Towards an ICME methodology: Current activities in Europe

Dr. Georg J. Schmitz

Access e.V. at the RWTH Aachen

Stockholm, June 2016

Towards an ICME methodology: Current activities in Europe

Overview of European communities being active in the field

- politics
- communication channels
- organisatorial

Overview of current scientific/technological activities

- Interoperability
- Metadata and Metadata schemata
- Platform concepts
- …more…

Towards an ICME methodology: Current activities in Europe

Overview of European communities being active in the field

- politics
- communication channels
- organisatorial

Overview of current scientific/technological activities

- Interoperability
- Metadata and Metadata schemata
- Platform concepts
- …more…

European ICME communities & communication channels

10/2013 – 09/2016	ICMEg project (Coordination Support Action CSA)
01/2014 – 12/2016	EU Multiscale Modelling Cluster („5 projects“)
11/2014 – now	European Materials Modelling Council EMMC (bottom up activity)
11/2015 – future	International Materials Modelling Board IM2B
09/2016 – future	EMMC- CSA (proposal approved)
01/2016 – future	several proposals submitted for research activities

7th Framework Program (2007-2013), **Horizon 2020 Program (2014-2020)**

plus national and multilateral projects within the different European Countries

European ICME communities & communication channels

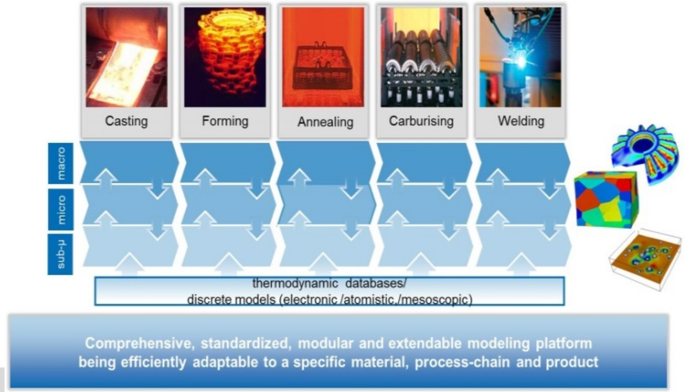
10/2013 – 09/2016	ICMEg project (Coordination Support Action CSA)
01/2014 – 12/2016	EU Multiscale Modelling Cluster („5 projects")
11/2014 – now	European Materials Modelling Council EMMC (bottom up activity)
11/2015 – future	International Materials Modelling Board IM2B
01/2016 – future	EMMC- CSA (proposal submitted)
01/2016 – future	several proposals submitted for research activities

7th Framework Program (2007-2013), **Horizon 2020 Program (2014-2020)**

plus national and multilateral projects within the different European Countries

The European Materials Modeling Council

- EU project ICMEg -



consortium: 11 partners, 6 countries

vision: plug&play in ICME

approach: global, open standards

How to do in practice? Read more:

ICMEg - the Integrated Computational Materials Engineering expert group - a new European coordination action

Integrating Materials and Manufacturing Innovation 2014, **3**:2 doi:10.1186/2193-9772-3-2

Georg J Schmitz (G.J.Schmitz@access.rwth-aachen.de)
Ulrich Prahl (Ulrich.Prahl@iehk.rwth-aachen.de)

www.icmeg.eu
www.icmeg.info

Expected outputs:

A) 2 International Workshops with minimum100 participants each

B) 2 books (e.g. Wiley) on:
- „Handbook of software solutions for ICME
- „Software standards for successful ICME“

C) Specifications of standards for information exchange in ICME settings

D) Foundation of an Association of Software providers for ICME

ICMEg e.V. founded on June 24th 2014 in Rolduc

Pavel Korzhavyi
(KTH Stockholm)

Borek Patzak
(CTU Prague)

Anders Engstrom
(Thermo-Calc)
vice-president

John Agren
(KTH Stockholm)

Laurent Adam
(e-xstream)

Georg J. Schmitz
(Access)
president

Andreas Kreutzer
(K&S)
treasurer

Albert Konter
(M2i)
vice-president

Ulrich Prahl
(RWTH Aachen)
secretary

1st ICMEg workshop in June 2014

- > 160 participants
- 24 countries
- 4 continents
- Abstract booklet available under www.icmeg.info
- pdf's of authors presentations also under www.icmeg.info
- Next workshop :

April 2016 Barcelona

2^{nd} ICMEg workshop in April 2016 in Barcelona

> 110 participants
24 countries, 5 continents

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

40% academia

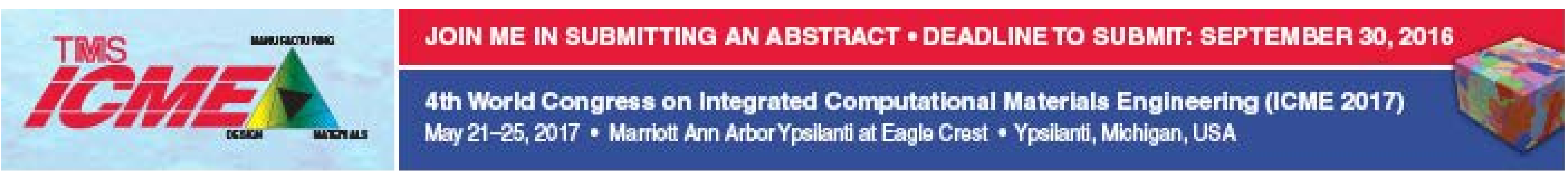
13 software companies

9 manufacturing industry

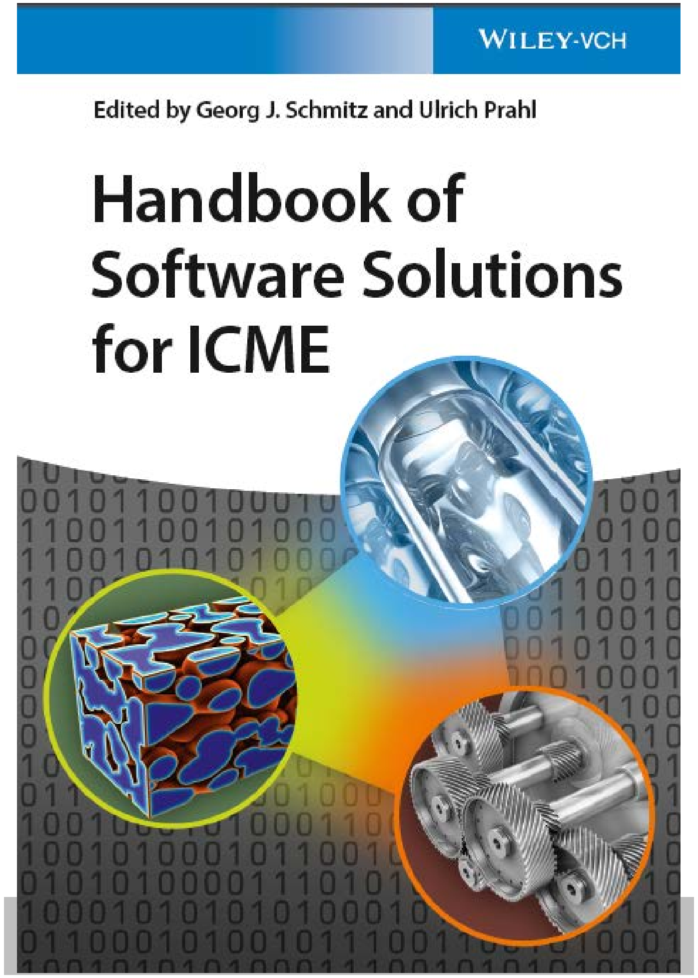
several governmental institutions

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 Ypsilanti (MI) in May 2017



Handbook of Software Solutions for ICME



in production: tentative release Sept/Oct 2016

93 authors
14 countries
~ 600 pages
~ hundreds of codes (thematically structured)

