



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 extent
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)



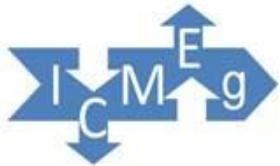
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current EU projects on interoperability/platforms



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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
Nanostructures
<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 **D**evelopment of micro- and **N**anostructures
<http://modena.units.it/>



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



Simulation **f**ramework for multi-scale phenomena in micro- and nanosystems
<http://www.simphony-project.eu/>



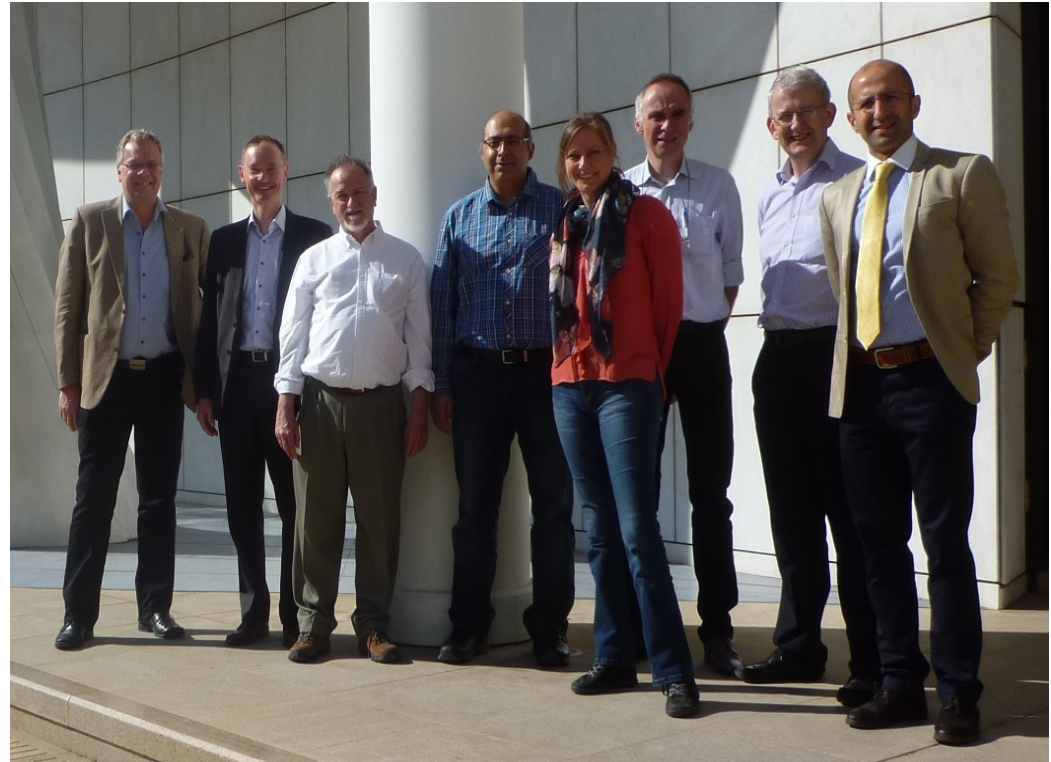
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EU - Multiscale Modelling Cluster „5+1“

*Kick-off :
Athens Feb 2014*

*1st Cluster workshop:
Oct. 2014 MSE
Darmstadt*

*2nd Cluster workshop:
Jyväskylä University
Finland 28/29 May 2015*



(left to right):

*Georg J. Schmitz (ICMEg) , Gerhard Goldbeck (EU-PTA),
Heinz A. Preisig (MoDeNa), Adham Hashibon (SimPhoNy) ,
Erica Coenen (MMP), Jan-Paul Krugers (MMP) ,
Eoin O Reilly (DEEPEN), Shahriar Amini (NanoSim.)*



cluster of 5 research projects and 1 networking project

Proposals for Communication Standards

Generic and structured list of metadata keywords

Alias Table for keywords describing the same metadata in different software packages

Overall data structure for file based information exchange.

Each project will make their own platform adhering to these standards.

ICMEg:

