



EMMC-Workshop

**“Integration of materials modelling into business decision:
Approaches, Models and Licenses”**

**E-MRS Fall Meeting
September 18th 2017, Warsaw**

EMMC-CSA H2020-NMPB-2016-2017 Grant 723867





The European Materials Modelling Council

EMMC-Workshop: Agenda

09:00 - 9:30		Welcome and presentation of EMMC Translation/Training activity by Natalia Konchakova (Helmholtz-Zentrum Geesthacht, GERMANY)
09:30 – 10:15	Unit 1	Advanced composite materials/ nanocomposites for industrial use: modelling challenges and translation experience Impulse presentation # 1 by Ronan Le Goff (IPC, FRANCE) Impulse presentation # 2 by Roger Assaker (e-Xstream Engineering, LUXEMBOURG)
10:15 – 10:30		Coffee Break
10:30 – 11:10	Unit 2	Materials modelling for electronic devices / sensors: successful translation expertise and modelling aspects Impulse presentation # 1 by Tomasz Krupicz (Comsol Multiphysics, GERMANY) Impulse presentation # 2 by Tobias Neumann (Nanomatch GmbH, GERMANY)
11:10 – 11:15		Break
11:15 – 12:00	Unit 3	Effective translation strategy and materials model creation for Energy & Funktional Materials Impulse presentation # 1 by Thierry Deutsch (CEA, Grenoble, FRANCE) Impulse presentation # 2 by Daniele Stradi (QuantumWise A/S, DENMARK)
12:00 – 12:30		Discussion and Conclusion (morning session)
12:30 – 14:00		Lunch break
14:00 – 14:20	Unit 4	Hydrides for Energy Storage: modelling approaches and translation realization Impulse presentation by Marcello Baricco (University of Turin, ITALY)
14:20 – 15:00		Funding opportunities, EMMC Translation Actions Discussion and Conclusion
15:00 – 15:15		Coffee Break
15:15 – 18:00		Tutorial / Training





EMMC: Translation and Training Activity

Natalia Konchakova, Daniel Höche,
Denka Hristova-Bogaerds, Pietro Asinari
European Materials Modelling Council (EMMC)

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Outline

- EMMC: Goal and Structure → How can you join the EMMC?
- Translator as a stakeholder → Translation process
- Translation → Code of conduct, Training activity
- Efficient Translation → Materials modelling for business decisions
 - EMMC-Workshop: Goal and Agenda**
 - EMMC Translation Actions**
 - Funding opportunities**





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Leadership in Enabling and Industrial

Translators

(non exhaustive list)



27th Feb. 2014, Brussels

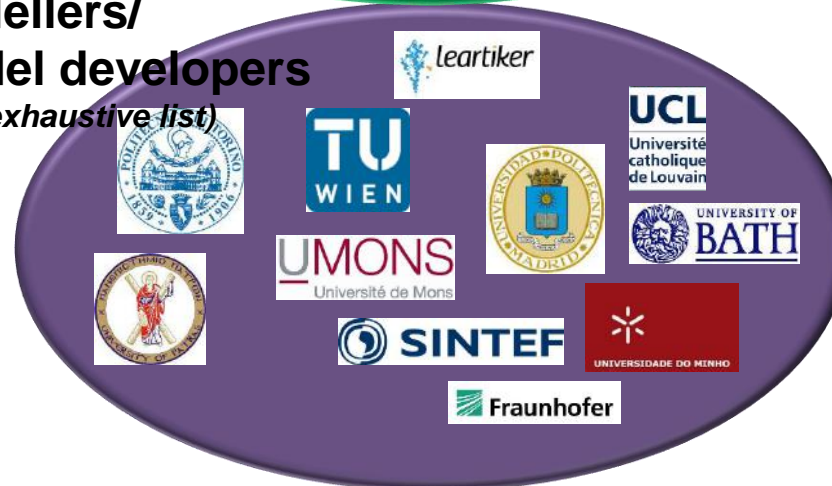
End-Users

(non exhaustive list)



Modellers/ model developers

(non exhaustive list)



Software Owners

(non exhaustive list)



Goal → to connect & coordinate & enlarge existing activities of the European materials modelling community

EMMC-Workshop, Warsaw 18th September 2017





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EMMC Working Groups

Working Groups

A number of working groups representing all material modeling stakeholders in Europe have been formed.



