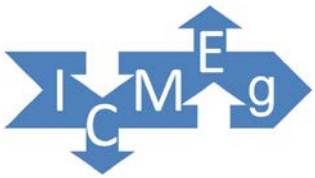

ICMEg

Final Report

(publishable summary)

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[1] **Nature:** R = Report, P = Prototype, D = Demonstrator, O = Other
Dissemination level PU = Public
PP = Restricted to other programme participants (including the Commission Services)
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C O N F I D E N T A L until public release by the ICMEg project consortium

Version	Date	Description
0.1	14.10.2016	First version by GJS
1.0	14.11.2016	Revised G.J.Schmitz
2.0	24.11.2016	Final version by G.J.Schmitz

1 Executive Summary

Materials are one of the Key Enabling Technologies for Europe allowing European products and industrial processes to become more competitive and sustainable, or even allowing for completely new, knowledge-based materials with tailored properties, new products and new processes. Modern materials research requires an integrated and multidisciplinary approach involving chemistry, physics, engineering sciences, as well as theoretical and computational modelling at different scales.

The present report summarizes the scopes and the output of the ICMEg ("Integrated Computational Materials Engineering expert group") coordination and support action, which was operational during the period 1.10.2013 until 30.9.2016 and aimed at an integrated approach toward solving modern materials engineering tasks.

The ICMEg objectives at a glance read as follows:

- Establishing a network of stakeholders in the area of ICME
- Organisation of two International Workshops with a minimum of 100 participants
- Foundation of an Association of Software providers for ICME
- Compilation of a „Handbook of Software Solutions for ICME"
- Elaboration of proposals for standards for information exchange in ICME

Besides successfully establishing a vital network of about 200 stakeholders in the area of interoperability and ICME around the globe, organising two well attended "International Workshops on Software Solutions for ICME" in Rolduc (2014) and in Barcelona (2016), founding of the ICMEg e.V. association in 2014, and publishing the „Handbook of Software Solutions for ICME" the major output of the ICMEg project relates to proposing communication standards to increase interoperability.

The essence of the proposed communication standard, being fully documented in related publications, is based on a digital description of a materials state being stored in a hierarchical manner in a suitable file format like HDF5 and on a limited number of canonical descriptors naming the different datasets within the file. Different types of models then can evolve this state or extract properties from it in a flowchart typeof configuration.

This modelling strategy will not only lead to the development of new materials but also to the improvement of existing materials and their processing thus fostering European industry in a number of sectors.

2 Project Context and Main Objectives

Materials are one of the Key Enabling Technologies for Europe allowing European products and industrial processes to become more competitive and sustainable, or even allowing for completely new, knowledge-based materials with tailored properties, new products and new processes. Modern materials research requires an integrated and multidisciplinary approach involving chemistry, physics, engineering sciences, as well as theoretical and computational modelling at different scales.

A fundamental requirement to meet the ambitious objective of designing materials for specific products resp. components is an integrative and interdisciplinary computational description of the history of the component starting from the sound initial condition of a homogeneous, isotropic and stress free melt resp. gas phase and continuing via subsequent processing steps and eventually ending in the description of failure onset under operational load.

Most relevant current research on the rational design of functional materials presently is performed in the areas of 3D-Materials Science ("3D-MS"), by the Materials Genome Initiative "MGI" and in Integrated Computational Materials Engineering "ICME", all of which are mutually strongly interrelated. While MGI focuses on the properties of new phases and 3D-MS aims at experimental and numerical descriptions of materials in 3 dimensions, ICME comprises all these aspects and even further also includes materials processing.

Focus of ICME is on engineering the properties of the component as a function of the local properties of the material inside the component by multiscale modelling approaches even extending across the manufacturing cycle. These properties experience an evolution and depend on the entire process history as well as on shape of the component and on the actual alloy composition. The realization of such a scale and process spanning modelling scenario to be available for generation of material-by-design is one of the key objectives of Integrated Computational Materials Engineering ("ICME").

The ultimate vision of the ICMEg – "Integrated Computational Materials Engineering expert group" is a new strategy of materials and process development, where a variety of academic and commercial simulation tools – present and future – can be easily combined across different process steps and bridging several length scales in a

"plug&play" type architecture being based on an object oriented, standardized information exchange.

Scope of the ICMEg coordination and support action is to establish a network of stakeholders aiming at the creation of an open, global standard for information exchange between the heterogeneous variety of commercial and academic simulation tools.

The Mission of ICMEg is to

a) establish and to maintain a network of contacts to

- simulation software providers around the world
- governmental and international standardization authorities
- ICME type users of simulation software
- different associations in the area of materials and processing
- academic developers of simulation software

b) stimulate knowledge sharing in the field of multiscale materials design

c) define - in discussions with all interested stakeholders and volunteers - an ICME language in form of an open and standardized communication protocol

d) communicate this standard worldwide to make it widely accepted

e) discuss - with all the interested stakeholders and volunteers - and to decide about future amendments to the initial standard

f) establish a legal body (not for profit) being open to all interested stakeholders for a sustainable further development

The work of ICMEg to realize both its vision and its mission is to create a global network of all stakeholders in the area of ICME software and users by

a) identifying all actors in the field of ICME related simulations

b) creating an inventory of these stakeholders

c) networking of all identified stakeholders in two international conferences

d) composing a directory of all available simulation approaches

e) proposing a common language for standardized information exchange

f) secure sustainable further the common language by foundation of an international association

The target of the project is the "creation of an open, global standard for information exchange between a heterogeneous variety of commercial and academic simulation tools covering multiple length and time-scales". Multi-scale in this context covers electronic, atomistic, mesoscopic and continuum models.

To secure a sustainable development of the standard formulations being developed the foundation of an association is intended. The project public website is www.icmeg.eu. It will be discontinued after the end of the project in favour of a more comprehensive, future "one-stop"-site being operated by the European Materials Modelling Council (EMMC-CSA project; www.emmc.info). Relevant information content will be moved to this new site.