Open workshops to get wide endorsement

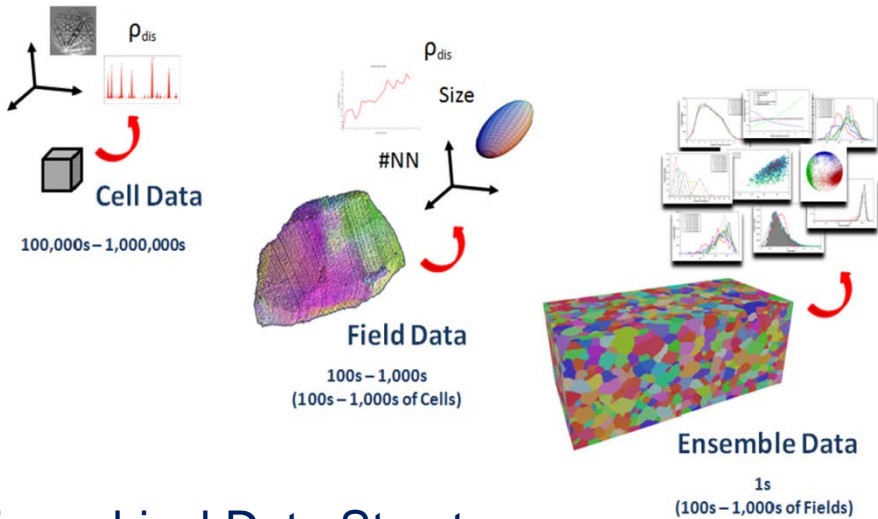


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Towards a data structure for file based communication

Possible approach currently being investigated:

HDF5
„Hierarchical Data Format“



Hierarchical Data Structure
(Source: dream3d Manual)

The screenshot shows the HDFView 2.10.1 interface. The main window displays a hierarchical tree structure for the file 'GIACC.dream3d'. The tree includes:

- Pipeline (0-6)
- VoxelDataContainer
 - CELL_DATA
 - EulerAngles
 - GoodVoxels
 - GrainIds
 - IPFCOLOR
 - Phases
 - SurfaceVoxels
 - DIMENSIONS
 - EDGE_DATA
 - ENSEMBLE_DATA
 - CrystalStructures
 - NumFields
 - PhaseTypes
 - ShapeTypes
 - Statistics
 - FACE_DATA
 - FIELD_DATA
 - Active
 - AvgQuats
 - EulerAngles
 - NeighborList
 - NumNeighbors
 - Phases

On the right, a table titled 'NumNeighbors at /VoxelDataCont' displays a list of values. A grey box labeled 'Metadata keywords' has red arrows pointing to the 'CELL_DATA', 'ENSEMBLE_DATA', and 'FIELD_DATA' nodes in the tree, and to the 'NumNeighbors' node in the table.

Index	Value
241	9
242	8
243	21
244	8
245	16
246	11
247	14
248	14
249	7
250	8
251	4
252	3
253	4
254	5
255	13
256	8
257	17
258	9
259	10
260	10
261	14
262	5
263	6
264	10
265	10
266	16
267	10
268	17
269	8



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Approach towards metadata keywords

Use HDF5 type directory data structure as a guidance

- a) Categorise: Cell Data, Field Data and Ensemble (RVE) Data
- b) further categorise according to type of „experimental data acquisition“

- RVE type data: RVE size, origin, orientation, units, ..
- LOM type data: grain sizes/topology, neighbors etc...
- EBSD type data: crystal orientations, texture, .., ..
- EDX type data: element concentrations

Indentation data: dislocations etc

other type data: ..to be defined

Per-phase properties will be „ensemble data“ e.g. to Abaqus mtl format

Inclusion of e/a/m data is straightforward

	A	B	C	D	E
1	0	AA_Nomenclature/property/entity	short description	Symbol	HDF-Type
14	1002	NAME = 0			
15	1003	NAME_UC = 12			
16	1099	RVE geometry			
17	1100	RVE_Origin		SDO	ensemble
18	1100	x,y,z number voxels		Nx,Ny,Nz	ensemble
19	1100	SIMULATION_DOMAIN_ORIGIN = 28		SDO	
20	1100	SIZE = 22			
21	1100	SCALING_COEFFICIENT = 34			
22	1101	SIMULATION_DOMAIN_DIMENSIONS = 27		Nx,Ny, Nz	
23	1102	cell_size		dx,dy,dz	ensemble
24	1199	RVE_chemistry			
25	1200	Phase_Fractions			Ensemble
26	1200	Number moles			Ensemble/RVE
27	1200	Number_Phases			Ensemble/RVE
28	1200	CONCENTRATION = 50			Ensemble
29	1200	DENSITY = 49			Ensemble
30	1200	MASS = 23			
31	1200	MATERIAL_ID = 4			

.....to be continued....



targeted timeline for the 5+1 cluster of projects:

- June 2015: Public cluster proposal for **metadata keyword list** published on the ICMEg project and EMMC websites for wide discussion
- Dec 2015: Public cluster proposal for a file data structure
- Dec 2017: Public Cluster proposal for platform(s) (coupling, distributed)



EMMC Interoperability Work Group

Complemented the cluster

Target: widely accepted, thus de-facto standards.

The EMMC recommends to the EC to support the development of an

Open Simulation Platform

- **Workflow tool(s) to orchestrate a number of different materials modelling tools; on one computer; first for linking than for coupling of simulations.**
- **Tools for distributed simulations.**
- **Accounting schemes (not for the use of the platform but for the use of commercial codes used in the platform operation by the user e.g. SME).**