Introductions to different topics:

- Electronic, atomistic, mesocopic models
- Continuum models (Phase-field, Phase-field Crystal, Crystal plasticity, Cellular Automata)
- Thermodynamics
- Effective properties (mean field, homogenisaton, virtual testing)
- Numerical methods
- Process simulations (from casting to recycling)
- Simulation platforms

remaining outputs:

A) 2 International Workshops with minimum100 participants each

B) 2 books (e.g. Wiley) on:
- „Handbook of software solutions for ICME
- „Software standards for successful ICME“

C) Specifications of standards for information exchange in ICME settings

D) Foundation of an Association of Software providers for ICME

European ICME communities & communication channels

10/2013 – 09/2016	ICMEg project (Coordination Support Action CSA)
01/2014 – 12/2016	EU Multiscale Modelling Cluster („5 projects“)
11/2014 – now	European Materials Modelling Council EMMC (bottom up activity)
11/2015 – future	International Materials Modelling Board IM2B
01/2016 – future	EMMC- CSA (proposal submitted)
01/2016 – future	several proposals submitted for research activities

7th Framework Program (2007-2013), Horizon 2020 Program (2014-2020)

plus national and multilateral projects within the different European Countries

The European Materials Modeling Council

current EU projects on interoperability/platforms

René Martins, Anne de Baas,
Sophia Fantechi (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/

European ICME communities & communication channels

10/2013 – 09/2016	ICMEg project (Coordination Support Action CSA)
01/2014 – 12/2016	EU Multiscale Modelling Cluster („5 projects“)
11/2014 – now	European Materials Modelling Council EMMC (bottom up activity)
11/2015 – future	International Materials Modelling Board IM2B
01/2016 – future	EMMC- CSA (proposal submitted)
01/2016 – future	several proposals submitted for research activities

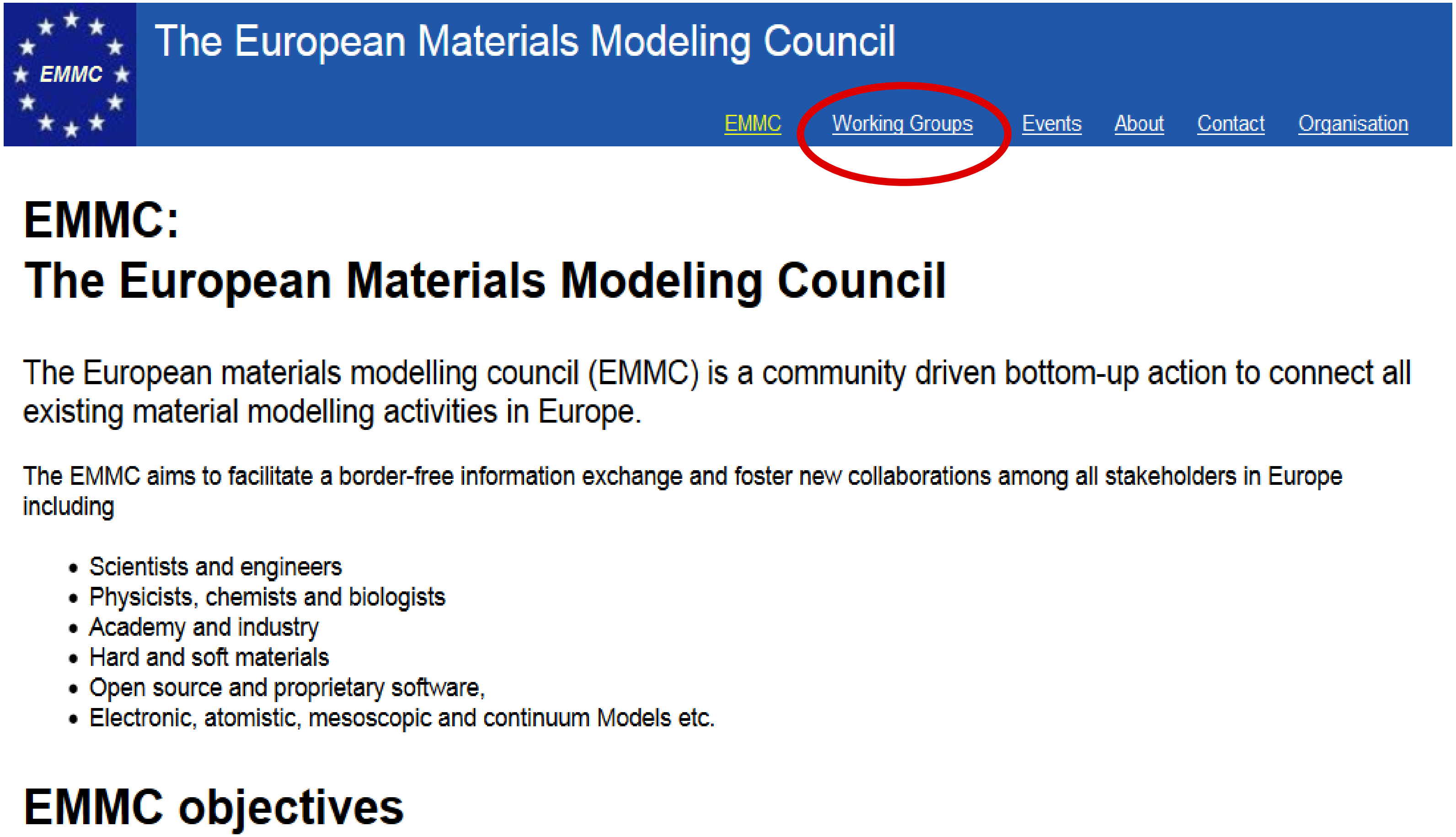
7th Framework Program (2007-2013), Horizon 2020 Program (2014-2020)

plus national and multilateral projects within the different European Countries

The European Materials Modeling Council

Kick-off 11/2014, Brussels

European Materials Modelling Council www.emmc.info



EMMC
The European Materials Modeling Council

EMMC | Working Groups | Events | About | Contact | Organisation

EMMC:
The European Materials Modeling Council

The European materials modelling council (EMMC) is a community driven bottom-up action to connect all existing material modelling activities in Europe.

