EMMC

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

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Georg Schmitz

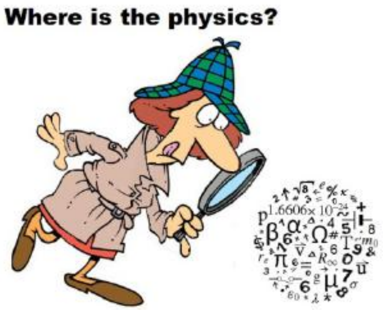
Workshop on

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



EU Multiscale Projects Cluster

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

„5+1“

Integrated **C**omputational **M**aterials **E**ngineering expert **g**roup
www.icmeg.eu/

From atom-to-**D**evice **E**xplicit simulation **E**nvironment for **P**hotonics and **E**lectronics **N**anostructures http://www.nmp-deepen.eu/

Multiscale **M**odelling **P**latform: Smart design of nano-enabled products in green technologies http://www.mmp-project.eu/

Modelling of morphology **De**velopment of micro- and **Na**nostructures
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

9:30 – 10:10	Classification of materials models, vocabulary, workflows and modelling elements MODA (user case, models, computation, post-processing)	P. Asinari
10:10 – 10:50	Computational related metadata: strategies for their specification/classification/organisation and their required attributes.	A. Hashibon, T. Hagelien, H. Preisig

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

+ Concluding Panel discussion:
1.Discrete electronic SWOs : Nicola Marzari (psi-K)
…

Industrial Materials Design: challenges for metadata and interoperability from an engineering workflow and database perspective	D. Cebon
Industrial Materials Design: challenges for metadata and interoperability from a discrete software owner perspective	A. Blom, E. Wimmer
Industrial Materials Design: challenges for metadata and interoperability from a manufacturer perspective	B. Rijksen, DOW
Response to Challenges: Meta level description of the challenge cases.	J. Friis, A. Hashibon, H. Rusche G.J. Schmitz

Purpose of Meeting

- 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.