Each working group has an operational team manager (OTM) and a vice OTM.

If you would like to join a working group or even start a new one please visit the [Participation Page](#).

1. Business Decision Support
2. Continuum Models
3. Discrete Models (including Electronic Models, Atomistic Models, Mesoscopic Models, Coupling and Linking)
4. Interoperability
5. Open Simulation Platform Concept
6. Materials Model Marketplace
7. Manufacturers
8. Software Owner
9. Translator
10. Validation





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Open community: www.emmc.info

Everybody from the
European Materials Modelling Community
is invited to join and express their opinion



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[EMMC](#) [Working Groups](#) [News & Events](#) [Participation](#) [Member Wiki](#)

Participation

You can join us and help shape Europe's Material Modelling vision, here is how:

The EMMC is a bottom-up organisation! In practice this means that anybody can start an activity.

[Join us!](#)

GET INVOLVED

[Advice for LEIT Proposers](#)

[Industrial Advisory Board](#)

[International Material Modelling Board](#)

[EMMC Roadmap](#)

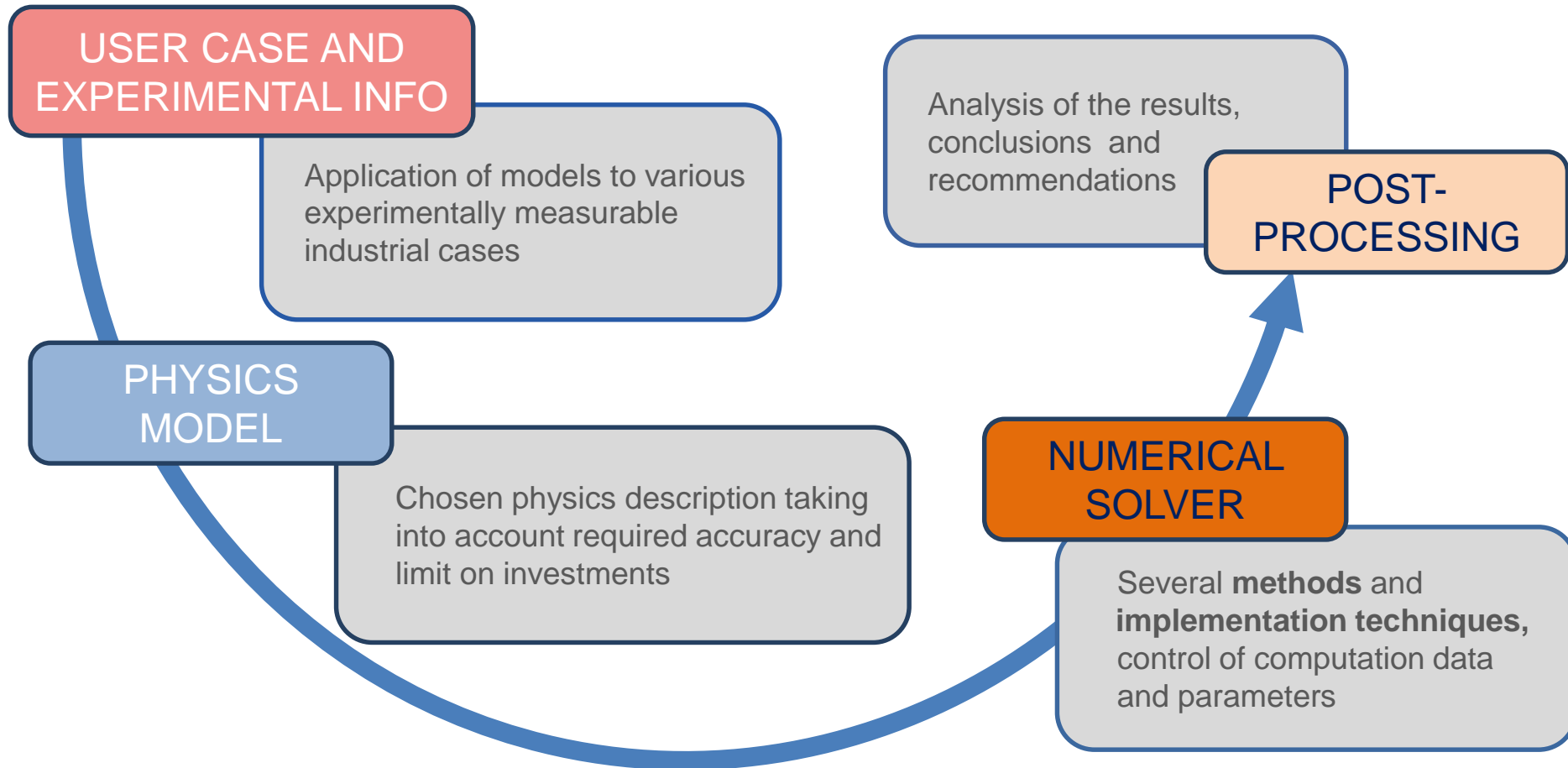
[Participation](#)