The EMMC aims to facilitate a border-free information exchange and foster new collaborations among all stakeholders in Europe including

- Scientists and engineers
- Physicists, chemists and biologists
- Academy and industry
- Hard and soft materials
- Open source and proprietary software,
- Electronic, atomistic, mesoscopic and continuum Models etc.

EMMC objectives

EMMC Working groups

1. Business Decision Support
2. Continuum Models
3. Discrete Models (including Electronic Models, Atomistic Models, Mesoscopic Models, Coupling and Linking)
4. Interoperability
5. Open Simulation Platform Concept
6. Materials Model Marketplace
7. Manufacturers
8. Software Owner
9. Translator
10. Validation

Towards an ICME methodology: Current activities in Europe

Overview of European communities being active in the field

- politics
- communication channels
- organisatorial

Overview of current scientific/technological activities

- Focus on Interoperability

large variety of existing codes

only a very small subset of a possible logo collection

Plugs and sockets for plug & play: benefits of standardization

Have you ever tried
to get

that one

into

that one?

Interoperability: Objectives

Scope:

improve interoperability between the heterogeneous variety of commercial and academic modeling tools

Communication Standards

will be based on existing standards and solutions to the largest possible extend

will allow sequential i.e. file based interoperability

- Generic and structured list of metadata keywords
- Overall data structure for file based information exchange

Open Simulation Platform(s)

will allow strong coupling resp. interoperability in each time step

- Workflow tool(s) to orchestrate a number of different materials modeling tools
- Tools for distributed simulations
- *Long term*: Accounting schemes (not for the use of the platform but for the use of commercial codes used in the platform)

Highest level metatdata for materials modelling

Three chapters
Chapter 1: Model
Chapter 2: System to be simulated
Chapter 3: Computational

Metadata are essential prerequisites to describe ***models and simulations interoperability*** of models (multi-scaling) and databases.

slides with courtesy of Pietro Asinari
Polytechnico di Torino

Chapter 1 Model

1.1. entity: finite volumes, grains, atoms, electrons
1.2. physics/chemistry equation and its physics quantities
materials relation (closure/constitutive equation) and its physics quantities/descriptors
1.3 Publication documenting the model

slides with courtesy of Pietro Asinari
Polytechnico di Torino

Model classes: e/a/m/c

A new way of building an overview of materials models.
Classification via the **entity** whose behaviour is described by the physics equation

1. electrons,
2. atoms,
3. nanoparticles/beads/grains
4. continuum finite volumes/elements

Models are strictly classified according to the entity whose behaviour is described by the physics equation in the model

not according to the size of the application or system
nor according to the lengthscale of the phenomena to be simulated

slides with courtesy of Pietro Asinari, Polytechnico di Torino

Physics equations and Materials relations

Materials Models consist of Governing Equations

- Physics or chemistry Equations (PE)

  Generic equations describing the behaviour of electrons, atoms, particles or finite volumes (the model entities).

  Underdetermined equations

- Materials Relations (closure relations, constitutive equations) (MR)

  Specifications of the specific material necessary to close the PE

Note the difference with coupled equations!

Governing Equations= Physics Equation with Materials Relation

slides with courtesy of Pietro Asinari, Polytechnico di Torino

Model classes

1.1 Ab initio quantum mechanical (or first principle) models
1.2 Many-body models and effective Hamiltonians
1.3 Quantum mechanical in response to time dependent fields
1.4 Statistical charge transport model

2.1 Classical (Dynamic) Density Functional Theory
2.2 Molecular Mechanics
2.3 Statistical mechanics models: Molecular Dynamics
2.4 Statistical mechanics models: Monte Carlo molecular models
2.5 Atomistic spin models
2.6 Statistical atomistic models
2.7 Atomistic phonon models (Boltzmann Transport Equation)

From „Review of Materials Modelling V" ,
eds. A.de Baas and L.Rosso European Commission 2015

Model classes II

3.1 Mesoscopic (Dynamic) Density Functional Theory
3.2 Coarse Grained Molecular Dynamics
3.3 Discrete lattice dynamics model
3.4 Statistical Mechanics mesoscopic models
3.5 Micromagnetism model
3.6 Mesoscopic phonon models ((Boltzmann Transport Equation)

4.1 Solid Mechanics
4.2 Fluid Mechanics
4.3 Heat flow and thermo-mechanics
4.4 Continuum Thermodynamics and continuum Phase Field models
4.5 Chemistry reaction (kinetic) models (continuum)
4.6 Electromagnetism (including optics, magnetics, electrical)
4.7 Process and device modelling

From „Review of Materials Modelling V" ,
eds. A.de Baas and L.Rosso European Commission 2015

The European Materials Modeling Council

Metadata materials model(s) : example continuum

“Generic physics of the model equation(s)”: examples for continuum equations

Diffusion:
e.g. Fick-Onsager

$$\dot{\vec{c}} = \nabla\left(\sum_{\alpha} \phi_\alpha \vec{\vec{D}}_\alpha \nabla \vec{c}_\alpha\right)$$

FluidFlow:
e.g. Navier-Stokes

$$\frac{\partial}{\partial t}[\rho v_{mix}] + \nabla\cdot\left[\frac{1}{\phi_l}\rho v_{mix} v_{mix}\right] = -\phi_l\left[\nabla p_L - \frac{\partial\rho}{\partial c} c_{liq}^{k*}\vec{g}\right] + \nabla\cdot[\mu\nabla v_{mix}] - h^*\mu_l\frac{\phi_s}{\phi_l}\frac{v_{mix}}{\delta}|\nabla\phi_l|$$

PhaseEquilibria:
e.g. Thermodynamic models

$$\Delta G(c_i, T, p) = 0$$

PhaseTransformations:
e.g. Phase-Field models,
Phase-Field-Crystal models

$$\dot{\phi}_\alpha = \sum_{\beta}^{n} \mu^*_{\alpha\beta}\left[\sigma^*_{\alpha\beta}\left(\phi_\alpha\nabla^2\phi_\beta - \phi_\beta\nabla^2\phi_\alpha + \frac{\pi^2}{2\eta^2_{\alpha\beta}}(\phi_\alpha-\phi_\beta) + \sum_{\alpha\neq\beta\neq\gamma}^{n} J_{\alpha\beta\gamma}\right) + \frac{\pi}{\eta_{\alpha\beta}}\sqrt{\phi_\alpha\phi_\beta}\,\Delta G_{\alpha\beta}\right]$$

$$\psi = \psi_0 + \sum_j A_j \exp(i\vec{k}_j\cdot\vec{r}) + \text{complex conjugate}$$

