



### 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)



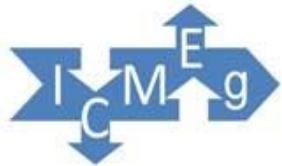
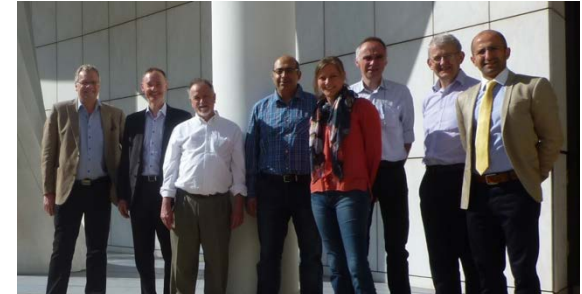
# The European Materials Modeling Council

## 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/](http://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/>



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



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



A Multi-scale Simulation-Based Design **P**latform for Cost-Effective CO<sub>2</sub> 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***

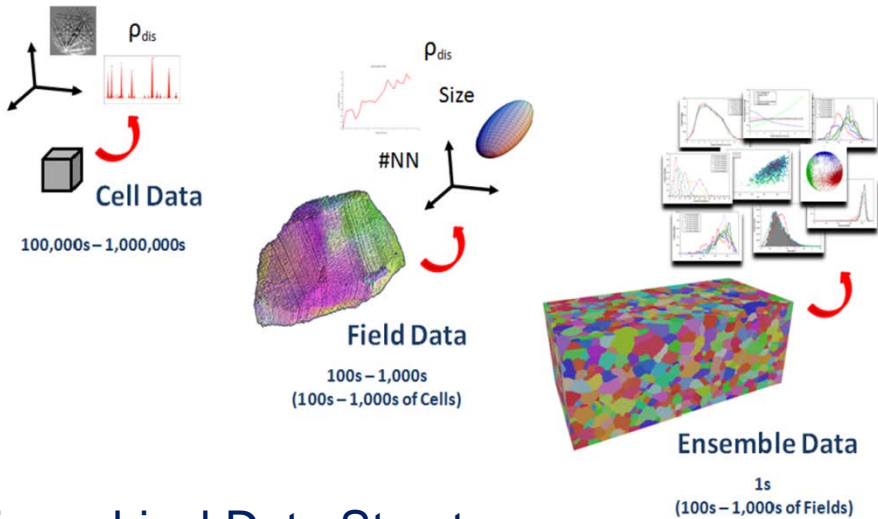


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## Towards a data structure for file based communication

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 file tree on the left is expanded to show the following structure:

- GIACC.dream3d
  - 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

A grey box labeled "Metadata keywords" has red arrows pointing to the following items in the tree:

- EulerAngles (under CELL\_DATA)
- NumNeighbors (under FIELD\_DATA)
- Active (under FIELD\_DATA)

On the right, a table titled "NumNeighbors at /VoxelDataCont" displays the following data:

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).**