The ICMEg objectives at a glance read as follows:

- Establishing a network of stakeholders in the area of ICME
- Organisation of two International Workshops with a minimum of 100 participants each
- Foundation of an Association of Software providers for ICME
- Compilation of a „Handbook of Software Solutions for ICME"
- elaboration of proposals for standards for information exchange in ICME

The list of ICMEg project partners reads as follows:

No	Name	Short name	Country
1	ACCESS e.V.	ACCESS e.V.	Germany
2	K&S GMBH PROJEKTMANAGEMENT	K&S	Germany
3	E-XSTREAM ENGINEERING SA	e-Xstream	Belgium
4	FUNDACION IMDEA MATERIALES	IMDEA	Spain
5	THERMO-CALC SOFTWARE AB	Thermo-Calc	Sweden
6	STICHTING MATERIALS INNOVATION INSTITUTE (M2I)	M2i	Netherlands
7	CESKE VYSOKE UCENI TECHNICKE V PRAZE	CVUT	Czech Republic
8	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	RWTH	Germany
9	CENTRE INTERNACIONAL DE METODES NUMERICS EN ENGINYERIA	CIMNE	Spain
10	SIMUFACT ENGINEERING GMBH	simufact	Germany
11	KUNGLIGA TEKNISKA HOEGSKOLAN	KTH	Sweden

3 Scientific and Technological Results

The work performed by the ICMEg partners at the beginning essentially focused on networking stakeholders originating from different areas and forming a coherent community, on creating global awareness of the “plug&play vision for ICME” and on identifying possible standardisation approaches improving the interoperability between the large and heterogeneous variety of simulation tools. Major activities in this context have been the successful organisation of the two "International Workshops on Software Solutions for ICME" (www.icmeg.info). A survey of these tools has been created and eventually was published as a “Handbook of Software Solutions for ICME” [Schmitz/Prahl 2016]. This book will also serve as a tutorial for future ICME engineers and scientists. Based on the feedback from the community a scheme for a standardized, file based information exchange has been proposed. In summary, the ICMEg consortium made following achievements all being fully detailed in the respective deliverables and a number of related publications:

- Networking of stakeholders in ICME especially during the two International Workshops on Software Solutions for ICME
- Foundation of ICMEg e.V.
- Publication of a “Handbook of Software Solutions for ICME”
- Proposal for an approach towards a communication standard for file based interoperability
- identification and assessment of the HDF5 file format as a suitable candidate for interoperability
- elaboration and publication of a metadata description for microstructures
- Numerous publications in journals, social media, Wikipedia etc.

The ICMEg project operated as a CSA. In the following sections the different coordination actions will be presented related to

identification of the field/creation of a network

collecting input from the field

digestion of the feedback by the ICMEg consortium

presentation of results to the field

agreement to the results by the field

3.1 Creating a network

3.1.1 Identification of the field

In order to structure the field of stakeholders in ICME, different types of stakeholders were identified and classified as follows:

a) users of modelling tools
- academic users
- industrial users /manufacturers

b) developers/providers of modelling tools
- academic developers of modelling tools
- providers of open source/open access codes
- commercial providers of modelling tools
    - small enterprises with very dedicated solutions
    - large enterprises with proprietary platform type approaches

c) governmental bodies
- funding agencies
- standardisation authorities

A number of measures were taken to identify the actual people representing these different stakeholders. These include e.g. web search for software providers, mailing activities through large mailing lists (EU, TMS, DGM, news-letters of e.g. European Community of Computational Mechanics), mailings to ICMEg partners mailing lists, personal contacts of the ICMEg partners, the ICMEg website and its forum, specifically developed questionnaires, a Wikipedia entry, entries in social media, numerous presentations on workshops an conferences, to name the most relevant.

In summary, the networking activities being performed by the ICMEg consortium have been manifold and very effective. Almost from scratch a network comprising about 700 stakeholders (people and software tools) from different communities of stakeholders like manufacturers, software owners, academic software providers and others could be generated. This network also encompasses and integrates people from different scientific communities like small scale modellers (electronic, atomistic, mesoscopic), the thermodynamic modelling community, continuum modellers both at the scale of the microstructure and at the process scale, governmental bodies, industrial users, and commercial software providers.

3.1.2 International Workshops

The community being identified as described above was then brought into first contact and then further networked in two “International Workshops on Software Solutions for ICME”.

Scopes of the “1st International Workshops on Software Solutions for ICME” being held in Rolduc/Aachen in June 2014 were

- to convene and to network software providers/developers – both commercial and academic – being interested in providing their solutions to the growing ICME community
- to create awareness about solutions and models presently being available along all processing steps and across all scales
- to generate a comprehensive overview and a thematically structured inventory of such software solutions
- to identify options emerging for individual codes by coupling them to other models/tools
- to identify needs for model functionalities up-stream the process chains on the basis of requirements by models downstream the value chain
- to discuss necessary steps to create a global and open standard for information exchange between different models/tools
- to outline a first concept for such a standard

This 1st workshop attracted more than 160 participants from 24 countries in 4 continents. About 40% of the attendees originated from academia. A large number of software companies resp. software tools was represented either in person or via different contributions like e.g. metatech, msc-software, gtt-technologies, Dassault Systemes, Sente Software, Thermo-Calc Software, e-xstream, Quantum Espresso, MatCalc, Phase 3D, Materials Design , Accelrys, esi calcom, DAMASK, MICRESS, simufact, OOF, ÅF, Materials Ressources, Enginsoft, simpleware, Itochu-Solutions, Magma, SCM, Homat, Geonx and others[1st_ICMEg].

The 2nd International Workshop on Software Solutions for Integrated Computational Materials Engineering (ICME 2016) took place on 12-15 April 2016 in Barcelona, Spain. The objectives of ICME 2016 were to re-convene and to foster the network of software providers/developers –both commercial and academic-- being interested in providing their solutions to the growing ICME community, to discuss the actual status

and further necessary steps for a global and open standard for information exchange between different models/tools in ICME, to create awareness about existing and newly emerging models and solutions along all the process steps and across all the scales (e/a/m/c), to identify options and needs for coupling of individual codes, and to identify needs for model functionalities up-stream the process chains on the basis of requirements by models downstream the value chain.