RoMM V

Workflow Description MODA

Each model in the chain is described in four chapters

Chapter 1: Part of the User Case

Chapter 2: Model

Chapter 3: Computational

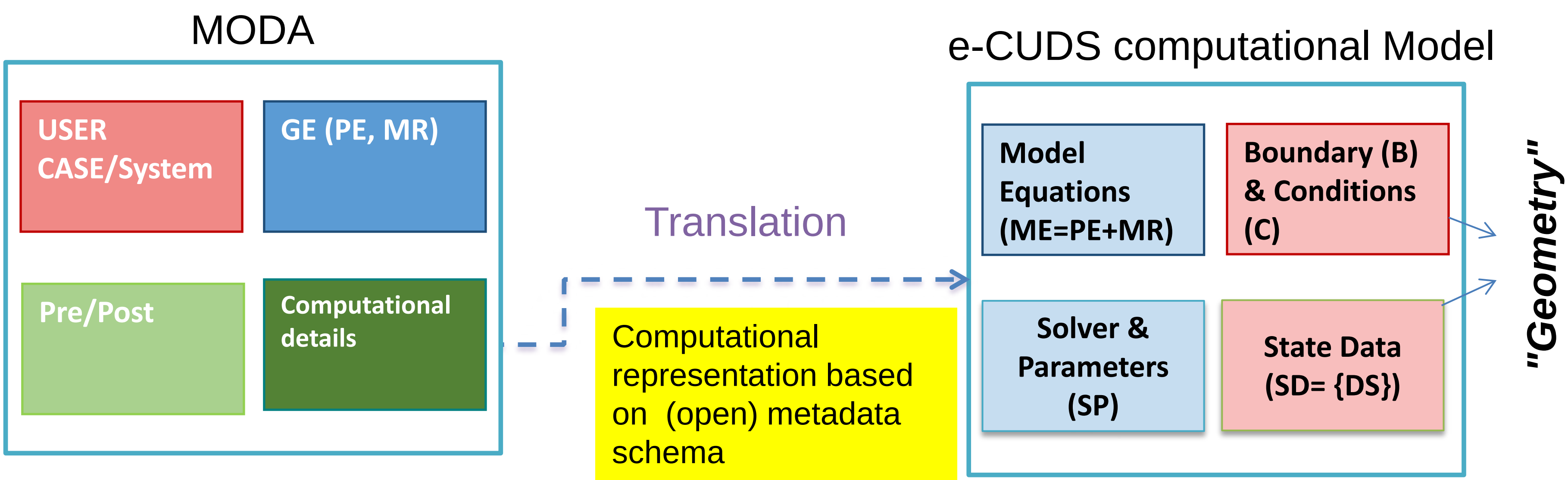
Chapter 4: Postprocessing

→A vocabulary across the materials modelling world

→Basis for Metadata definition and development

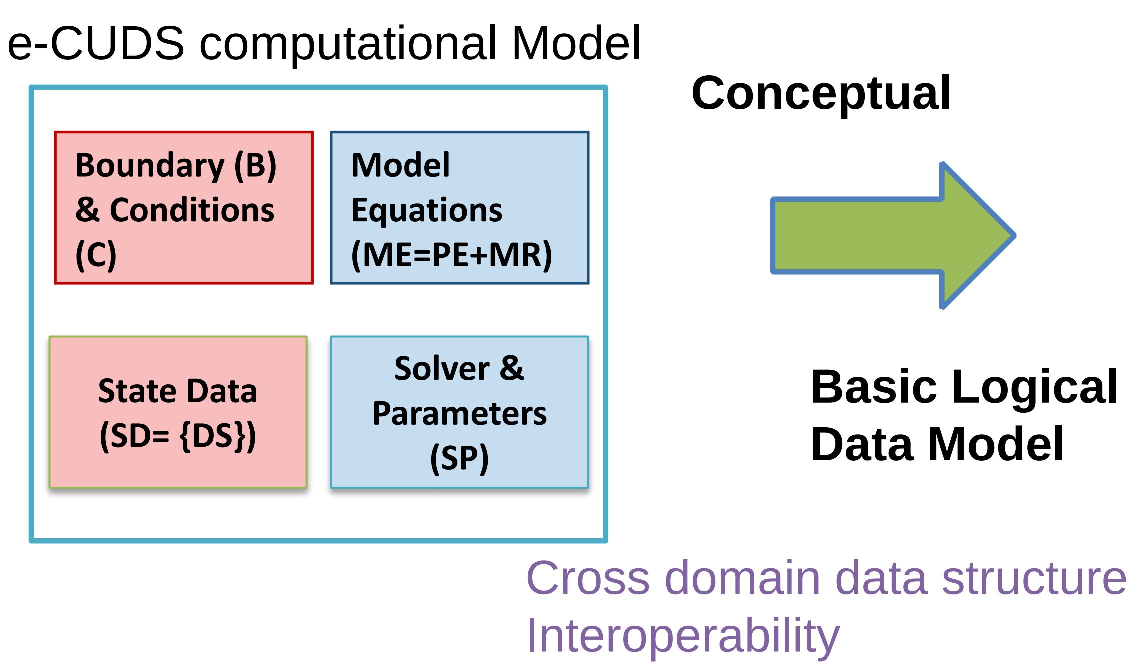
Beyond the MODA: Towards a Computational Material Modelling Metadata

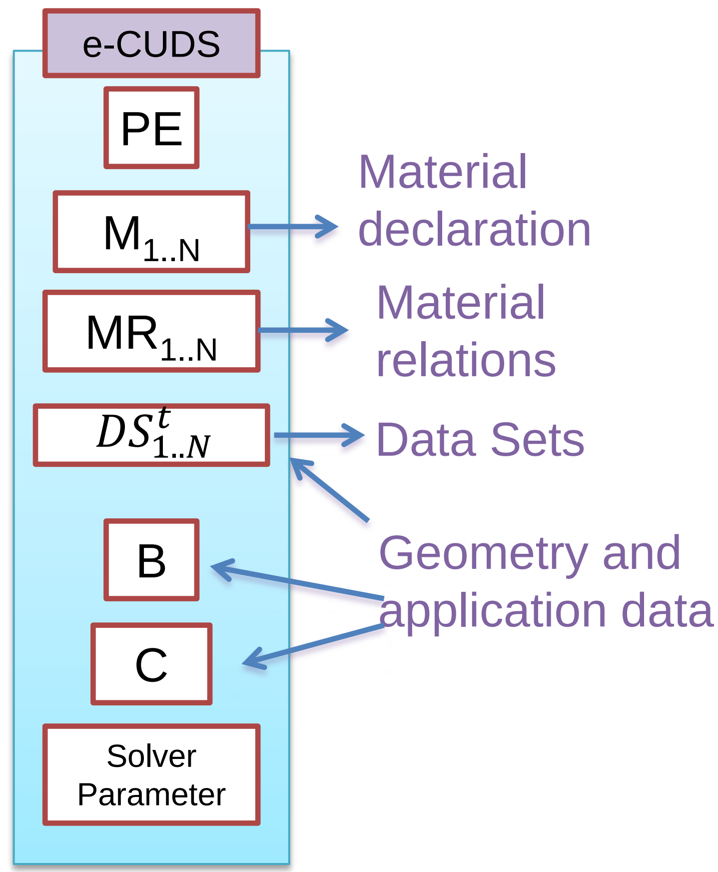
- A European Common Unified Data Structure: e-CUDS
  - provide a schema for semantic interoperability
- A European Common Unified Basic Attributes: e-CUBA
  - provide reference agreed upon keywords for syntactic interoperability



e-CUDS: One Conceptual
Many Logical Models, Many Implementations!