Elasticity:
e.g. mechanical equilibrium

$$0 = \nabla\sigma = \sum_{\alpha} \nabla\phi_\alpha C_\alpha\left(\varepsilon_\alpha - \varepsilon^*_\alpha - \varepsilon^{th}_\alpha(T-T_0)\right)$$

Plasticity:
forming models,

e.g. Crystal Plasticity

$$\dot{\varepsilon} = \sum_{\alpha=1}^{n} M^{\alpha}_{sym}\,\dot{\gamma}^{\alpha}$$

The European Materials Modeling Council

Ontology for models

	equations	*res*	*vars*	*given*
integrals	$n_{\mathcal{NS}} := \int_0^t \dot{n}_{\mathcal{NS}}\, dt + n^o_{\mathcal{NS}}$	$n_{\mathcal{NS}}$	$\dot{n}_{\mathcal{NS}}$	$n^o_{\mathcal{NS}}$
differential balances	$\dot{n}_{\mathcal{NS}} = F^n{}_{\mathcal{NS},\mathcal{AS}} \overset{\mathcal{AS}}{\star} \hat{n}_{\mathcal{AS}}$	$\dot{n}_{\mathcal{NS}}$	$\hat{n}_{\mathcal{AS}}, F^n{}_{\mathcal{NS},\mathcal{AS}}$	
constants	$F^n{}_{\mathcal{NS},\mathcal{AS}} = F^m{}_{\mathcal{N},\mathcal{A}} \overset{\mathcal{N},\mathcal{A}}{\odot} S_{\mathcal{NS},\mathcal{AS}}$	$F^n{}_{\mathcal{NS},\mathcal{AS}}$		$F^m{}_{\mathcal{N},\mathcal{A}}, S_{\mathcal{NS},\mathcal{AS}}$
flows	$\hat{n}_{\mathcal{AS}} := \hat{V}_{\mathcal{A}} \overset{\mathcal{A}}{\odot} c_{\mathcal{AS}}$	$\hat{n}_{\mathcal{AS}}$	$\hat{V}_{\mathcal{A}}, c_{\mathcal{AS}}$	
	$\hat{V}_{\mathcal{A}} := -K^V{}_{\mathcal{A}} \cdot F^m{}_{\mathcal{N},\mathcal{A}} \overset{\mathcal{N}}{\star} p_{\mathcal{N}}$	$\hat{V}_{\mathcal{A}}$	$p_{\mathcal{N}}$	$K^V{}_{\mathcal{A}}, F^m{}_{\mathcal{N},\mathcal{A}}$
state variable transformations	$c_{\mathcal{AS}} := d_{\mathcal{A}} \overset{\mathcal{A}}{\odot} F^n{}_{\mathcal{NS},\mathcal{AS}} \overset{\mathcal{NS}}{\star} c_{\mathcal{NS}}$	$c_{\mathcal{AS}}$	$d_{\mathcal{A}}, F^n{}_{\mathcal{NS},\mathcal{AS}}, c_{\mathcal{NS}}$	
	$d_{\mathcal{A}} := \mathrm{sign}\left(F^m{}_{\mathcal{N},\mathcal{A}} \overset{\mathcal{N}}{\star} p_{\mathcal{N}}\right)$	$c_{\mathcal{AS}}$	$p_{\mathcal{NS}}$	$F^m{}_{\mathcal{N},\mathcal{A}}$
	$c_{\mathcal{NS}} := V^{-1}_{\mathcal{N}} \overset{\mathcal{N}}{\odot} n_{\mathcal{NS}}$	$c_{\mathcal{NS}}$	$V_{\mathcal{N}}, n_{\mathcal{NS}}$	
	$p_{\mathcal{N}} := \rho_{\mathcal{N}} \cdot g \cdot h_{\mathcal{N}}$	$p_{\mathcal{N}}$	$h_{\mathcal{N}}$	$\rho_{\mathcal{N}}, g$
	$h_{\mathcal{N}} := A^{-1}_{\mathcal{N}} \cdot V_{\mathcal{N}}$	$h_{\mathcal{N}}$	$V_{\mathcal{N}}$	$A_{\mathcal{N}}$
	$V_{\mathcal{N}} := \rho^{-1}_{\mathcal{N}} \cdot m_{\mathcal{N}}$	$V_{\mathcal{N}}$	$m_{\mathcal{N}}$	$\rho_{\mathcal{N}}$
	$m_{\mathcal{N}} := \lambda_{\mathcal{S}} \overset{\mathcal{S}}{\ddagger} n_{\mathcal{NS}}$	$m_{\mathcal{N}}$	$n_{\mathcal{NS}}$	$\lambda_{\mathcal{S}}$

slide with courtesy of Heinz Preisig, University Trondheim, Norway

Chapter 2 System to be simulated

2.1 Material properties, behaviour and/or material manufacturing processes
2.2 Size, form, geometry, picture of the system and time lapse of the process
2.3 Other physics metadata for system
2.4 Publication documenting the simulated case

slides with courtesy of Pietro Asinari, Polytechnico di Torino

getting the initial conditions: example microstructure

preceeding simulation

digital experimental data
e.g. CT scans, SEM/EDX,LOM, EBSD stacks

experimental data
e.g. images

synthetic microstructures
e.g. voronoi tesselation
designed structures, assumptions

microstructure database

SD
System Description

- outer geometry of the system
- material composition
- initial state, *(time lapse)**
- boundary conditions/process condition

*not addressed yet

The following slides only address metadata keywords to describe a

static microstructure

Adding any dynamics will happen in future steps/activities

The European Materials Modeling Council

Huge variety of existing codes

different scales; different objectives;
different properties; different materials

only common denominator:
MATERIAL

What is a material ?

Any material is

„a number of atoms arranged in a volume“

The number of atoms may be large and they typically will belong to several chemical elements

What is a material in terms of keywords?

Any material is

„*a* NumberAtoms

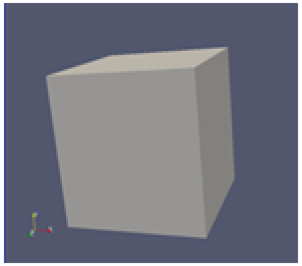
***arranged in a* Volume“**

The **NumberAtoms** may be large (**NumberMoles)** and they typically will belong to a **NumberChemicalElements**

How to describe arranged?

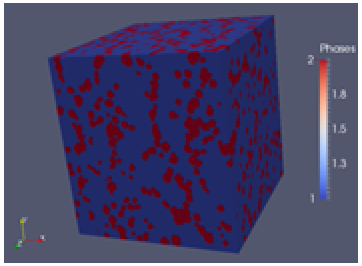
- Atoms may „self arrange“ (see also e/a/m models) and form **objects/features** and **ensembles** of objects/**features** e.g.
  - molecules, particles, precipitates, crystals/grains
  - different phases/crystal structures
  - defect structures….and eventually
  - multiphase, polycrystalline materials

RVE



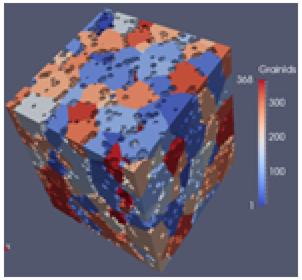
effective material

Ensemble(s)



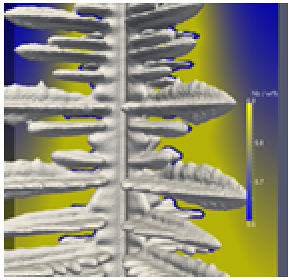
e.g.phases

Feature(s)



e.g. grains

Fields



e.g. concentration

- Materials reveal an inherent hierarchical structure!