The 2nd workshop in April 2016 in Barcelona attracted more than 110 participants from 24 countries in all 5 continents. The major participating nations were Germany (29), USA (16), Spain (14), Japan (11), and the UK (6). 40% of the participants originated from academia.13 software companies and 9 manufacturing industry as well as several governmental institutions were represented.

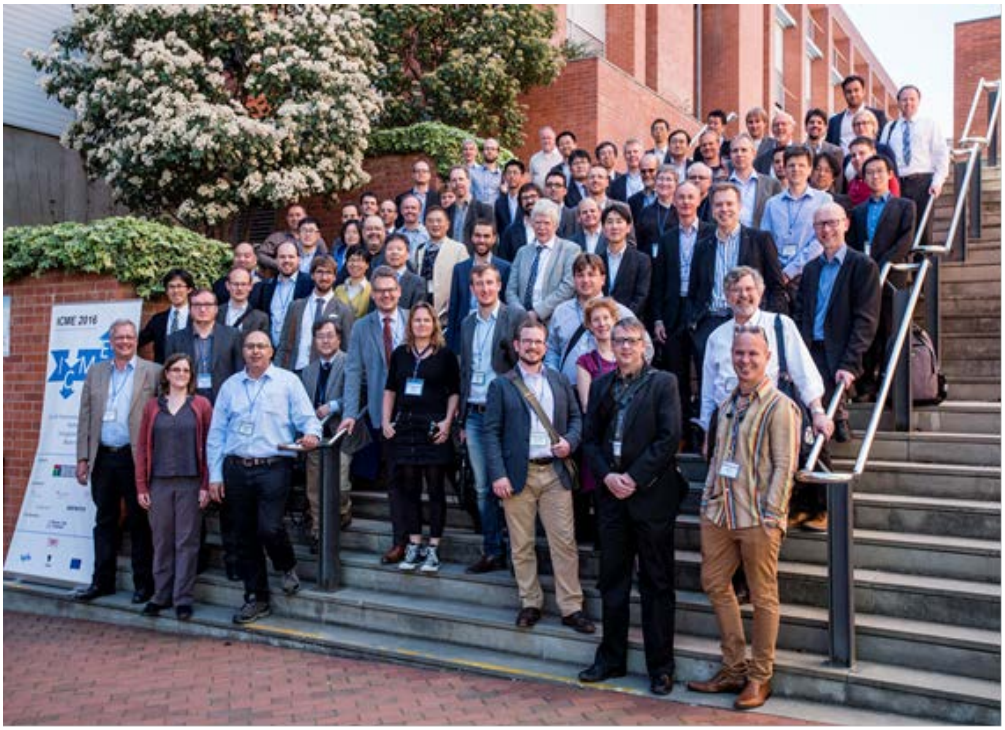
At the end of the ICMEg project (status Sept 2016) it can be stated that a community network of about 200 people around the world working on different aspects of interoperability is clearly emerging. The current activities of this community around the world can broadly be assessed as follows:

The US is strong in the “big data” type approaches: collecting and curation of data, generation of data and metadata schemes, maintenance of repositories, databases etc.

The EU is strong in interoperability aspects of different simulation tools (e.g. CUDS, CUBA, metadata keywords, HDF5..).

Japan in few areas is strong in first applications for complex materials and processes disregarding any specific metadata approaches.

Participants of the 1st ICMEg workshop in June 2014 in Rolduc Abbey near Aachen



Participants of the 2nd ICMEg workshop in April 2016 in Barcelona

3.2 Input from the field and its digestion

3.2.1 Chronological Overview

The following section provides a short chronological overview of the major input the received from the network by the ICMEg project during its 3 years of operation.

In December 2013 the ICMEg partners received first hints on HDF5 as an interesting approach towards interoperability during a meeting of Germany‘s Computational Materials Science expert group.

In June 2014, during the 1st Workshop, needs for a hierarchical data structure comprising both a spatially resolved and simultaneously also a statistical description of data were identified. Especially for microstructures a spatially resolved description was identified as a mandatory basis for a sound physics description of phenomena.

In October 2014, during a meeting of five European projects on simulation platforms in Darmstadt (5+1), the needs and benefits of a common list of keywords bridging across these different platforms were identified. The need for metadata schema was raised.

In November 2014, a publication on „Dream.3D“ [Dream3D] describes the first customisation of the HDF5 file format to the purposes of the materials modelling community.

In January 2015, a first possible structure of a metadata keyword list was discussed jointly with EU project Simphony.

In February 2015, during an EMMC workshop in Brussels, HDF5 was proposed as a basis for a possible communication standard in a first short presentation along with a proposal for a first draft structure of a metadata keyword list. A number of other EU projects already using HDF5 were identified, and a positive general feedback on HDF5 was received.

In February 2015 the HDF5 idea was further discussed in Tokyo during a workshop of the Structural Materials for Innovation Initiative (SM4I) of the Japanese government. Several institutions in Japan have ideas on HDF5 or even already use it.

In March 2015, the HDF5 based „Common Data Format CDF“ was internally circulated as a deliverable by EU-project DEEPEN. Intense discussions within ICMEg about pro‘s, con‘s and potential no-go‘s for HDF5 took place.

Also in March 2015, the HDF5 approach was discussed during the TMS annual meeting with several representatives from user industry and from software owners all being positive about HDF5. During a meeting with the developers of Dream3D joint activities and requirements in establishing HDF5 as a possible future standard were discussed.

In April 2015 keywords of the MMP and DEEPEN projects were integrated into a preliminary metadata keyword list. The need for a structured procedure for the compilation of a keyword list was identified.

In May 2015, during a meeting of five European projects on simulation platforms in Finland (5+1) metadata keywords, possible metadata schemata, and metadata attributes were intensely discussed.

Also in May 2015, during the 3rd ICME World Congress in Colorado, the HDF5 approach was discussed with representatives from user industry, software owners and experimentalists all being positive about HDF5. First ideas about a minimum „canonical set of keywords“ were raised by NIST and ICMEg during this congress.

