



Software Focus Area Kickoff Meeting





Outline



- Initial Team
- Background and related CSA activities
- EMMC International Workshop 2021
- Task Groups
- Next Steps



Software Focus Area: The Initial Team



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EMMC: Our Mission



- The development of new and improved materials and the use of existing materials in new applications are a key factor for the success and sustainability of European industry and society in general.
- The European Materials Modelling Council considers the integration of materials modelling and digitalisation critical for more agile and sustainable product development.
- Created in 2014, the EMMC undertook numerous consultation and networking actions with representatives of all stakeholders including modellers, materials data scientists, software owners, translators and manufacturers in Europe.



EMMC: Our Goals



- Improve interaction and collaboration between all stakeholders
- Facilitate integrated modelling and digitalisation of materials
- Increase awareness & adoption of materials modelling in industry
- Support the software industry for materials modelling in Europe
- Identify main obstacles to increased use of modelling of materials in European industry and develop strategies to overcome them
- Coordinate & support actors & mechanisms by creating bridges between academic research and industrial exploitation
- Support sustainability of modelling and digitalisation in Europe



EMMC: Roadmaps



The EMMC elaborates [Materials Modelling Roadmaps](#) after intensive consultation and networking with all stakeholders. The EMMC Roadmaps

- identify major obstacles to widening the use of materials modelling in European industry and
- recommends strategies to overcome them.



EMMC: Focus Areas



Model Development



Interoperability



Digitalisation



Software

Impact in Industry



Policy





Software Focus Area



The main purpose of this Focus Area is on motivating, facilitating, and promoting the transfer of software for computational materials science into ready-to-use tools for industry, and on providing a forum especially for industrial end users to express their evolving requirements for materials modelling software.



Software Focus Area: Objectives



- Materials science (materials and materials properties)
- Methodologies and algorithms
- Integrability and interoperability, multiscale modelling
- Ownership, licensing, and legal issues
- Verification and validation
- Distribution, documentation, and training
- Maintenance and support
- Models for sustainable software ecosystems



Background: CSA activities 2016-2019



White paper
for standards of modelling software development

Volker Eyert, Materials Design and Kurt Stokbro, Synopsys

 **EMMC-CSA WEBINAR**
Volker Eyert, Materials Design and Kurt Stokbro, Synopsys
Best Practices for Software Development
EMMC-CSA WEBINAR #2 www.emmc.info May 29, 2018 10-11 am GMT


 **Expert Meeting on**
Open source, free software and commercially supported software for materials modelling
October 25-26, 2018 @ Paris / France
Erich Wimmer, Volker Eyert, Materials Design and Kurt Stokbro, Synopsys

 **EMMC-CSA Expert Meeting on**
"Sustainable economic framework for materials modelling software"
Report online now!!
July 4, 2018 – Cambridge, UK
Alexandra Simperler and Gerhard Goldbeck, Goldbeck Consulting


BUSINESS MODELS AND SUSTAINABILITY FOR MATERIALS MODELLING SOFTWARE
Alexandra Simperler and Gerhard Goldbeck, Goldbeck Consulting
<https://zenodo.org/record/2541723>

 **EMMC-CSA WEBINAR**
Alexandra Simperler, Goldbeck Consulting
Introductions to Standards in Software Development for Beginners
Presentation & Recording available now!!
January 18, 2019

 **EMMC WORKSHOP**
Alexandra Simperler, Gerhard Goldbeck, Goldbeck Consulting, Natalia Konchakova, HTZ
Business Models for Materials Modelling Software
May 20-21, 2019 / St John's Innovation Centre, Cambridge, UK

 **EMMC WEBINAR**
Georg J. Schmitz, ACCESS
MICRESS, a commercial software... developed and maintained by a non-profit organization
EMMC WEBINAR #7 July 15, 2019 10:00-11:30 am CEST

 **EMMC Documentation on**
Alexandra Simperler, Goldbeck Consulting
Training material for standards in software development and where to find it
Published on July 17, 2019

 **EMMC-CSA WEBINAR**
Malgorzata Celuch, QWED
"Why set up a modelling SME when you are student? The economic impact of QuickWave software"
Recording available!
EMMC-CSA WEBINAR #8 August 23, 2019 – 12-1.30 pm CEST

 **EMMC WEBINAR**
Alexandra Simperler, Goldbeck Consulting
"How to find the right business model for materials modelling software"
EMMC WEBINAR #10 August 28, 2019 10:00 am CEST



EMMC International Workshop 2021



Plenary Speaker: **Nicola Marzari, EPFL**
The digital infrastructures for 21st-century science



Guideline for Sessions:

The main purpose of this Focus Area is on motivating, facilitating, and promoting the transfer of software for computational materials science into ready-to-use tools for industry, and on providing a forum especially for industrial end users to express their evolving requirements for materials modelling software.



EMMC International Workshop 2021



Session 1: Industrial Requirements to Materials Modelling Software

- Impulse talks shall kick off a discussion about actual and future requirements of industrial end users for materials modelling software
- Speakers preferably from industry
- Possible issues to be addressed
 - Accuracy vs. complexity
 - Integrability and interoperability
 - Multiscale modelling



Confirmed speakers

- Kurt Stokbro
- Sophie Loehle, TOTAL



EMMC International Workshop 2021



Session 2: From Materials Science Software to Industrial Tools

- Impulse talks shall illustrate ways for better transfer of materials science software into industrial tools
- Speakers from all areas
- Possible issues to be addressed
 - Sustainable software ecosystems
 - Multiscale modelling
 - “Software chain”



Confirmed speakers

- Scott M. Woodley, UCL
- Flavio Souza, Siemens
- Ellad Tadmor, UMN



Task Group Suggestions



- International Workshop Organisation
- Software Survey
- Success Stories
- From Software to Industrial Tools
- Best Practices for Software Development
- Benchmark Collection in Literature
- Documentation, Training, and Support
- Business Models and Sustainability
- ...



Next Steps



- Evaluate survey ([questionnaire](#))
- Finalize sessions of International Workshop 2021
- Establish and support Task Groups



THE EMMC ACTIONS



Thank you!

Join the EMMC ASBL!

<https://emmc.eu/register/>