basic schema-"language"**

- Building block for the domain specific schemas
- Enforce versioning for sane handling of change
- Minimalistic
- Be able to define itself

**Supersets of this language already exists!**

- JSON
- YAML
- XML
- ANS.1
- +++

```plaintext
<table>
<thead>
<tr>
<th>type</th>
<th>name version namespace dimensions types properties</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>nil</td>
</tr>
<tr>
<td></td>
<td>dimensions dimension</td>
</tr>
<tr>
<td>types</td>
<td>nil</td>
</tr>
<tr>
<td></td>
<td>types type</td>
</tr>
<tr>
<td>properties</td>
<td>nil</td>
</tr>
<tr>
<td></td>
<td>properties property</td>
</tr>
<tr>
<td>dimension</td>
<td>name description</td>
</tr>
<tr>
<td>property</td>
<td>name type dimensions description</td>
</tr>
<tr>
<td>name</td>
<td>string</td>
</tr>
<tr>
<td>version</td>
<td>string</td>
</tr>
<tr>
<td>namespace</td>
<td>nil</td>
</tr>
<tr>
<td></td>
<td>string</td>
</tr>
<tr>
<td>description</td>
<td>nil</td>
</tr>
<tr>
<td></td>
<td>string</td>
</tr>
</tbody>
</table>
```
Defining the CUDS 1.0 Schema from the Basic Schema

```json
{
    "name": "cuds",
    "version": "1.0",
    "namespace": "http://simphony.eu.org/metadata",
    "dimensions": [{
        "name": "num_parents"
    }, {
        "name": "num_models"
    }, {
        "name": "num.physics_quantities"
    }, {
        "name": "num_properties"
    }],
    "properties": [{
        "name": "definition",
        "type": "string"
    }, {
        "name": "key",
        "type": "string"
    }, {
        "name": "models",
        "type": "http://simphony.eu.org/metadata/cuds_1.0",
        "dims": ["num_models"]
    }, {
        "name": "parents",
        "type": "http://simphony.eu.org/metadata/cuds_1.0",
        "dims": ["num_parents"]
    }, {
        "name": "type",
        "type": "http://simphony.eu.org/metadata/cuds_1.0"
    }, {
        "name": "physics_quantities",
        "type": "http://simphony.eu.org/metadata/cuds_1.0",
        "dims": ["num.physics_quantities"]
    }, {
        "name": "id",
        "type": "string"
    }, {
        "name": "description",
        "type": "string"
    }, {
        "name": "name",
        "type": "string"
    }, {
        "name": "properties",
        "type": "http://simphony.eu.org/metadata/properties_1.0",
        "dims": ["num_properties"]
    }]
}
```
MODA and the e-CUDS Metadata Schema

```json
{
    "name": "symphony_task_4_4",
    "version": "1.0",
    "initial_state": "continuum_model",
    "states": [
        {
            "name": "continuum_model",
            "type": "ecuds://emmc.info/metadata/continuum_model/1.0",
            "transitions": [
                {
                    "target": "proc_velocity_fluctuations",
                    "event": "normal_exit"
                }
            ]
        },
        {
            "name": "proc_velocity_fluctuations",
            "type": "ecuds://emmc.info/metadata/proc_velocity_fluctuations/1.0",
            "transitions": [
                {
                    "target": "atomistic_model",
                    "event": "normal_exit"
                }
            ]
        },
        {
            "name": "atomistic_model",
            "type": "ecuds://emmc.info/metadata/atomistic_model/1.0",
            "transitions": [
                {
                    "target": "proc_average_wall_velocity",
                    "event": "normal_exit"
                }
            ]
        },
        {
            "name": "proc_average_wall_velocity",
            "type": "ecuds://emmc.info/metadata/proc_average_wall_velocity/1.0",
            "transitions": [
                {
                    "target": "continuum_model",
                    "event": "continue"
                },
                {
                    "target": "finished",
                    "event": "normal_exit"
                }
            ]
        },
        {
            "name": "finished",
            "type": "final"
        }
    ]
}
```
Keywords (Syntactic level) and HDF5 implementations

- NumberChemicalElements
- ChemicalElementID „CEID“
- ChemicalElementName(CEID)
- NumberMoles(CEID)
- NumberAtoms; NumberMoles
- AtomPercent(CEID)
- Composition

Figure 6:

The major descriptors for the description of the composition of an RVE

EMMC Metadata Workshop, 10th March 2016, Brussels
Addressing the SWO delamination challenge: Using MODA, Metadata and e-CUDS

- for each grain/pair of grains:
  - Crystallographic Structure
  - Chemical Composition
  - Reference Frame
  - Orientation/Miss-orientation
  - ...