In November 2015, a first public presentation of metadata descriptors during the EMMC-ICMEg Workshop in Brussels received positive feedback, and raised discussions about needs/options/benefits of specifying further attributes.

In December 2015, a publication on a full metadata description of microstructures has been submitted upon invitation by NIMS to a special issue on „Materials Genome” of the open access journal „Science and Technology of Advanced Materials“ [STAM]

In January 2016, the revised version of the STAM publication profited from including multiple comments by the referee, an obvious expert in ontology.

In February 2016, both the HDF5 file format and the metadata descriptors were presented within an invited presentation at the TMS annual meeting in Nashville. Hints for the needs of attributes especially w.r.t uncertainty propagation were raised. Also the need for statistical descriptions/statistical representations was raised in the discussions.

In April 2016, during the 2nd International ICMEg Workshop, HDF5 is present in many presentations. Metadata, metadata schemata, data curating and others are increasingly in focus. Hints are received for the need of recording data history in metadata attributes in view of interoperability.

In July 2016, the metadata descriptors [STAM] are eventually published online and received about 600 views within the first month

In August 2016, a positive feedback on the metadata descriptors as detailed in the STAM publication was received from ASM. ASM International is quite interested in the development and dissemination of open materials data schema, and would welcome any opportunity to participate in collaborative efforts with ICMEg.

Also in August 2016, during an international data format workshop for atomistics (simulation/experiment) organised by MPIE Düsseldorf, HDF5 was a central topic playing a role in almost any presentation.

The community feedback and related actions by the ICMEg consortium can be summarized as follows:

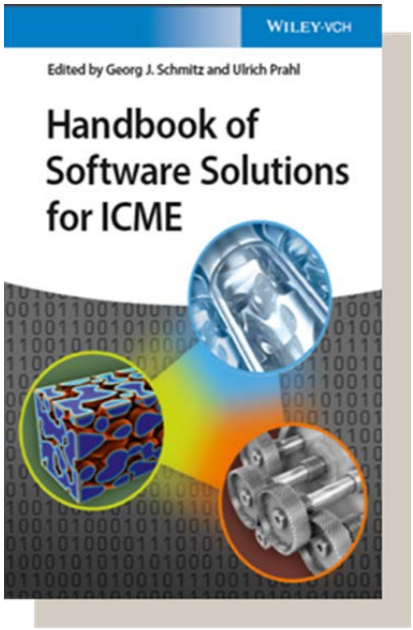
Community feedback	related ICMEg actions
Need for establishing a community	Community established (approx. 200)
Need for an overview of existing solutions	Compiled „Handbook of Software Solutions“
Need for statistical AND spatial data	proposed HDF5
Need for hierachical materials description	proposed HDF5
Strong, positive feedback on HDF5	further elaborated/ promoted HDF5 approach
need for keyword scheme raised	Proposed metadata descriptors
wish for Interoperability	Proposed FlowChart scenario
enable handling of uncertainity propagation	Compiled attributes to metadata descriptors
alllow to record data history	Compiled attributes to metadata descriptors

3.2.2 Handbook of Software Solutions for ICME

Quite a substantial support was received from the community when composing the "Handbook of Software Solutions for ICME". 93 authors from 14 countries compiled more than 600 pages. Hundreds of simulation codes have been identified and were thematically structured. Along with introductions to a number of different topics, this community effort allowed to define the current state of the art in materials modelling, to summarize available resources, and to provide a holistic view for future scientist and engineers being interested in:

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

The book has been officially released by Wiley VCH (Weinheim) on Nov. 9th 2016 (ISBN 978-3-527-33902-0)



Handbook of Software Solutions for ICME
being edited during the course of the
ICMEg project
Editors G.J.Schmitz and U.Prahl
ISBN 978-3-527-33902-0

3.3 Proposal for standards

Towards the formulation of a global standard several constraints, conditions and requirements could be identified by interactions with the network. Three important ingredients of a possible future standard for the description of microstructures could be identified: a hierarchical schema, a defined file format, and a keyword ontology. A most interesting approach meeting all these constraints and being proposed by the community is based on an HDF5 type data structure to describe the state of a material. This approach - along with identified approaches on a unified nomenclature for microstructures and thermodynamic data - have been further elaborated by specifying necessary metadata descriptors [STAM]. The resulting standard has been discussed with the stakeholders and volunteers in a number of workshops and eventually was challenged and refined on the basis of specifically designed sand-box scenarios being of commercial interest.

3.3.1 HDF5 file formats

Materials in general reveal a hierarchical structure ranging from atoms and molecules to clusters, grains, phases and eventually to polycrystalline, multicomponent and multiphase engineering materials. Thus there is strong a need for a hierarchical description comprising both spatially resolved information about the microstructure and also statistical information like average phase fractions, grain size distributions and many others. Such data may originate from a large variety of simulations tools or from experiments. A strong benefit is to be expected from integration of such data into a coherent, hierarchical data structure. One pragmatic approach towards interoperability is to specify a common data file format. HDF5 has been shown to have great potential for evolving into such a standard, since HDF5 can be used to describe continuum data, discrete atomistic data, and also statistical data.

In short HDF5 not only is a data format, but also an open and freely available suite of software tools for handling respective HDF5 files. It provides:

- A versatile data model that can represent very complex data objects and a wide variety of metadata.
- A completely portable file format with no limit on the number or size of data objects in the collection.
- A software library that runs on a range of computational platforms, from laptops to massively parallel systems, and implements a high-level API with C, C++, Fortran 90, and Java interfaces.

- A rich set of integrated performance features that allow for access time and storage space optimizations.
- Tools and applications for managing, manipulating, viewing, and analyzing the data in the collection.

HDF5 is best practice in numerous applications like geophysics, earth observation, medicine, particle physics, astronomy, biology, financial engineering, computation, mechanical engineering, and electronics to name only a few. HDF5 is an established *standard data format* in computational fluid dynamics.

