



## Workshop on

### Metadata and Interoperability in Integrated Computational Materials Engineering (ICME) and Multiscale Materials Modelling (MMM)

Thursday 26 November 2015, 09:20 - 17:00 h  
Covent Garden Brussels

#### Organized by

*The Integrated Computational Materials Engineering expert group (ICMEg)  
The EU Multiscale Modelling Cluster (EU-MMC)  
The Interoperability (IntOP) and Open Software Platform (OSP) working groups of the  
The European Materials Modelling Council EMMC*

#### AGENDA

09:00 – 09:20	Registration	Attendees, Commission Services
09:20 – 09:50	Welcome and Introduction - EMMC/ EMMC-IntOP/EMMC-OSP - EU Multiscale Modelling Cluster - ICMEg <i>Includes an overview of metadata classes</i>	A. Hashibon G. Goldbeck G.J. Schmitz
09:50 – 10:15	Motivation and Vision (1): Requirements on meta data and interoperability to answer industrial material design questions (Engineering perspective)	D. Cebon and S. Donders
10:15 – 10:40	Motivation and Vision (2): Requirements on metadata arising from industrial needs for identification of results/data generated by modelling ( <i>Chemistry and physics perspective</i> )	M. Noro
10:40 – 11:10	Coffee break	
11:10-11:40	Classification of materials models and corresponding physics-based metadata (the highest level of metadata)	P. Asinari
11:40-12:10	Computational related metadata: strategies for their specification/classification/organisation and their required attributes	A. Hashibon
12:10-12:35	Examples for materials metadata: proposals for metadata keywords for the description of a microstructure	G.J. Schmitz
12:35-13:30	Lunch break	

13:30 – 14:00	The hierarchical data format HDF5 – a pragmatic basis and viable approach for linking of models in a file based interoperability approach?	F. Sacconi G.J. Schmitz B. Patzak
14:00 – 14:30	Implementation, benefits and handling of formal metadata schemata as enablers of Platform interoperability – From Data Structures to Modelling Platforms	T. Hagelien (with input from EU-MMC cluster)
14:30 – 15:00	How to facilitate information exchange between different communities by means of metadata and standards? <ul style="list-style-type: none"> <li>- Introduction of end user sandbox use case scenario.</li> <li>- Metadata description of the selected use case.</li> </ul>	D. Cebon, J. Friis, A. Hashibon, G.J. Schmitz
15:00-15:30	Coffee/Tea break	
15:30 – 17:00	Concluding Panel discussion Panellists: <ol style="list-style-type: none"> <li>1. Discrete: SWO owner from psi-K: Mike Payne (t.b.c.)</li> <li>2. Continuum: SWO: Stijn Donders</li> <li>3. Characterisation: Marco Sebastiani (t.b.c.)</li> <li>4. Industrial End Users: Massimo Noro (Unilever)</li> <li>5. Databases: David Cebon (Granta Design)</li> <li>6. Standardisation: Philipp Albrecht (DIN)</li> </ol>	Moderators: G.J. Schmitz, A. Hashibon