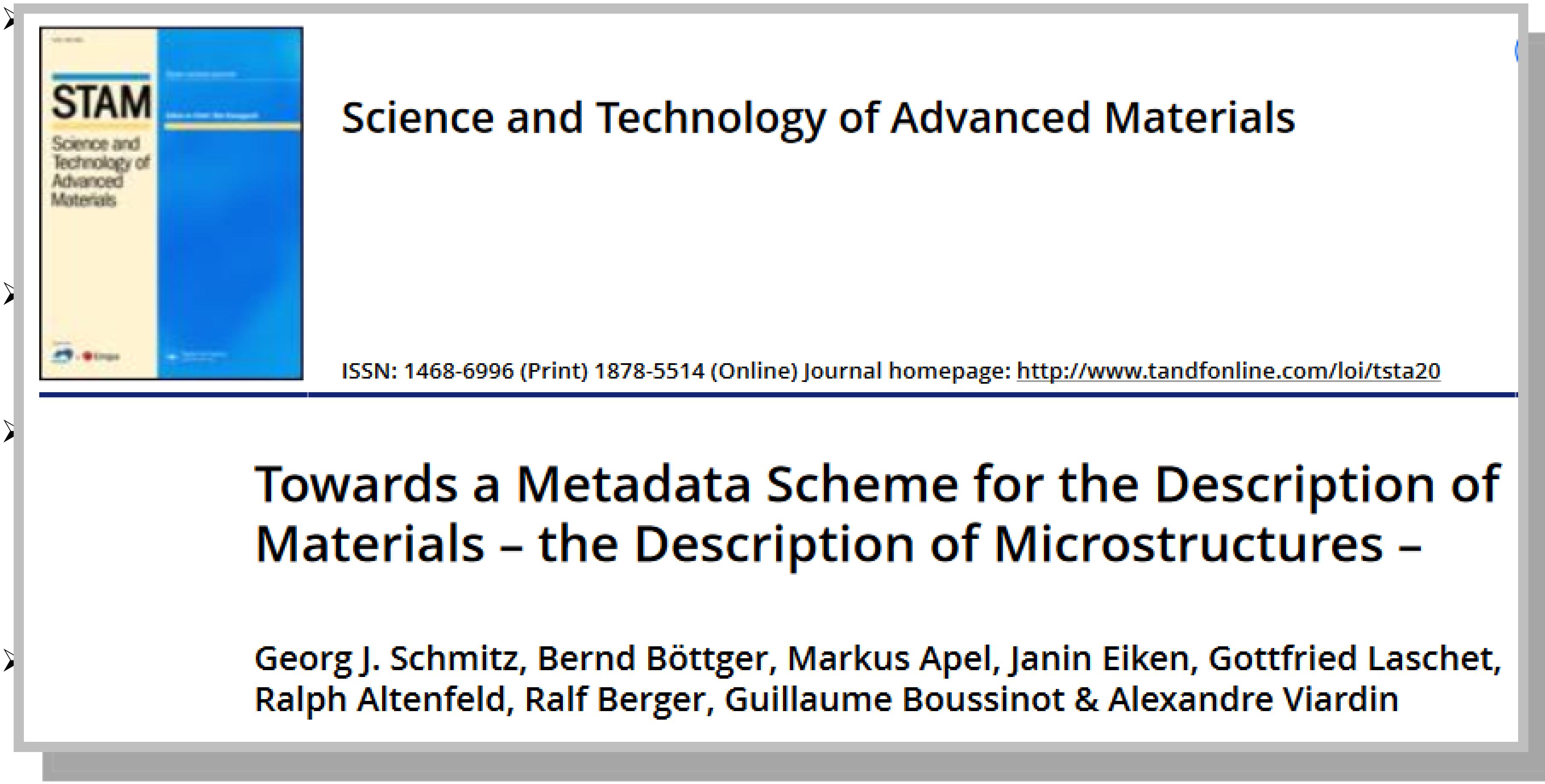
Canonical keywords (Volumetric)

RVE	Phase/ensemble	Feature	Field at Cell
NumberChemical Elements	NumberChemical Elements	NumberChemical Elements	NumberChemical Elements
NumberAtoms	NumberAtoms	NumberAtoms	NumberAtoms
NumberPhases			
	PhaseID	PhaseID	
NumberFeatures	NumberFeatures		
		FeatureID	FeatureID
NumberDefects	NumberDefects	NumberDefects	NumberDefects
Composition	Composition	Composition	Composition
Volume	Volume	Volume	Volume
Centroid	Centroid	Centroid	Centroid
Orientation	Orientation	Orientation	Orientation
Crystallinity	Crystallinity	Crystallinity	Crystallinity

EMMC

The European Materials Modeling Council

metadata description of a static microstructure



Science and Technology of Advanced Materials

ISSN: 1468-6996 (Print) 1878-5514 (Online) Journal homepage: http://www.tandfonline.com/loi/tsta20

Towards a Metadata Scheme for the Description of Materials – the Description of Microstructures –

Georg J. Schmitz, Bernd Böttger, Markus Apel, Janin Eiken, Gottfried Laschet, Ralph Altenfeld, Ralf Berger, Guillaume Boussinot & Alexandre Viardin

- **The proposed metadata keyword structure may even be applicable to e/a/m models**
  - ***to be verified….***