HDF5 as a general purpose data scheme reveals no inherent keyword ontology. However, keywords used in DREAM.3D [Dream.3D], which defines a hierarchical schema and exploits HDF5 to store its data, triggered a first customization of HDF5 keywords for the materials research and engineering community. Besides for communication with Dream3D, the use of HDF5 files can further extended for mutual information exchange between any pair of different tools.

One method for submitting information is the use of HDF5 files/data containers already matching both the format and the keyword nomenclature as used by Dream3D (.dream3d). There is, however, also a strong interest and benefit for a number of further tools in providing and retrieving 3D-microstructure information. Examples are reconstructions of 3D experimental microstructures or synthetic microstructures as input for the simulation of the further evolution of such structures.

With a view to future file-based plug&play-type interoperability among a range of experimental datasets, numerical simulations describing microstructures, software tools extracting properties from such structures, a well-defined structure of such files as available in HDF5 and their defined nomenclature are most beneficial for all stakeholders. Information from any simulation tool or experimental procedure can easily be integrated into the hierarchical framework as the structure is separate from the tools themselves. This has been successfully demonstrated resp. discussed for the examples MICRESS, DAMASK and Abaqus [HDF5]

In the long term, 4D data, i.e. time-dependent microstructures, may be thought of as a sequence of HDF5 files. All spatially resolved data could be described in .vtk format only. However, the description of per phase data, RVE statistics, RVE effective properties and others, requires an additional data structure as provided by HDF5 (with vtk resembling a subset). A description of workflows and the temporal evolution of materi-

als will require combinations of HDF5 (and other data and file types) and is probably achievable on the basis of xdmf, with HDF5 then a subset.

The hierarchy of HDF5 presents as a directory-type structure which is exploitable using the free tool HDF5view [HDFview]. The name(s) of the individual directory entries represent keywords, which have to be specified. Specification of suitable set of metadata keywords is not an easy task since even the keywords used in some individual applications are “moving targets”. Creating a generic keyword ontology within an open source development like Dream3D seems quite difficult as most of the actors typically contribute solutions focused on their topics of interest. A respective list of keywords resp. descriptors thus has been elaborated and was proposed by the ICMEg project and is summarized in the following section. An important feature of a well-defined keyword list – besides indicating the availability of specific information in a file – is the identification of *information not being available* in case a particular keyword is not specified.

3.3.2 Metadata Descriptors

In view of an improved interoperability of a host of different software tools it is highly desirable to establish a standardized nomenclature and methodology for the exchange of data based on a comprehensive system of metadata descriptors for the description of a 3D microstructure. The descriptors - as detailed in [STAM] - are limited to a mere geometric description of a static microstructure and have to be complemented by further descriptors e.g. for properties, for numerical representations, for kinetic data and others in the future. The proposed descriptors are meant to be independent of any specific numerical representation and may serve as a first basis for standardization. They will simplify the data exchange between different numerical models, as well as promote the integration of experimental data into numerical models of microstructures.

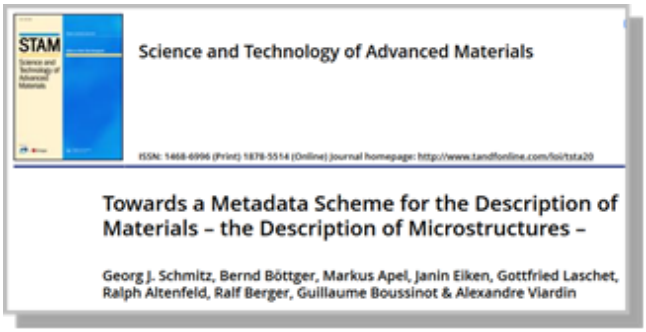
The following section summarizes descriptors allowing the mere geometric description of any static microstructure, their comprehensive list being fully detailed in [STAM]. Numerous early efforts to generate such a list by simply collecting descriptors/keywords from a variety of different codes and trying to harmonize them into a unique set of descriptors all failed. This is essentially due to the fact that many descriptors/keywords can be derived from other descriptors/keywords and the amount of possible descriptors thus tends to infinity. Thus the need for a basic set of descriptors was identified, being minimal in their number, but allowing deriving anything which is needed by suitable relations between the basic descriptors. The major concepts being followed to generate a descriptor list are:

- Starting from the most generic notion of a material as being an arrangement of atoms in space
- Considering a dimensional hierarchy of 3D volumes, 2D surfaces, 1D lines and 0D points
- Considering a hierarchy in terms of data resolution with the highest resolution data (the “Field”) being the basis for lower resolution and averaged data for Features, for Ensembles and eventually for statistical data of the full RVE
- Proposing a scheme to derive relations between descriptors by different mathematical operations
- Securing that the selected descriptors are independent of any numerical representation in view of interoperability with experimental data and with available analytic solutions
- Attempting to specify descriptors which hold for both continuum and discrete models i.e. allowing the description of discrete features in the volume and also of continuous fields
- Attempting to specify descriptors that may even be applicable to electronic, atomistic and mesoscopic models.

A fundamental concept of the description of the microstructure representing the material state by a minimum set of “canonical descriptors” with the basic descriptors being Volume, Surface, Composition, Orientation, Position, Centroid, ReferenceFrame to name the most relevant. These basic descriptors in combination with the hierarchical data structure allow deriving a host of further parameters like the phase-fraction as the volume of the phase divided by the volume of the RVE. The strength of this approach is fully detailed in [STAM].

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

	http://www.tandfonline.com/doi/pdf/10.1080/14686996.2016.1194166?needAccess=true

In summary, the proposed metadata keyword structure describes

- a volume
- distinct features in the volume like grains, precipitates, defects
- ensembles of features in a volume e.g. all grains of a specific phase
- continuous fields e.g. composition, defects, stresses/strains
- interfaces
  - 2D grain resp. phase boundaries
  - 1D triple lines
  - 0 D quadruple junctions
- surfaces/boundaries

The proposed metadata keyword structure accounts for

- the hierarchical structure of materials
- possible future amendments

The metadata structure proposed in [STAM] allows assigning

- attributes to ensembles/phases e.g. their mechanical properties
- attributes to features like dislocation densities,
- attributes to interfaces like interfacial energies or interfacial mobilities
- conditions on boundaries e.g. for temperature and/or composition, for flow velocity and others.

