



Software Focus Area Meeting





Outline



- Overview of the Software Focus Area
- Recent Activities
 - EMMC International Workshop 2021
 - Model Development & Software Survey 2021
- Establish Task Groups
- Next Steps



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.

Details: <https://emmc.eu/focus-areas/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



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



Speakers

- Kurt Stokbro, Stokbro Invest
- Sophie Loehle, TOTAL
- Jonathan Mueller, VW

Rapporteur

- Michael Seaton, STFC



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”



Speakers

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

Rapporteur

- Guiseppe Fiscaro, CNR



Survey 2021



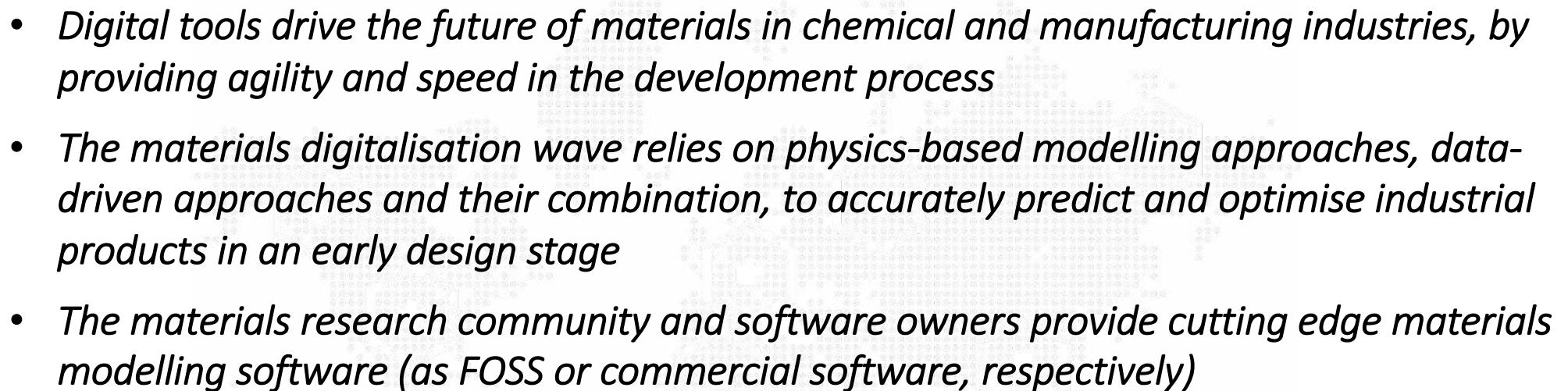
- Kick-off initiative by the Software (FA4) and Model Development focus areas (FA1) of the European Materials Modelling Council (EMMC) after its reincarnation from CSA into an ASBL in 2020
- Organized by Ilian Todorov, UKRI Science and Technology Facilities Council, UK
- December 2020 – January 2021
- 98 responders



Survey 2021 - Purpose



- To survey the opinion of the wider community of materials modellers and clarify the communities' interests to the benefit of EMMC
- FA4 and FA1 are closely linked, connected and bound by the subject of scientific methodology. Hence overlap of audiences, despite different stakeholder groups
 - FA1 – a modelling and simulation researcher, modeller and theorist
 - FA4 – a software owner, computational/computer scientist, and research software engineer
- Identify: our audiences, materials modelling interests, types of funding, incentives and bottlenecks in adopting technologies relevant to the FAs, changes to how research is carried out – 5-year backward and forward views, most targeted material properties in research, digital twinning software integration, and finally, the ways EMMC can address community





Survey 2021 – Conclusions II



- *The EMMC focus areas Model Development and Software lead the EMMC activities in their domains and the key researchers' needs are:*
 - *FA4 – more accurate, robust, well-documented and validated/verified software, with better availability of parameters data (easy generation of input), applicability (general purpose/demonstrators), scalable performance & lower complexity to use*
 - *FA1 – improved capability, accessibility and performance of methods, with better applicability (general purpose over specificity)*





Task Groups: Status



1. Success Stories
2. Best Practices for Software Development
3. From Software to Industrial Tools
4. Documentation, Training, and Support
5. Business Models and Sustainability



Background: CSA activities 2016-2019



White paper for standards of modelling software development

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

EMMC WORKSHOP
Alexandra Simperler, Gerhard Goldbeck, Goldbeck Consulting,
Natalia Konchakova, IZG
Business Models
for Materials Modelling Software

May 20-21, 2019 / St John's Innovation Centre, Cambridge, UK

Recording available!
EMMC-CSA WEBINAR
Małgorzata Celuch, QWED
"Why set up a modelling SME when you are student?
The economic impact of QuickWave software"

EMMC CSA WEBINAR #6
August 23, 2019 – 12-1.30 pm CEST

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

BUSINESS MODELS AND
SUSTAINABILITY FOR
MATERIALS MODELLING
SOFTWARE

Alexandra Simperler
and Gerhard Goldbeck,
Goldbeck Consulting

<https://zenodo.org/record/2541723>

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

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 WEBINAR
Alexandra Simperler, Goldbeck Consulting
Introductions to Standards in
Software Development for Beginners