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Materials Modelling - Complexity



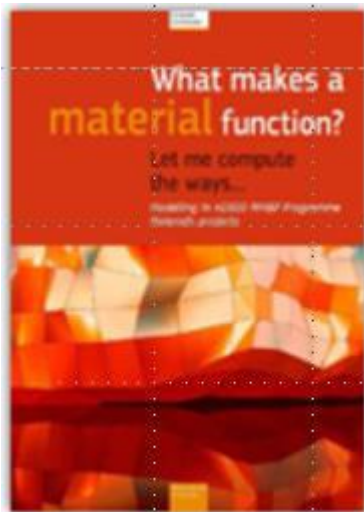
Each part contains complex info on cases, approaches, methods
(a user case can be simulated in a multitude of different ways)





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Review of Materials Modelling - MODA



Review of Materials Modelling VI
RoMM

Vocabulary, classification and metadata for materials modelling (130 FP7 and H2020 projects)

Source:

<https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/>



MODA (M**OD**elling D**AT**a)

is a **template** for the **standardised description** of **materials models** (<https://emmc.info/moda-workflow-templates/>)

The **MODA** is meant to **guide users** towards a complete **high-level documentation** of material models, starting from the **end-user case** via the **computational details** to the **results**.

It provides all necessary aspects for: **description**, **reproducibility**, **curation** and **interfacing** with other models and databases.

The MODA -- **model concepts**

PHYSICS ENTITY

EQUATIONS
(physics- or data-based)



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MODA - Materials Models Classification

In the **MODA**, physics-based Materials Models are classified via the

PHYSICS ENTITY

Self-contained, physically distinct, internally frozen, physical 'object'

WHOSE BEHAVIOUR IS DESCRIBED BY PHYSICS

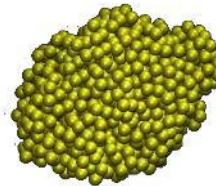
ELECTRONS



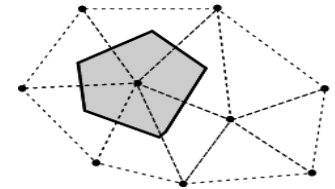
ATOMS



BEADS



CONTINUUM VOLUME



Bead: Discrete entity consisting of more than one atom (e.g. groups of atoms, nanoparticles, grains).

Continuum Volume: Volume in which the material properties are averaged.

The classification is

not according to the **size** of the application or system

nor according to the **length scale** of the phenomena to be simulated

nor according to the **solver type**





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Materials Modelling and Industrial feedback

Modelling offers unique insight into

- properties and in-service behaviour of materials,
- industrial manufacturing processes,
- provides understanding of the underlying physics of materials, devices and processes;

Modelling complements experiments by

- guiding experiments, replacing time and cost expensive trials,
- reducing cost and hardware for testing,
- interpreting the experiments;

THEORY

PRACTICE

Modelling helps design prototypes by enabling

- pre-screening, faster screening of alternative materials and designs,
- predicting final product properties and performance,
- determination if a design concept works without having to build it,
- optimisation of production processes;

Modelling reduce development time by

- shortening lead and qualification time,
- facilitating the debottlenecking,
- decreasing the time-to-market;

Source:

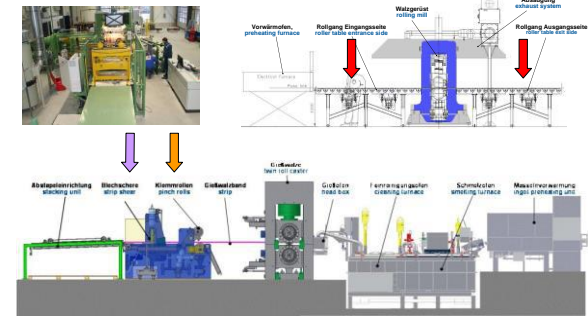
<https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/>





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Translation gap





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Mission of Translators

Goal





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Translators and Translation

BUSINESS

- all stages of the development:
 - design
 - testing
 - up-scaling
 - market introduction



TRANSLATOR

Business
Activities

Science

R&D



BUSINESS
AIM

TRANSLATION
FOCUS

INDUSTRIAL
PROBLEM

Necessary:
full understanding of
the problem and its
industrial context



support
the **implementation**
and **utilization** of
modelling and **simulation**
by enhancing the skills of
the industrial operators

TRAINING





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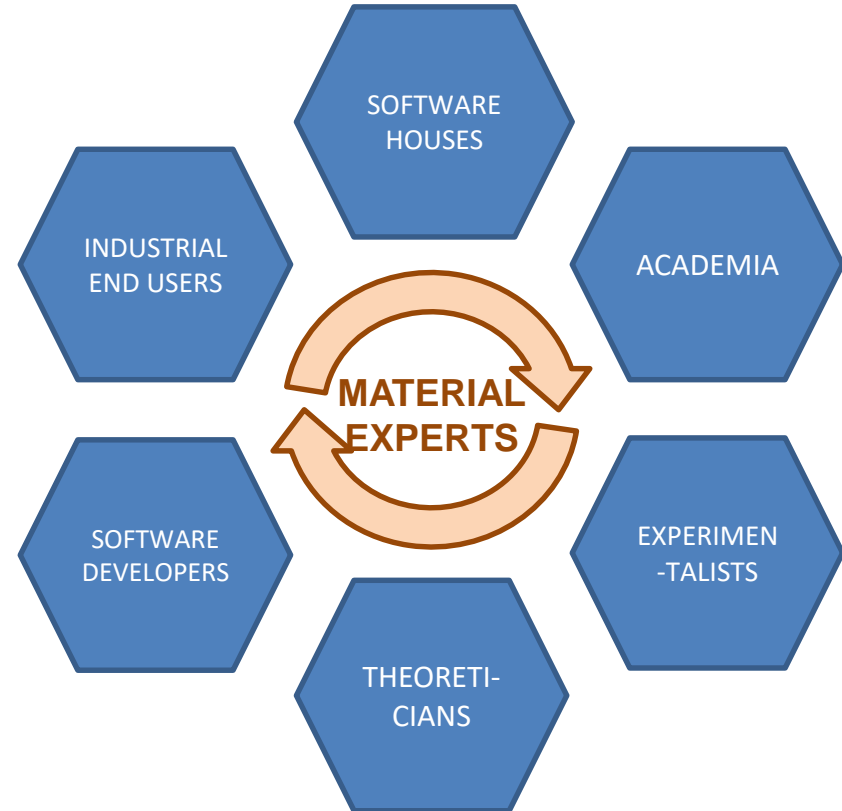
Translation process

Review the user case, existing models and previous success stories

Identify the suitable ones and, if not available, request modelling

Advise the company on the correct implementation

Consult the company on the analysis of the results



EACH COMMUNITY HAS ITS OWN TERMINOLOGY !!!

Specific language to explain modelling to non-modellers





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Current Translators Charter V5, <https://emmc.info>

Economical aspects

- **balance** between investments (resources and expertise) and expected return
- economic background to **advice** on costs and time to solution
- **human factors**: skills, readiness, management of subcontractors

Technical aspects

- **four different materials models** (electronic, atomistic, mesoscopic and continuum)
- **accuracy** of modelling efforts
- **input of data** from the industrial stakeholder \leftrightarrow **workflow/ simulation** tools
- **confidentiality** issues of industrial data
- **expertise** for results interpretation

Neutrality

- give **neutral advice**; third parties might be involved in the implementation of the modelling workflow
- be **free** from hidden **self-interests**: must place the interest of the clients before the interests of the Translator
- **more than one solution** should be proposed
- proposed solution should **not be biased** towards the Translators **favourite models, methods or software tools**

TRAINING





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Training for translators

TRAINING

TECHNICAL

input data
modelling solutions
simulation strategies
computational effort
accuracy & error
expected outcome
...