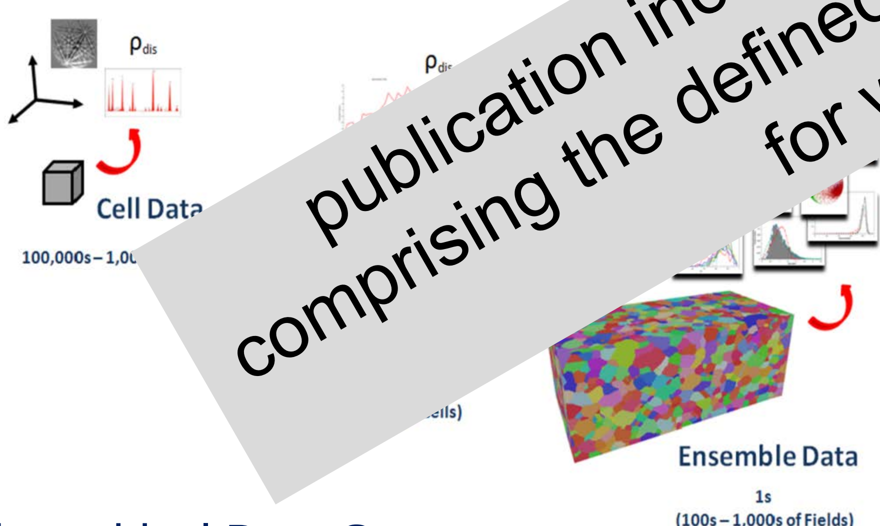
The European Materials Modeling Council

Towards a data structure for file based communication

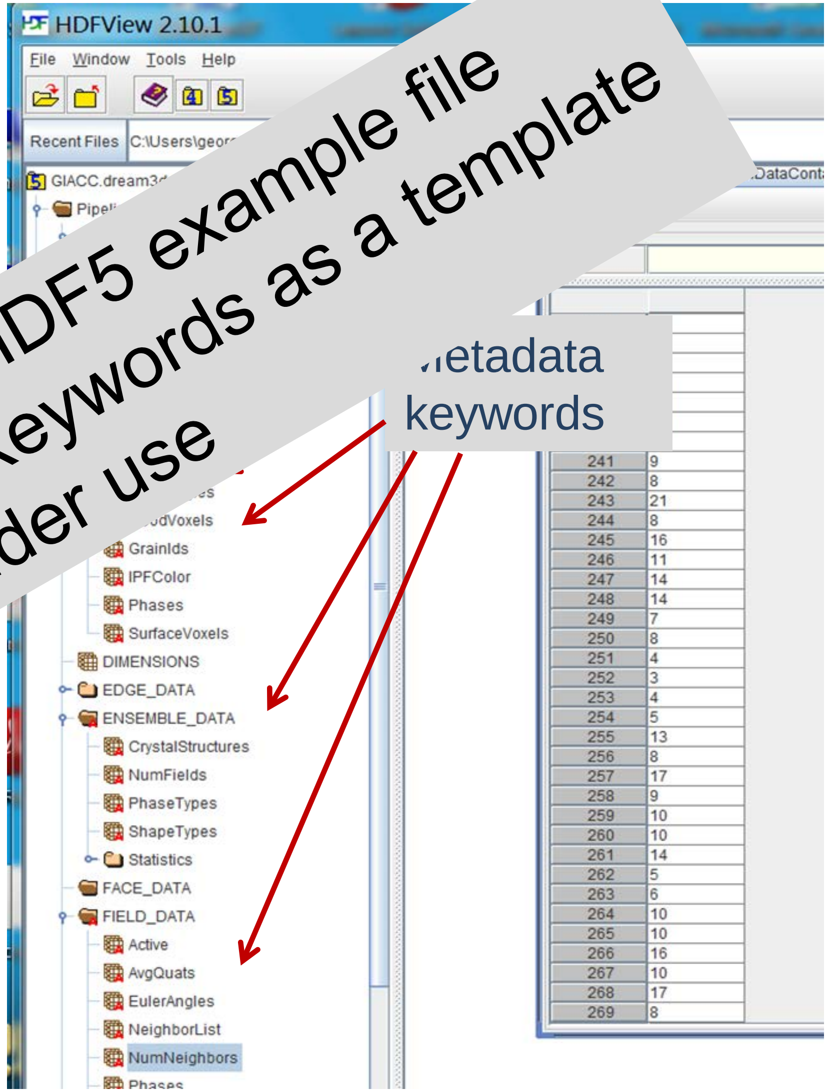
Possible approach
currently being investigated:

HDF5
„Hierarchical Data Format“

publication includes HDF5 example file
comprising the defined keywords as a template
for wider use

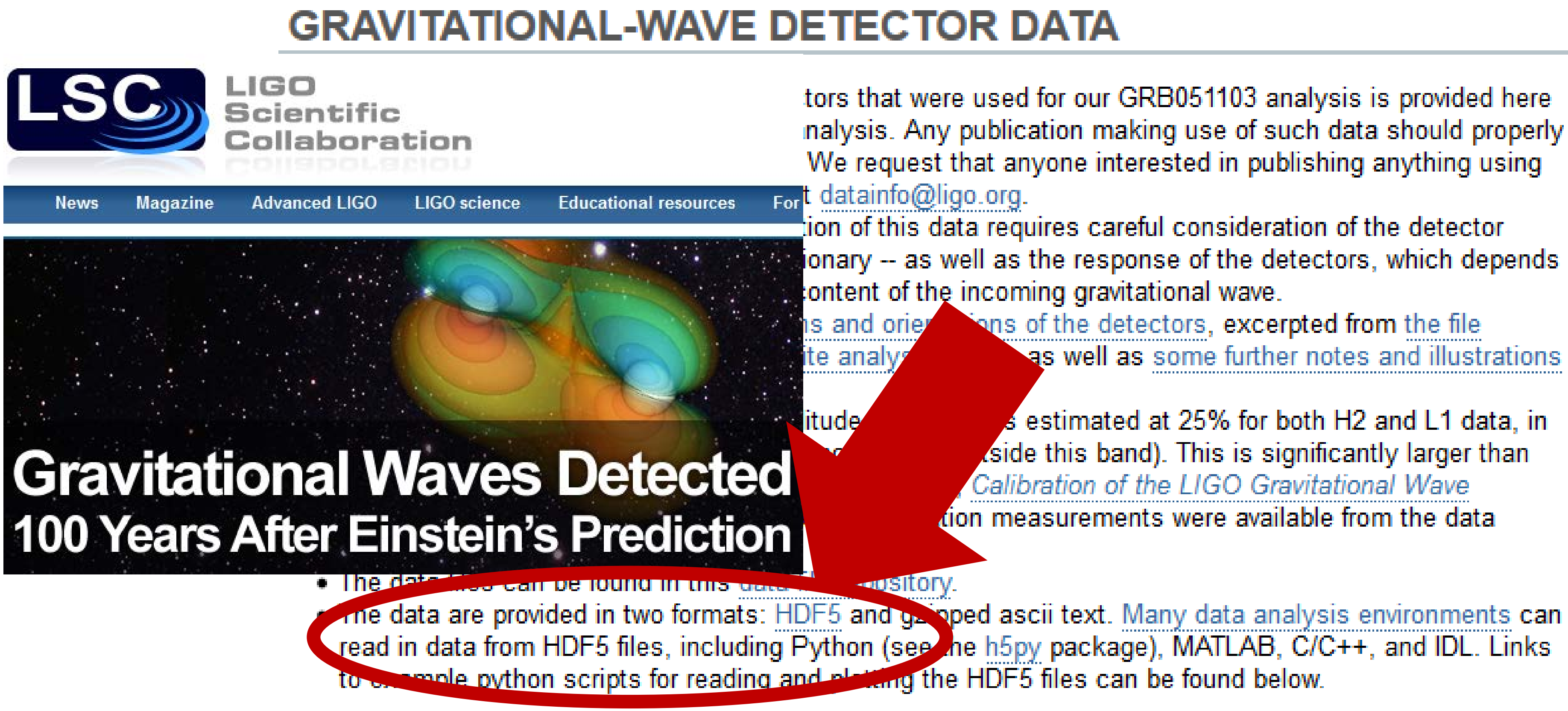


Hierarchical Data Structure
(Source: dream3d Manual)



