



EMMC-CSA

European Materials Modelling Council

H2020-NMBP-CSA-2016

NMBP-24-206

Network to capitalize on strong European position in materials modelling
and to allow industry to reap the benefits

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Duration: 36 months

DELIVERABLE REPORT

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| Task | 2.1 | Networking and Consultation |

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| Contributing beneficiaries | Fraunhofer |

¹ Dissemination level: **PU** = Public, **PP** = Restricted to other programme participants (including the Commission Services), **RE** = Restricted to a group specified by the consortium (including the Commission Services), **CO** = Confidential, only for members of the consortium (including the Commission Services).

² Nature of the deliverable: **R** = Report, **P** = Prototype, **D** = Demonstrator, **O** = Other.

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| Consortium | | |
|-------------|---|----------------|
| TU WIEN | Technische Universität Wien | Austria |
| FRAUNHOFER | Fraunhofer Gesellschaft | Germany |
| GCL | Goldbeck Consulting Limited | United Kingdom |
| POLITO | Politecnico di Torino | Italy |
| UU | Uppsala Universitet | Sweden |
| DOW | Dow Benelux B.V. | Netherlands |
| EPFL | Ecole Polytechnique Federale de Lausanne | Switzerland |
| DPI | Dutch Polymer Institute | Netherlands |
| SINTEF | Stiftelsen SINTEF | Norway |
| ACCESS e.V. | ACCESS e.V. | Germany |
| HZG | Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GMBH | Germany |
| MDS | Materials Design S.A.R.L | France |
| QW | QuantumWise A/S | Denmark |
| GRANTA | Granta Design LTD | United Kingdom |
| UOY | University of York | United Kingdom |

| | |
|-----------------------|--------------------------------------|
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1. Executive summary

1.1 *Description of the deliverable content and objectives*

In line with the objectives and actions described in Task 2.1, the Interoperability and Repositories Advisory Group (IRAG) has been formed together between WP2 and WP3 and a Charter for the work of the group drawn up and discussed with members. The Charter document is the subject of this deliverable.

1.2 *Deviation from objectives, corrective action (if applicable)*

None

1.3 *Major outcome*

IRAG formed and Charter (see Annex) agreed with current membership.

2. Progress report (main activities)

Invitations to join IRAG were sent to 44 people selected from the list of 82 people covering all FP7 and H2020 projects that have completed MODA. 31 people agreed to participate. Monthly telcos have been held together with EMMC-CSA members. They were attended by about 3-5 IRAG experts. An IRAG expert group meeting was held on 18 January 2017 in Brussels, attended by 7 IRAG members. The draft charter was discussed and elaborated at that workshop and a subsequent telco. The draft was also sent to all members by email for approval. The current leadership team includes

- Emanuele Ghedini (University of Bologna)
- Wolfgang Wenzel (Karlsruhe Institute of Technology)
- Peter Schiffels (Fraunhofer IFAM)
- Eoin O'Reilly (Tyndall Institute)
- Alejandro Franco (Univ Picardie)

3. Conclusions

The IRAG has been formed and a Charter agreed. Revisions to the Charter may be carried out in future as necessary.

4. Annex I: Charter



Charter of the EMMC Interoperability and Repositories Advisory Group (IRAG)

V3

13 February 2017

Introduction

The EMMC, supported by the EMMC-CSA Project³, aims to strengthen the integration of the field of materials modelling across its many sub-disciplines. It is recognised that integration will be strongly aided by establishing a common vocabulary and terminology, and a standardised classification of materials models and related metadata. Also, in order to facilitate a more efficient and effective way of carrying out materials modelling and developing the necessary software, the EMMC supports efforts to achieve interoperability and develop an open simulation platform, i.e. an environment which provides open standards for integration and interoperability of materials models. Furthermore, it is recognised that data, be it experimental or modelling derived, form a key part of materials modelling workflows and provide the crucial link between modelling and experimentation. Therefore, the integration with data repositories and achieving interoperability with repository systems is equally crucial in order to guarantee industrial impact.