- **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





Formal Computational Modellin Metadata

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 alread exists!

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

```
type        -> name version namespace dimensions types properties

dimensions  -> nil
             | dimensions dimension

types       -> nil
             | types type

properties  -> nil
             | properties property

dimension   -> name description

property    -> name type dimensions description

name        -> string

version     -> string

namespace   -> nil
             | string

description-> nil
             | string
```

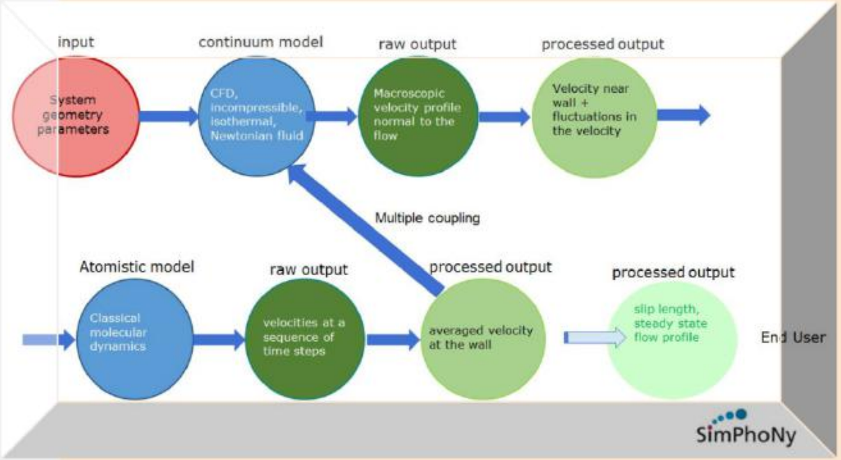
e-CUDS Schema

Defining the CUDS 1.0 Schema from the Basic Schema


```
{
        "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

```
{
        "name": "simphony_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