metadata
keywords

☺ ☺ HDF5 and gravitational waves ☺ ☺

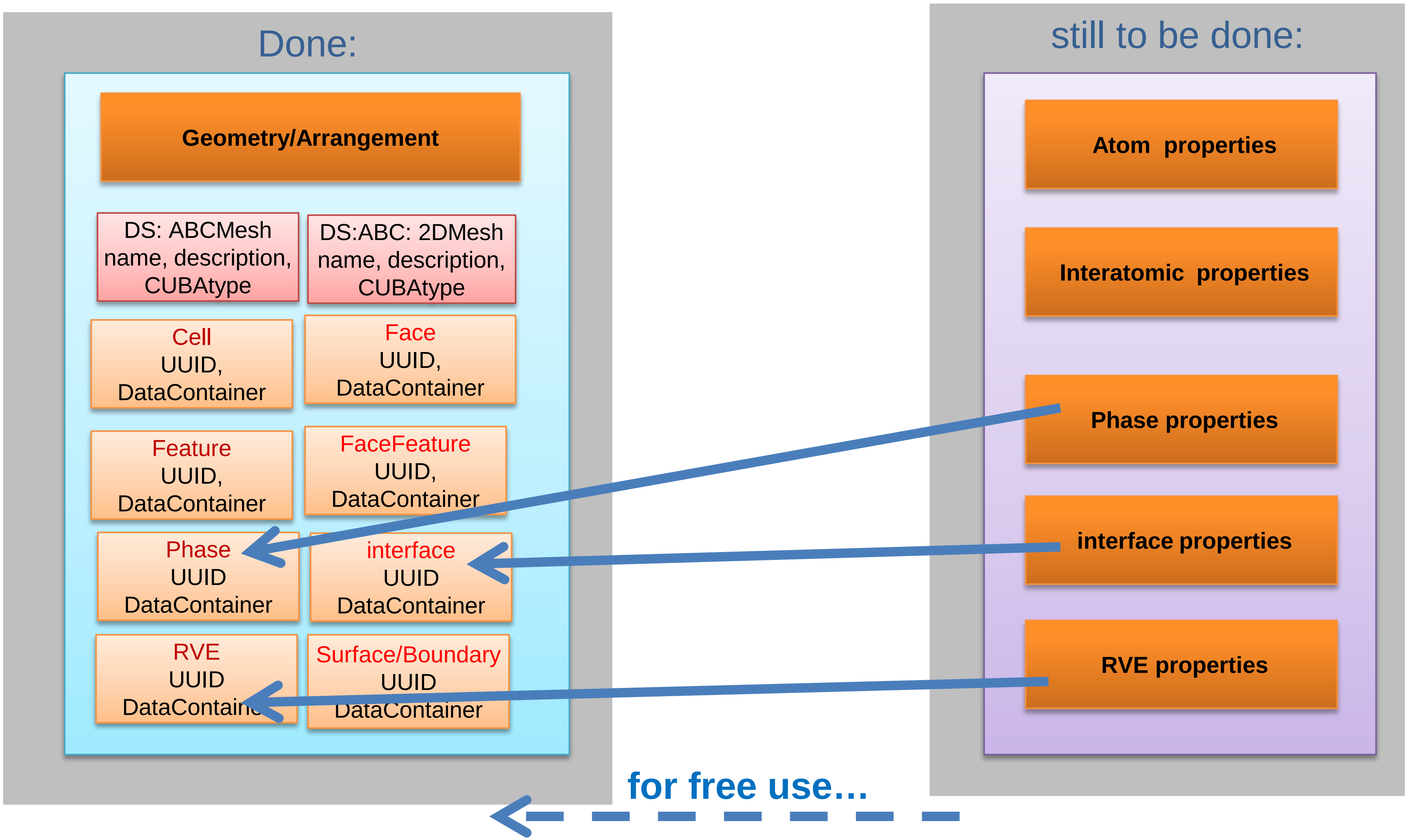


Length scales from light-years down to atto-meters
Time scales from billions of years to microseconds

EMMC

The European Materials Modeling Council

Next steps: keywords for properties



The European Materials Modeling Council

EMMC

first example: keywords for mechanical properties

An HDF5 file generated based on keywords from Abaqus-Python, showing Material Elasticity, Plasticity and Expansion, tables.

- mat.hdf5
  - Material
    - Mechanical
      - Elastic
        - elasticity
      - Expansion
        - expansion
      - Plastic
        - hardening

elasticity at /Material/Mechanical/Elastic/ [m...

Table — 0-based

Elasticity table

	0	1	2
0	93500.0	0.27	20.0
1	89250.0	0.27	100.0
2	85000.0	0.27	200.0
3	78200.0	0.27	300.0
4	66300.0	0.27	400.0
5	51000.0	0.27	500.0
6	40800.0	0.27	600.0
7	40800.0	0.27	700.0
8	0.0	0.0	0.0
9	0.0	0.0	0.0
10	0.0	0.0	0.0
11	0.0	0.0	0.0
12	0.0	0.0	0.0
13	0.0	0.0	0.0
14	0.0	0.0	0.0
15	0.0	0.0	0.0
16	0.0	0.0	0.0
17	0.0	0.0	0.0
18	0.0	0.0	0.0
19	0.0	0.0	0.0

expansion at /Material/Mechan...

Table — 0-based

Expansion table

	0	1
0	1.17E-5	20.0
1	1.17E-5	100.0
2	1.18E-5	200.0
3	1.22E-5	300.0
4	1.29E-5	400.0
5	1.32E-5	500.0
6	1.36E-5	600.0
7	1.38E-5	700.0
8	0.0	0.0
9	0.0	0.0
10	0.0	0.0
11	0.0	0.0
12	0.0	0.0
13	0.0	0.0
14	0.0	0.0
15	0.0	0.0
16	0.0	0.0
17	0.0	0.0
18	0.0	0.0
19	0.0	0.0

hardening at /Material/Mechanical/Plastic/ [...