TECHNICAL ACADEMY

SWO, MoDe

ECONOMICAL

cost assessment
resource investment
return on investment
risk assessment
decision making
...

ECONOMICAL ACADEMY?

EC expert? Prof. of economics?

TRAINING MATERIALS





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Translation process: successful workflow

Close academic/industrial
collaboration (60%)

Regulation of the
translation activity
(20%)

Realizable plans
(20%)

Correct interpretation/utilization of
the model and analysis of the results

- We should not forget the model accuracy...
- The language to address the SMEs (industry) representatives should be appropriate and balanced: neither too technical nor too basic...
- It is recommended for translators to visit the company production lines
- It is important to estimate the costs of the project and of the translation activity

EMMC, H1 Workshop in Vienna (April 2017)





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EMMC-Workshop

Goal:

- to find strategies for successful integration of materials modelling into industrial decision making based on efficient translation
- to understand the role of so-called translators

Agenda:

- **Unit 1** Advanced composite materials/ nanocomposites for Industrial use: modelling challenges and translation experience
- **Unit 2** Materials modelling for electronic devices / sensors: successful translation expertise and modelling aspects
- **Unit 3** Effective translation strategy and materials model creation for Energy & Funktional Materials
- **Unit 4** Hydrides for Energy Storage: modelling approaches and translation realization

Conclusion and Discussion; **EMMC Translation Actions; Funding opportunities**

Tutorial / Training -> test use of models





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Survey questions

1. Is it **important to know** the applicability and **limitations** of the software?





2. Are you able to make a **rough estimation** on the **cost/investments** for performing modelling project?





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Survey questions

3. Could you specify (at least three) and prioritize the **criteria** for choosing/using specific **model/software**?





4. Can you specify the **level of maturity** / development of the **models** you use/develop?





5. Can you provide, if needed, **special conditions/licences** for SMEs to use your software?





6. Which **training materials** are very important for Translators?





Advanced composite materials/ nanocomposites for Industrial use: modelling challenges and translation experience

Dr. Ronan Le Goff, IPC, FRANCE

Dr. Roger Assaker, e-Xstream Engineering, LUXEMBOURG





Materials modelling for electronic devices / sensors: successful translation expertise and modelling aspects

Tomasz Krupicz, Comsol Multiphysics, GERMANY

Dr. Tobias Neumann, Nanomatch GmbH, GERMANY





Effective translation strategy and materials model creation for Energy & Funktional Materials

Dr. Thierry Deutsch, Laboratoire de Simulation Atomistique,
CEA, Grenoble, FRANCE

Dr. Daniele Stradi, QuantumWise A/S, DENMARK





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Survey questions

- ❑ Is it **important (for Translators) to know** the applicability and **limitations** of the software?
 - Could you please briefly outline limitations of a software?
 - SWOs would not like to mention the limitations of their software. **Why?**
 - Is it possible to initiate SWO to describe **(for Translators)** the real limitations of software? **How?**





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Survey questions

- Could you specify (at least three) and prioritize the **criteria** for choosing/using specific **model/software**?

- Can you provide, if needed, **special conditions/licences** for SMEs to use your software?
 - 3 licensing models:
 - Commercial
 - R&D
 - Academic
 - **15-days demo licenses** and **extended (30 days)** trial licenses are available for SMEs interested in testing the software
 - For SMEs which do not have sufficient in-house computational resources to run the software, company offers a **flexible** and **cost-effective** new model to run the software in the cloud
 - **Other options? Which** special conditions/licences could be provided the for SMEs?

Lunch break





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Hydrides for Energy Storage: modelling approaches and translation realization

Prof. Marcello Baricco, University of Turin, ITALY





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Survey questions

- Are you able to make a **rough estimation** on the **cost/investments** for performing modelling project?
 - What do model developers need to know to estimate the modelling project cost/investments ?
 - Where can they find these knowledge?