Presentation & Recording available now!!
January 18, 2019

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 WEBINAR
Alexandra Simperler, Goldbeck Consulting
"How to find the right business model
for materials modelling software"

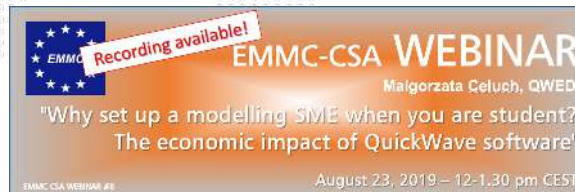
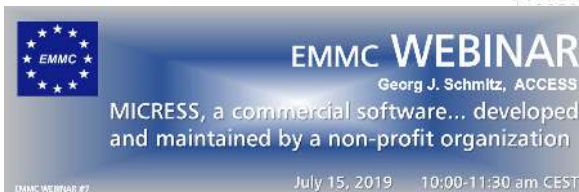
EMMC WEBINAR #10
August 28, 2019 10:00 am CEST



Task Group 1: Success Stories



- Objective: Demonstrate added value of MM in Industry and Society
- Actions
 - Collect success stories from across the EMMC (members, speakers, ...)
 - Propose/agree on requirements (papers, reports, no theses)
 - Publish online on EMMC website (EMMC internal)
- People: VE, UM, NN





Task Group 2: Best Practices for Software Development



- Objective: Provide guidelines for Software Development in MM
- Actions
 - Collect and make available information about best practices for MM software
 - Collect experiences (attention points, application, solver, data management, GUI, multiscale, cloud, FOSS and commercial, ...?)
- People: VE, NN, NN

White paper
for standards of modelling software development
Volker Eyert, Materials Design and Kurt Stokbro, Synopsys

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Software Development for Beginners
Presentation & Recording available now!! January 18, 2019



Task Group 3: From Software to Industrial Tools



- Objective: Encourage professionalization of MM software
- Actions
 - Identify requirements for transforming MM software into industrial tools
 - Identify software, which has successfully completed transition from academia to industry-readiness
 - Contact and learn from companies which successfully completed such transformation processes (Siemens DI SW, Global TCAD Solutions, Synopsys, VASP GmbH, Materials Design, ...)
- People: NN, NN, NN



Task Group 4: Documentation, Training, and Support



- Objective: Provide links to industry-level training material
- Actions
 - Survey to collect experiences with software documentation, training and support, as well as needs for improvements
 - Look at: in-house coding, FOSS, commercial software, ... ?
 - Achieve customer success
- People: NN, NN, NN

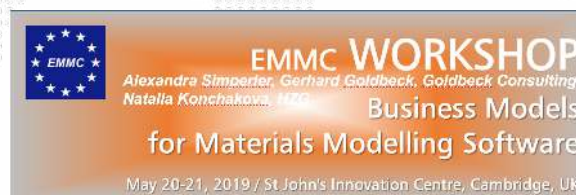




Task Group 5: Business Models and Sustainability



- Objective: Identify business models in industrial software deployment
- Actions
 - Collect information from Goldbeck Consulting from earlier studies in EMMC
 - Circulate some questions to software partners, ask for input from previous EC project participations in Materials Software area
- People: SD, AS, NN





Task Groups: Webpages



- Create webpages for each task group (Ernst-Dieter) ✓
- Add existing CSA material to TG webpages (Ernst-Dieter) ✓
 - EMMC → Focus Areas → Software → TG 4.2

TG 4.2 - Best Practices for Software Development

Objective

Provide guidelines for Software Development in Materials Modelling

Related documents

 WEBINAR  Best Practices for Software Development by Volker Eyert (MDS, FR) Kurt Stokbro (Synopsys, DK) LMMC CSA Webinar, recording	 WEBINAR  Introduction to Standards in Software Development for Beginner by Alexandra Simperler (Goldbeck Consulting Ltd., UK) EMMC-CSA Webinar, recording	
 WHITE PAPER  White Paper for Standards of Modelling Software Development by Volker Eyert (MDS, FR) Kurt Stokbro (Synopsys, DK) LMMC CSA White Paper	 REPORT  Open Source, free Software and Commercially Supported Software for Materials Modelling by V. Eyert, E. Wimmer (MDS, FR) K. Stokbro (Synopsys, DK) EMMC-CSA Expert Group Meeting, report	 DOCUMENTATION  Training Material for Standards in Software Development and where to find it by K. Stokbro (Synopsys, DK) G. Goldbeck, A. Simperler (Goldbeck Consulting, UK) V. Eyert, E. Wimmer (MDS, FR) EMMC-CSA Documentation, report



Task Groups: Next Steps



- Create webpages for each task group (Ernst-Dieter) ✓
- Add existing CSA material to TG webpages (Ernst-Dieter) ✓
- Establish Task Groups
 - Teams
 - Organization
 - TG meetings
- Check and update material (TG members)



Task Groups: Members



Task Group	Members			
1	Volker Eyert	Umberto Martinez		
2	Volker Eyert			
3				
4				
5	Stijn Donders	Alexandra Simperler		



Next Meeting



February-March 2022



Thank you!