Table — 0-bas

Plasticity table

	0	1	2
0	153.0	0.0	20.0
1	19278.0	0.25	20.0
2	153.0	0.0	100.0
3	18746.75	0.25	100.0
4	153.0	0.0	200.0
5	18215.5	0.25	200.0
6	129.2	0.0	300.0
7	17129.2	0.25	300.0
8	119.0	0.0	400.0
9	9681.5	0.25	400.0
10	85.0	0.0	500.0
11	1997.5	0.25	500.0
12	68.0	0.0	600.0
13	174.25	0.25	600.0
14	68.0	0.0	700.0
15	174.25	0.25	700.0
16	0.0	0.0	0.0
17	0.0	0.0	0.0
18	0.0	0.0	0.0

hardening (5904, 2)
32-bit floating-point, 40 x 3
Number of attributes = 1
title = Plasticity model

Work performed by Anshuman Singh

UPC BarcelonaTech

Keywords for Computational Implementaion

Chapter 3 Computational detail

3.1 Numerical Solver
3.2 Input you need to start computing
3.3 Initialisation of all quantities and parameters
3.4 Keywords describing “raw output” calculated by the model for the entities
3.5 Keywords for “post processed properties” calculated for the next model
3.6 Margin of error of property calculated under 3.5
3.7 Publication documenting the simulation

slide with courtesy of Pietro Asinari, Polytechnico di Torino

The European Materials Modeling Council

From metadata keywords to metadata schemata

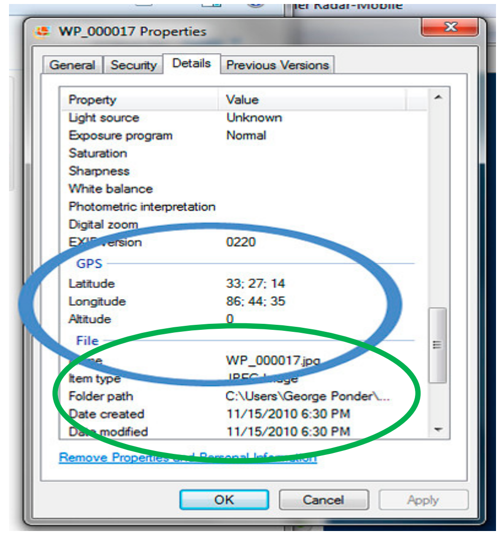
Tag	Value
Manufacturer	CASIO
Model	QV-4000
Orientation (rotation)	top - left [8 possible values[21]]
Software	Ver1.01
Date and Time	2003:08:11 16:45:32
YCbCr Positioning	centered
Compression	JPEG compression
x-Resolution	72.00
y-Resolution	72.00
Resolution Unit	Inch
Exposure Time	1/659 sec.
FNumber	f/4.0
ExposureProgram	Normal program
Exif Version	Exif Version 2.1
Date and Time (original)	2003:08:11 16:45:32
Date and Time (digitized)	2003:08:11 16:45:32
ComponentsConfiguration	Y Cb Cr -
Compressed Bits per Pixel	4.01
Exposure Bias	0.0
MaxApertureValue	2.00
Metering Mode	Pattern
Flash	Flash did not fire.
Focal Length	20.1 mm
MakerNote	432 bytes unknown data
FlashPixVersion	FlashPix Version 1.0
Color Space	sRGB
PixelXDimension	2240
PixelYDimension	1680
File Source	DSC
InteroperabilityIndex	R98
InteroperabilityVersion	(null)

Model

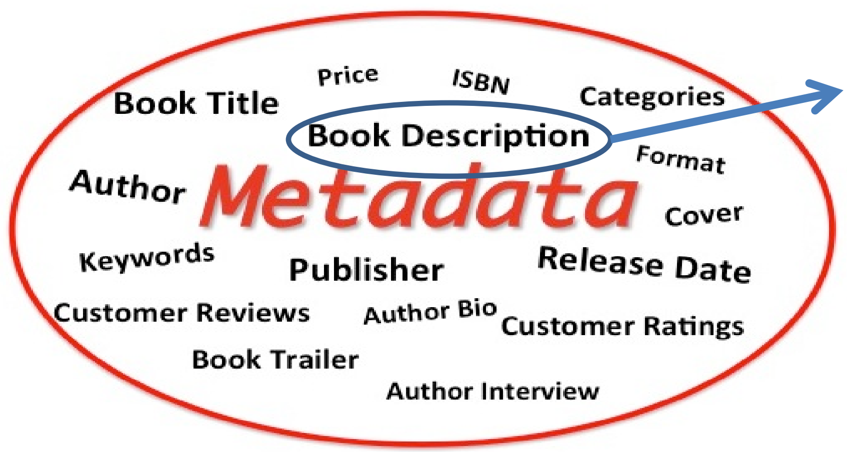
Model parameters

History

DataFile



and how does the picture look like ??



summarizes book content

From metadata keywords to metadata schemata

similar to books & jpeg pictures, each keyword describing a feature or an attribute benefits from further metadata information about e.g.

- data origin and data history
- models used for creation
- model parameters, software versions
- units and number formats
- creation date
- lower and upper limits of validity
- error estimates
- parent-child relations for hierarchical data
- ….

Need for formal metadata schemata

Open Simulation Platforms

Scope:

improve interoperability between the heterogeneous variety of commercial and academic modeling tools

Communication Standards

will be based on existing standards and solutions to the largest possible extend

will allow sequential i.e. file based interoperability

- Generic and structured list of metadata keywords
- Overall data structure for file based information exchange

Open Simulation Platform(s)

will allow strong coupling resp. interoperability in each time step

- Workflow tool(s) to orchestrate a number of different materials modeling tools
- Tools for distributed simulations
- *Long term*: Accounting schemes (not for the use of the platform but for the use of commercial codes used in the platform)

The European Materials Modeling Council

EMMC Working groups

1. Business Decision Support
2. Continuum Models
3. Discrete Models (including Electronic Models, Atomistic Models, Mesoscopic Models, Coupling and Linking)
4. Interoperability
5. Open Simulation Platform Concept
6. Materials Model Marketplace
7. Manufacturers
8. Software Owner
9. Translator
10. Validation

even this topic has only been partially addressed during this talk

For more:
visit www.emmc.info
and….

2nd International Workshop on Software Solutions for ICME

Home
About ICME
Committees
Invited Speakers NEW!
Program Overview NEW!
Supporting Organizations
Sponsorship & Exhibition
Format of the Workshop / Call for Contributions
Sessions List NEW!
Publications
Important Dates
Registration & Abst…
Submission
Location &…
Acco…
Secre…

Number o…

Welcome to Barcelona for the Second International Workshop on Software Solutions for Integrated Computational Materials Engineer…

ICME2016

It's too late ☹ : April 12th to 15th in Barcelona
But have a look at some of the presentations

http://congress.cimne.com/icme2016/

www.icmeg.info

Future events

- CECAM Workshop on Interoperability, Sept. 2016, Dublin, Ireland

Multiscale Simulation: from Materials through to Industrial Usage
Location : CECAM-IRL
September 5, 2016 - September 7, 2016

- Eoin O'Reilly
  Tyndall National Institute at University College Cork, Ireland
- Joan Adler
  Technion Haifa, Israel
- Heinz A. Preisig
  Norwegian University of Science and Technology, Chemical Engineering Department, Norway
- Shahriar Amini
  SINTEF Materials and Chemistry, Flow Technology Department, Norway

- 4th World Congress on ICME, May 2017, Ypsilanti (MI):