- For the polymer: e.g. the phase composition and orientation

Build a number of Atomistic e-CUDS of the different interface systems (I through IV) with specific statistical/thermal model for the exact structure.

return/store the average energy: “interfacial energy” for the different systems (I through IV)
Interoperability: where are we today?

Many are still not even here!

The cluster of 5+1 are already here: integrated OSP

...and then no one is here! YET... but the cluster is approaching this rapidly

Metadata is the vehicle of interoperability

Cross-domain interoperability
- Interoperability of metadata schemas
- Community strict agreements

Semantic interoperability
- Requires Metadata (Schema, Vocabulary, conceptual model)

Syntactic interoperability
- Technical Interoperability
- Specific cases
- Limited use of metadata

Metadata allows a resource to be understood by both humans and machines → promote interoperability.
2nd International Workshop on Software Solutions for ICME

Barcelona, Spain, April 12th to 15th 2016

Georg J. Schmitz, Access e.V., Aachen, Germany

Coordinator of ICMEg CSA
> 110 participants
24 countries, 5 continents

Germany (29)
USA (16)
Spain (14)
Japan (11)
UK (6)

40% academia
13 software companies
9 manufacturing industry
several governmental institutions
Participants (in detail)

- Commercial SWO:

- Academic SWO:
  - OOF, DAMASK, PRISMS, Dream3D and others

- Manufacturers:
  - Tata Steel *(late cancellation)*, MTU, Hydroaluminium, Safran, Philips, Bosch, Toyota, Hyundai and Hitachi

- Governmental institutions:
  - NIST (US), NIMS (Japan), DIN (Germany), EU
Scope and format

- **scope**: INTEROPERABILITY

- **for EMMC especially**:
  dissemination of 5+1 results to the global community

- about 100 presentations (almost all invited by the ICMEg consortium)

- plenary lectures, parallel sessions, posters, exhibition and sand-box scenario discussion sessions, closing panel discussion

Most talks from IntOP where also in ICMEg!
Preliminary assessment of the workshop

- A community working on different aspects of interoperability is clearly emerging.

- US is strong in the “big data” type approach: collecting and curing of data, generation of data and metadata schemes, maintenance of repositories etc.

- EU is strong in interoperability aspects of different simulation tools (e.g. CUDS, CUBA, metadata keywords, HDF5..). Presented approaches got positive feedback.

- Japan in few areas is strong in first applications for complex materials and processes.

Summary & Outlook

- Extendable, adaptable and interoperable open simulation platforms for multiple application fields
- Open Metadata Schema for materials modelling
  - Open in the sense it does not oblige any one to use the e-CUBA keywords outside of a specific domain
  - Can be used for closed as well as open source data
  - Can be used for high level model (GE) and low level computational data
- Easy to interoperate
  - Automatic discovery of information
  - Only relevant data for a model are included in each case
  - Basis for coupling and linking workflows (in the general sense, no specific implementation is implied here)
- Reference implementation for interoperability across all platforms!
The 4th World Congress on Integrated Computational Materials Engineering (ICME 2017) is the destination where leading researchers and practitioners of ICME convene to share the latest knowledge and advances in this discipline.

*Don't miss this opportunity to discuss and influence trends in the field—submit your abstract today.*

This congress will focus on ICME–related technical topics, such as:

- The wide range of materials programs where an ICME approach validated by experimental efforts is applicable, including computational- and experimental-based talks
- Individual computational methods utilized in an ICME approach, including both advantages and limitations
- Roles of ICME in graduate and undergraduate courses
- Digital infrastructure required for information sharing and model integration
- ICME implementation strategies
- Verification, validation, and uncertainty quantification issues
- Interoperability and communications standards
- ICME networking initiatives around the world

For more information on this congress and to submit your abstract today, visit [www.tms.org/ICME2017](http://www.tms.org/ICME2017).