The proposed metadata keyword structure is further independent of any models and numerics

- in view of interoperability with experimental data
- in view of possibly available analytic solutions

The proposed metadata keyword structure eventually may even be applicable to e/a/m models. This applicability to discrete models – after some minor amendments like the inclusion of a descriptor “Charge” - could be verified to a large extend as depicted in the following section.

3.3.3 Challenging the proposed approach

Procedures to challenge, to prove and validate the applicability of the developed approaches had to be specified. Multiple approaches have been taken towards these objectives like the specification of sandbox scenarios, the application of Moda Schemes [MODA], validation based on experience, validation based on applications of software codes available to the ICMEg partners and more.

In the end the validation of the metadata description was limited to the different types of physics equations being listed in the [RoMM]. These physics equations and materials relations essentially act on the material state as depicted in section 3.3.5.

A fundamental requirement for validation and a validation procedure thus is that any symbol appearing in the equations has to be mirrored into a descriptor within the metadata namespace. It should be noted, however, that this descriptor may – and in general will be - be derived from the canonical set of descriptors outlined in section 3.3.2

A metadata namespace thus can be considered as validated for a model in case that for any symbol in the PE of the model a descriptor is available – or can be derived - within the namespace. Any physics equation is based on mathematics and in this context it seems worthy to stress that mathematics is an established – and probably the most accurate -metadata description

In this spirit, the ICMEg namespace has been validated for large number of models as listed in the [RoMM] comprising both discrete electronic/atomistic/mesoscopic and also continuum models.

3.3.4 Attributes to Metadata descriptors

Similar to books & jpeg pictures, each array in the materials state description being identified by its descriptor benefits from further metadata information. For each of the descriptors being depicted in section 3.3.2 the respective attributes may comprise:

- data domain, data origin and data history
- units, symbols and number formats
- models, model parameters, software versions
- data statistics
- parent-child attributes for hierarchical data

A comprehensive list of such attributes is under preparation and scheduled for publication. In the following a first listing of possible and meaningful attributes is compiled.

data domain, data origin and data history

The origin of the data being stored in the respective array can be classified by a *DataOriginID* which may take different values depending whether the data are of synthetic, experimental, simulation or theoretic origin. Each of these data sources can be further classified by own IDs like e.g. *SyntheticID, ExperimentID, SimulationID, TheoryID*. Respective ID lists still have to be compiled. A *SourceListID* may relate to a list of references and other sources of information documenting the origin and nature of the data being used. This list may accompany the overall data set and may also include e.g. DOI numbers of external literature references.

Especially in simulation chains, where in many cases only subsets of the overall state description will be updated, it is most important to control the *DataVersion*. This *DataVersion* is best organized by a *TimeStamp*, including a *DateStamp*. These stamps can indicate the *TimeFirst* and the *TimeLast* i.e. the date and time of the first creation and of the last modification of the dataset. In a *DataLog* the history of the data for each array can be tracked by recording *TimeStamps* and activities acting on that particular data set resp. data array.

data types, symbols and units

Most important attributes of any array are the *DataType* (e.g. integer, real, complex, character) and the *ArraySize* (e.g. 3x10 for the description of positions (vectors of dimension 3) of 10 objects). Eventually a short Description of the data content (which could read “positions of objects” for this example) is most helpful for future metadata schemata.

Physics entities do have units. These units by default should be recorded in SI, i.e. m (meter), g (grams), s (seconds), A (Ampere), K (Kelvin) which define the *UnitName*. A *ScalingFactor* or in a synonymous way a *ScalingName* can be added to account for very large or very small values of the respective units like 10^{-9} = nano, 10^{-6} =micro, 10^{-3} = milli, 10^{3}=kilo etc.This will basically allow assigning independent units to each of the datasets i.e. each array. However, this also implies that units have to be carefully checked by the different tools operating on the state and should be harmonized across all arrays describing the materials state.

In view of aligning with existing mathematical formulations/notations of physics equations it seems beneficial to consider also the symbol being commonly used for the entity being described by the descriptor and adding it as a character string value to the metadata. An example would be Attribute=Symbol, Value= "ρ_m" for the descriptor of a mass density, where mass is indicated by the subscript m in order to distinguish from e.g. NumberDensity or ChargeDensity. Adaptation of the LaTex conventions for symbols and their ASCII representation seems meaningful in this context.

models used for creation, model parameters, software versions

In many case it may be meaningful to define model classes and models typically acting on a specific array in the state description. Such *ModelClasses* may read electronic, atomistic, mesoscopic, continuum, analytic, or eventually unknown

Eventually a *SoftwareToolLabel* may identify a specific software tool from a list. This list may be based on a first compilation of software tools being published in the Handbook of Software Solutions for ICME [Schmitz/Prahl 2016]. This list will be further be maintained by the European Materials Modelling Council [EMMC].

data statistics

A number of statistical and other values are most beneficial for evaluation of data, for check of data consistency and especially for error propagation. *LowerBound* and *UpperBound* are the minimum and maximum allowable values for the entries in the individual arrays. Examples are phase-fractions which have to take values between 0 and 1 or concentrations of alloy elements which have to be between 0 and 100(%). Other interesting statistical values for many arrays are *AverageValue*, *MeanValue*, *RelativeError*. The values for these attributes are most important for any future efforts to track error propagation in modelling chains. Existing standard formulations for statistical data as compiled in the ISO 3534-1:2006(en) standard on "Statistics — Vocabulary and symbols" provide a valuable and sound basis here.

parent-child attributes for hierarchical data

Parent and *Child* attributes allow identifying the location of the array in an overall hierarchical data structure disregarding in which way it is actually represented. In the picture of a windows or HDF5 directory scheme, “Parent” corresponds to the name of “directory up” whereas “Child” corresponds to subdirectories. Such attributes are most important for the specification of future metadata schemata aiming at cross domain interoperability.