Objectives

- Review, analyse, provide feedback and make recommendations regarding updates to the [Review of Materials Modelling](#) including the MODA.
- Review, analyse, provide feedback and make recommendations regarding the metadata, interoperability standards and open simulation platform design proposed by the EMMC CSA.
- Review, analyse, provide feedback and make recommendations regarding the design requirements for concerted interoperable databases for materials modelling data covering all relevant models, all industrial application fields and all materials and all databases etc.
- Build collaborations and interactions with national and international standards organizations such as DIN, IUPAC, ISO, ASM and NIST.

³ EMMC-CSA project has received funding from the European Union's Horizon 2020 research and innovation programme, under Grant Agreement No.723867



Stakeholders

IRAG should represent all different types of materials modelling, modelling software, data providers and repositories, translation and industrial applications.

Topics

1. Materials Modelling Terminology, Classification and Metadata (incl. MODA)
2. Metadata Schema and Materials Modelling Ontology for semantic interoperability
 - a. A basic metadata schema supporting cross-domain interoperability will be proposed by EMMC-CSA for review by IRAG. Materials Modelling domain specific metadata will be developed based on the basic metadata schema with keywords from the Ontology. These will be reviewed by IRAG and checked for redundancy and compliance.
3. Design requirements for concerted interoperable databases for materials modelling data, aimed at describing and sharing the information in the different subfields so that a catalogue can be built of available data for all industrial application fields and materials and models in the repositories scattered across Europe without altering what already exists, but building on top of it. The metadata elaborated should be sufficient to describe all concepts of the MODA. New concepts (elements) to add to the existing chapters in the MODA will be proposed as needed based on input gathered throughout the consultation process. In addition it should be explored how to combine experimental characterisation and modelling data into the same metadata schema.

Governance and structure of IRAG

Membership

IRAG membership is subject to invitation by the EMMC OMB (Organisational Management Board). Initial membership of IRAG consists of persons involved in EU FP7 and Horizon2020 projects that have completed MODA descriptions for their projects.

EMMC-CSA participants are not IRAG members.

Membership will be extended to cover all stakeholders.

IRAG members may propose new IRAG members to the EMMC OMB.

Leadership and management

IRAG is run by a leadership team with support of EMMC-CSA members (acting as Secretariat). The current leadership team consists of:

- Emanuele Ghedini (University of Bologna)
- Wolfgang Wenzel (Karlsruhe Institute of Technology)
- Peter Schiffels (Fraunhofer IFAM)
- Eoin O'Reilly (Tyndall Institute)
- Alejandro Franco (Univ Picardie)



Communication within IRAG

A collaboration environment for IRAG members will be made available on the EMMC Wikix.

Interactions between IRAG and EMMC-CSA

Regular interactions are facilitated by

- Monthly online calls
- Email
- Shared Wikix environment

In addition, physical meetings focused on the issues of IRAG are planned annually.

5. Annex II: List of current IRAG members

| | First Name | Last Name | Active |
|----|-------------------|--------------------------------|---------------|
| 1 | Jaakko | Akola | |
| 2 | Peter | Bobbert | |
| 3 | Jesús | Carrete Montaña | x |
| 4 | Marie-Liesse | Doublet | x |
| 5 | Naiara | Elejalde | x |
| 6 | Ivo | Filot | |
| 7 | Alejandro | Franco | x |
| 8 | Emanuele | Ghedini | x |
| 9 | Jianguo | Lin | x |
| 10 | Nuria | Lopez | |
| 11 | Philippe | Maincon | x |
| 12 | Adrián | Quesada | |
| 13 | Daniela | Reccardo | |
| 14 | Peter | Schiffels | x |
| 15 | Christoph | Sprengard | x |
| 16 | Alison | Walker (Bridget Jensen) | x |
| 17 | Aron | Walsh | |
| 18 | Wolfgang | Wenzel | x |
| 19 | Dhammika | Wideanalage | x |
| 20 | Lukasz | Figiel | x |
| 21 | Mathieu | Lusier | x |
| 22 | Javier | Llorca | x |
| 23 | Vincenzo | Carravetta | x |
| 24 | Lukasz | Figiel | x |
| 25 | Susanna | Monti | x |
| 26 | Costas | Kiparissides | x |
| 27 | Eoin | O'Reilly | x |
| 28 | Natalio | Mingo | x |
| 29 | Liliang | Wang | x |
| 30 | Luigi | Gurreri | x |
| 31 | Antonino | Campione | x |