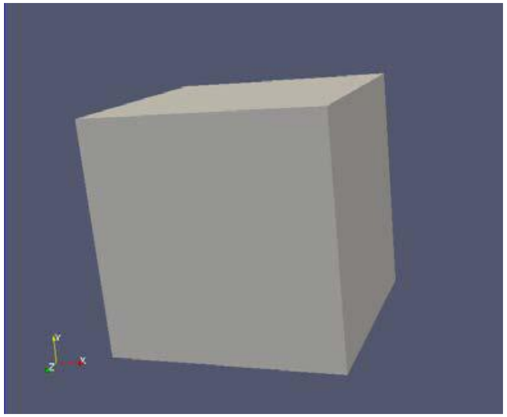
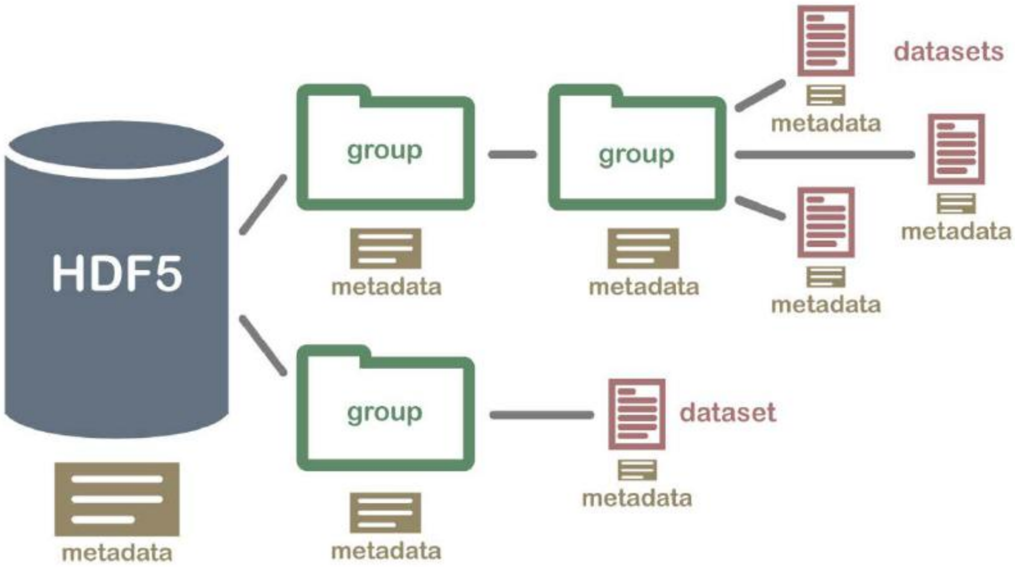
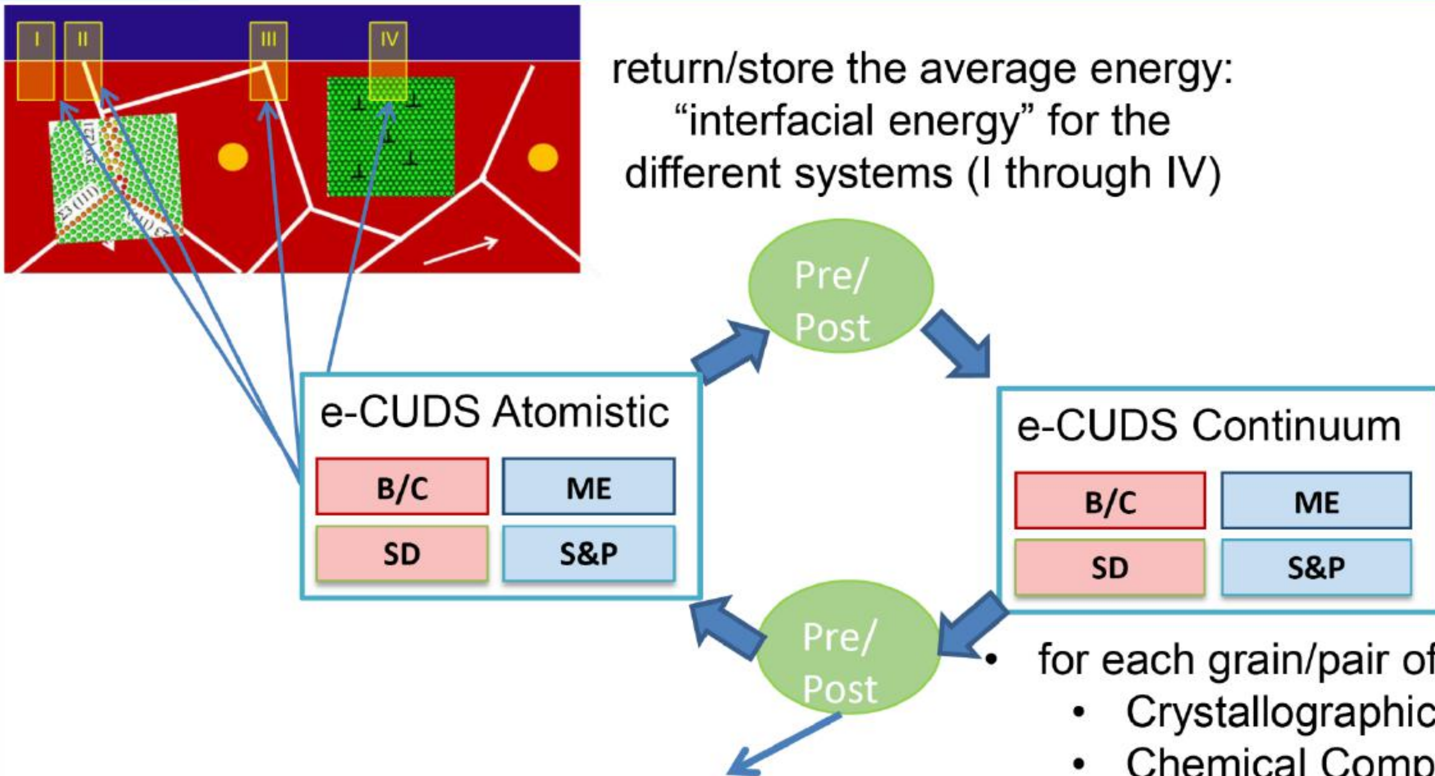


Figure 6:

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



Addressing the SWO delamination challenge: Using MODA, Metadata and e-CUDS

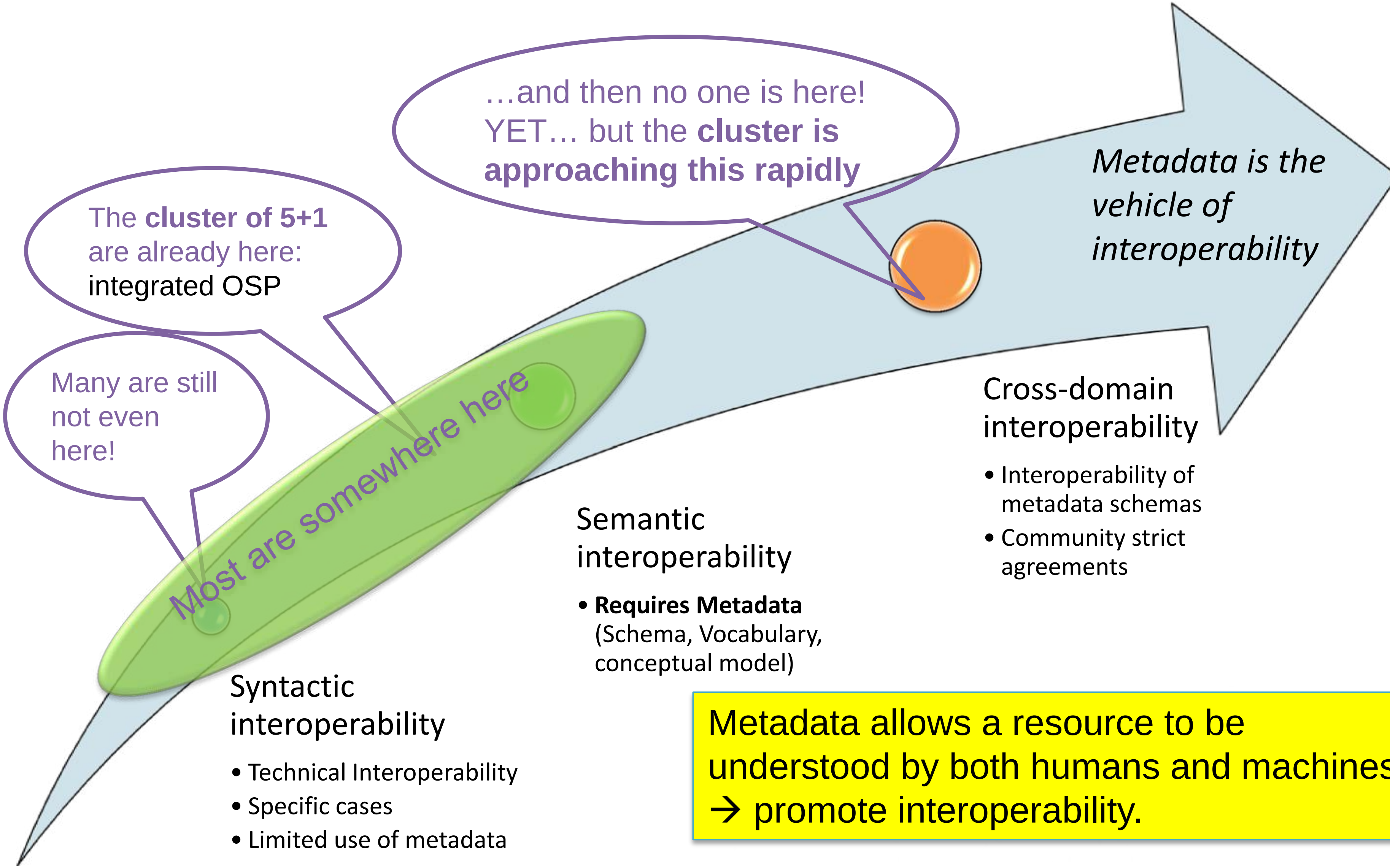


return/store the average energy: "interfacial energy" for the different systems (I through IV)

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

- 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

Interoperability: where are we today?



Metadata allows a resource to be understood by both humans and machines → promote interoperability.

EMMC

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

Attendance

> 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:
  - msc-software, gtt-technologies, Dassault Systemes, Thermo-Calc Software, e-xstream, Materials Design, MICRESS, simufact, Materials Ressources, simpleware, Itochu-Solutions, Granta Design, Tiberlab
- 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.
- Next related event: 4th ICME World Congress in the US in May 2017

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!

TMS ICME
MANUFACTURING DESIGN MATERIALS

4th World Congress on Integrated Computational Materials Engineering (ICME 2017)

May 21–25, 2017 • Marriott Ann Arbor Ypsilanti at Eagle Crest
Ypsilanti, Michigan, USA

SUBMIT YOUR ABSTRACT BY SEPTEMBER 30, 2016.

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

Georg's Advertisement!

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visit **www.tms.org/ICME2017**.