3.3.5 Flow chart approach for interoperability

Once a perfect metadata description of a materials state is available, and multiple namespaces can easily be combined, then the next steps to be taken relate to the interoperability of models and tools. Interoperability between models implies the need for the definition of a flow of information or a “workflow” and also the specification of timing between the different operations of the different models acting on the materials state or on subsets of the materials state description. Different types of workflows have been proposed in the MoDa scheme [MoDa] for linking and different types of coupling of models in workflows.

Getting such workflows eventually well-defined, operational and also extendable to future decision making processes needs further considerations. An instructive and helpful approach is having a look at the specification of workflows and decision making in different areas, where different types of flowchart tools are needed to control the workflow.

The classes in the MoDa scheme essentially correspond to the models (blue), the “post-processing” (green) and the “state description” (red). To allow informatics type workflows these models, states and post-processors have to be complemented by further tools like INPUT/OUTPUT and especially by DECISIONS allowing steering the workflow. In the overall scenario being depicted in the present report all I/O operations are based on reading/writing to the state description as specified and stored in the HDF5 file as depicted in the sections above.

The scenario underling the present report is based on the description of a materials state and its evolution being influenced by all types of phenomena occurring at all scales. The materials state further defines the properties and these can be extracted from the materials state information by suitable methods/algorithms/models at all scales in a post-processing mode of operation. A sound description of the materials

state has been provided in the preceding sections. This materials state description is based on a suitable set of arrays of scalars, vectors, tensors.

Different types of models/tools then can operate on this materials state and a further classification scheme being based on the character/functionality of the physics equation is proposed for the models in addition to the 24 types of models being classified in [RoMM]:

Creator tools “CREATORS”
Evolution equations “EVOLVERS”
Property equations “EXTRACTORS”
Balance equations “EQUILIBRATORS”

CREATORS serve the design of an initial materials state. Examples are Voronoi tessellation, synthetic microstructures, homogeneous liquid assumption, but also experimental microstructures

EVOLVERS further evolve an existing materials state. They are characterized by any time dependency within the physics equation or within the materials relations e.g.: Schrödinger equation (time dependent), Molecular Dynamics equations, Phase Field equations, Diffusion equations, Navier-Stokes equation. EVOLVERS address the central paradigm of materials engineering “processing determines microstructure” corresponding to “EVOLVERS alter materials states”

EQUILIBRATORS allow predicting conditions at equilibrium and thus specifying criteria e.g. for thermodynamic equilibrium, for thermomechanical equilibrium, and for stationary states.

EXTRACTOR type models „post-process“ existing materials states without altering the state and extract desired properties from a state. Examples are mathematical homogenization models & tools, volume averaging, statistics tools, virtual testing, visualization tools to name a few. EXTRACTORS address the central paradigm of materials engineering “microstructure determines properties” corresponding to “EXTRACTORS extract properties from a materials state”. The data generated by EXTRACTORS may serve to enrich the information in the HDF5 file.

Conservation laws provide constraints and criteria to be met by any type of above models anywhere and anytime e.g. energy conservation, momentum conservation, mass/species conservation, conservation of angular momentum, charge conservation positive entropy production to name the most important principles.

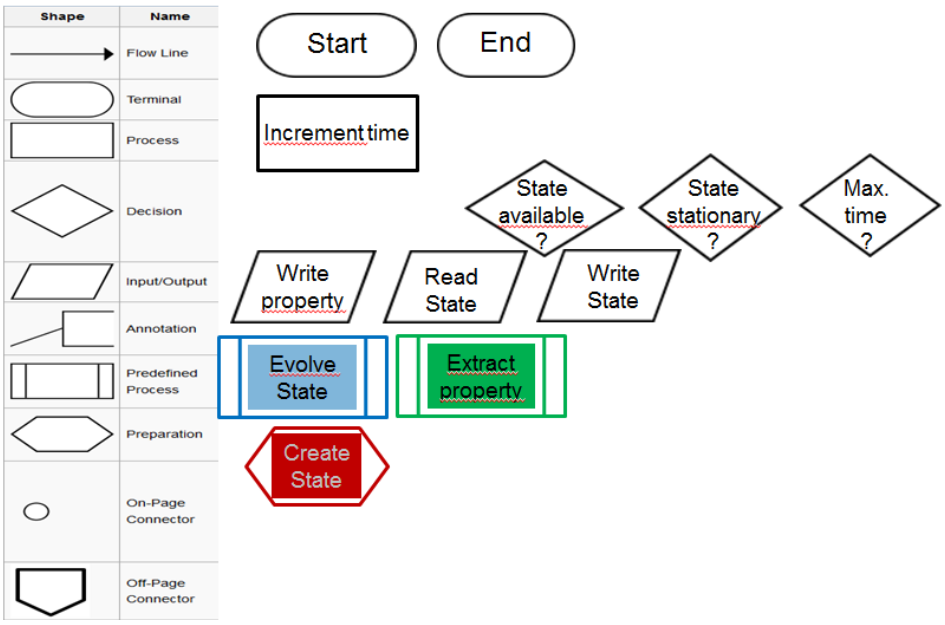
Besides the models themselves a number of tools allowing to control and steer the information flow between the different models and their mutual timing are necessary.

DECISIONS check for a criterion to be met and redirect the workflow. They can act on logical values and on scalars only.

PROCESSOR tools steer the workflow. Examples are counters and timers

I/O-TOOLS allow to store and get data by “Read data” and “Write data” operations

In summary, all objects being depicted above (in capital letters) provide the building blocks for the specification of a flow chart as known from informatics but also from business decision model. Details of this flow chart approach will be published in the proceedings of the 4th World Congress on ICME in 2017.