- Can you specify the **level of maturity** / development of the **models** you use/develop?
 - How would you define the **model maturity**?





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Survey questions

- ❑ Which **training materials** are very important for Translators?
 - Who can/should provide the training material for Translators?
 - Where could Translators find training materials?





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Conclusion

- **strategies** for successful integration of materials modelling into industrial decision making based on efficient translation
- **role** of Translators
- **recommendation** for the integration of materials modelling into industrial decision making
- **additional steps** for EMMC-Translation activity





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Funding opportunities

- There are many different funding available:
 - Regional funding
 - National funding
 - EUREKA (intergovernmental, for SMEs)
 - H2020 funding:
 - ✓ There are many H2020 funding opportunities: ERC (science), e-INFRA (infrastructures), NMPB (industry: *Nanotechnologies, Advanced Materials, Biotechnology and Production*), etc.
 - ✓ There is a strong emphasis on **industrial exploitation!**
 - ✓ NMPB deals with materials modelling, including electronic, atomistic, mesoscopic and continuum models
 - ✓ Many NMPB projects deal with materials modelling, see

http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

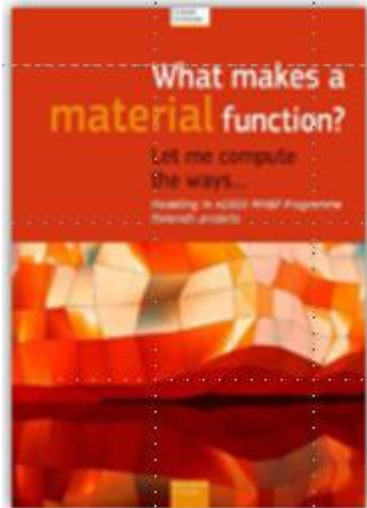




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Review of Materials Modelling (RoMM)

<https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/>
(free!)



- ❑ Modelling is a powerful tool that supports materials research in the development of novel or improved applications
- ❑ The **sixth version** of the Review of Materials Modelling (RoMM) defines the necessary concepts and proposes names which harmonies the language of modelling subfields
- ❑ The common language is hoped to foster dialogue between industrial end-users, software developers and theoreticals
- ❑ The RoMM also makes new classification (taxonomy) and the relation between concepts from the basis for ontology
- ❑ This in its turn can be a basis for metadata development necessary for interoperability
- ❑ The scope and achievements of the modelling in 36 H2020 *projects* are presented with this harmonized language using the MODA template





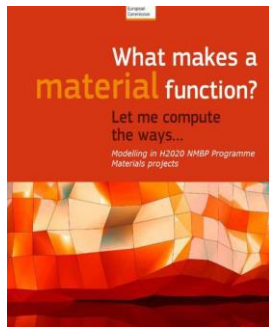
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EMMC Translation Activity

- Translation - Benefits for industry:
 - to cover gaps between industry and research/science innovation
 - to integrate material modelling into business decisions
 - to show modelling potential:

powerful tool that supports materials research in the development of novel or improved applications

MODA Aspects --
in the RoMM VI



Modelling in
H2020 LEIT-NMBP Programme
Materials and Nanotechnology projects

- **Translation Workshop EC and EMMC**, September, 21, 2017, Brussels
- **ECCM 6/ECFD 7 (ECCOMAS) 2018**, June 11-15, Glasgow
- **MS147 “Materials modelling for industrial use“**
- **CECAM** Trainings/ Workshop “Economical aspects of modelling” -> in 2019
- **CALL’s: 2019-2020** (Translation)

Acknowledgements: Anne F de Baas, EC





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Tutorial/Training

- Unit 1: **Ronan Le Goff** (IPC, FRANCE) – Room **210**, FMB*
- Unit 2: **Tomasz Krupicz** (Comsol Multiphysics, GERMANY) – Room **231**, MB**
Tobias Neumann (Nanomatch GmbH, GERMANY) – Room **212**, FMB
- Unit 3: **Daniele Stradi** (QuantumWise A/S, DENMARK) – Room **213**, FMB
- Unit 4: **Marcello Baricco** (University of Turin, ITALY) – Room **231**, MB

* FMB - Faculty of Mathematics building

** MB - Main building





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EMMC-Workshop, Warsaw 18th September 2017