3.4 Assessment of acceptance

As a measure for the agreement to the data structure and strategy for interoperability as proposed by the ICMEg consortium following indicators are taken:

- Invitations of ICMEg members to join/establish national and international expert groups aiming at interoperability e.g. TMS Committee on ICME, VDI expert group „Digital Materials“, International Data Format activity, EMMC,…
- Invitations of ICMEg members to join editorial boards of internationally renowned journals in the field like e.g. the IMMI journal where 3 out of 5 non-american members of the editorial board are ICMEg partners (http://immijournal.springeropen.com/about/editorial-board)
- Invitations of ICMEg members to join the board of renowned international conferences in the field. where e.g. the ICMEg coordinator is the only European representative in the board of the highly visible “4th World Congress on ICME”
- A number of citations of publications by ICMEg members on the subject already shortly after publication and also personal feedback being received
- Adaptation of the HDF5 concept as observed during Second Workshop, where HDF5 explicitly appeared in the tile of a number of presentations and further a number of presentations where HDF5 was mentioned in the abstract or during the presentation itself

4 Potential Impact

Reaching the vision of “plug&play type multi-modelling” will eventually accelerate the future development of new materials and processes and accordingly increase the pace of innovation for which materials have laid the grounds ever since. This modelling strategy will not only lead to the development of new materials but also to the improvement of existing materials and their processing thus fostering European industry in a number of sectors.

The project eventually has gone beyond mere conventional static descriptions of a material and provided a detailed description of 3 D microstructures and their evolution. As the microstructure is the carrier of all materials properties a sound description of a microstructure (in the sense of describing a “state variable” of the system) will allow for future predictions of materials properties and their evolution/variation e.g. with composition and temperature. This will tremendously advance the field of materials science and engineering for technical materials. Such predictions will need the interaction of various tools operating in different model worlds and at different length/time scales. The only common denominator for all types of models and for all scales is the subject they are targeting – the material. Scope of the standard formulations to be proposed by ICMEg thus is a hierarchical description of polycrystalline, polyphase and multicomponent materials being applicable to all length scales and to both discrete and continuum models. The HDF5 type hierarchical approach being identified and proposed as a basis for a standard seems most promising in this context.

The ICMEg project has outlined a scenario for data exchange at the microstructure scale. This scenario is based on the definition of a state, which can be evolved and analysed by different types of models and tools.

The state essentially corresponds to a comprehensive digital description of the microstructure. It provides the initial condition for any evolution type model. The output state of such models again represents a state, which then can be further forwarded along the simulation chain.

Models and tools have been classified into evolution type and extractor type models/tools allowing either to evolve resp. to process the state corresponding to the “pro-cessing determines microstructure” paradigm or to extract property data from the state, corresponding to the “microstructure determines properties” paradigm.

The digital representation of the state is characterized by a suitable set of arrays of scalars, vectors, and tensors. A nomenclature/namespace for the metadata descriptors for each of the arrays has been proposed. This nomenclature has been elaborated on the basis of continuum models. However, it also considers descriptors for electronic, atomistic, and mesoscopic models.

A major conceptual approach is the hierarchical arrangement of the individual arrays describing the state resp. the microstructure. This allows for different representations of the microstructure like statistical representation and spatial representation in a coherent way within the same data structure. This inherent hierarchy of local and integral data is essential to bridge the scales between different physical phenomena and enables a seamless interaction e.g. with models/tools operating at the component scale.

The HDF5 file format is proposed as a specific realisation of such a hierarchical data structure. This open source format is very powerful and versatile and already has established itself as a standard in computational fluid dynamics and in several other areas of application.

Eventually a concept to specify workflows in simulation chains has been proposed. The state description, models describing the evolution of the state, and models extracting properties are the major building blocks. To allow for control and for steering of the workflow especially “Decisions” have been introduced as further mandatory building blocks of a flowchart.

In summary the basic concepts for interoperability between, simulated, experimental and synthetic microstructures being developed by ICMEg are now available and seem viable. These concepts are constructed as to enable/ensure interoperability also with models operating on components and processes as well as electronic/atomistic/mesoscopic models.

Future activities will relate to further spreading these concepts into the community, to applying them in industrial use cases, to further developing and incorporating them into workflows and simulation platforms, to broadening their scope toward uncertainty propagation and error estimates, to generating robust simulation chains, to harmonize namespaces, like e.g.:

- Open simulation platforms

- life-cycle predictions
- global optimisation of process chains
- fully documented data
- error propagation / robustness assessment
- surrogate models / reduced models
- Software as a Service („SaaS“) approaches
- Business decision support systems
- design to cost…
- …and many others.

The activities launched by ICMEg towards these grounds will be further continued and coordinated especially by the EMMC-CSA project which started in September 2016 (www.emmc.info) and by the ICMEg e.V. being founded as a non-profit association during the course of the ICMEg project.

5 Dissemination/References

5.1 Presentations/publications

ICMEg related results were presented at more than 50 international conferences, often as invited presentations. They were especially presented during the 1st and 2nd Workshop on Software Solutions for ICME being organized by ICMEg itself.

During these conferences and workshops and during expert group meetings the approaches being proposed by ICMEg were intensely discussed with stakeholders.

The most significant results were published in numerous publications (see separate listing) and to a large extend are documented in the “Handbook of Software Solutions” as well as in the deliverables of the project.

5.2 Books

The “Handbook of Software Solutions for ICME” [Schmitz/Prahl] was officially released by Wiley VCH on 9th of November 2016. 93 authors from 14 countries compiled about 600 pages. Hundreds of software codes are listed in a thematically structured way.

Introductions to following topics are included:

- 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

The book addresses readers seeking a holistic overview on things or introduction to fields adjacent to their own expertise. In this sense it is written not only for experts but also for a wider public.

5.3 Sustainability

An activity to secure a sustainable development of the standard formulations was the foundation of the ICMEg association ("ICMEg e.V."), which took place on 24th of June 2014 in Rolduc. Using the successful "template" of the OpenMP foundation, which created standards in parallel computing during the last two decades, the ICMEg e.V. will accompany the future development of a standardized communication protocol for ICME. The activities launched by ICMEg in addition will be further continued and coordinated especially by the EMMC-CSA project, which started in September 2016 (www.emmc.info).

5.4 References

[1st ICMEG] The abstract booklet is available under www.icmeg.info along with pdf's of authors presentations also under www.icmeg.info

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