EMMC International Workshop 2019
FEB 25-27, 2019 - Vienna / Austria

Venue

Parkhotel Schönbrunn

Hietzinger Hauptstr. 10-14, 1130 Vienna

Austria

Sponsors & Exhibitors

Responsible for content:
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TU Wien
Institute of Sensor and Actuator Systems
Gusshausstrasse 27-29, 1040 Vienna, Austria

The European Materials Modelling Council

is organising the

EMMC
International Workshop 2019

February 25-27, 2019

Vienna / Austria

Venue

Parkhotel Schönbrunn

Hietzinger Hauptstr. 10-14, 1130 Vienna

Austria

EMMC International Workshop 2019

Workshop organisation

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Erich Wimmer, Materials Design, France

Rudolf Koopmans, Koopmans Consulting, Switzerland

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EMMC International Workshop 2019

Introduction

Talk 1

Nadja Adamovic (EMMC Chair / TU Wien, AT)

The European Materials Modelling Council

Talk 2

Anne de Baas (European Commission)

European Commission: Activities in the Framework of Industrial Commons

Plenary Talks

Plenary Talk 1

Sandeep Namdeo (Airborne Oil & Gas, NL)

Materials modelling - A key enabler for the business

Plenary Talk 2

Eric Little (OSTHUS, US)

Beyond the Models: Applying Semantic Technologies Across the Enterprise

Plenary Talk 3

Berend Smit (EPFL, CH)

The nanoporous materials genome in action

Plenary Talk 4

Ben Anderson (RTI, US)

Technology Infrastructure to support Advanced Materials: Economic Analysis of Needs and Opportunities

Plenary Talk 5

Barbara Holtz (Dassault Systemes, UK)

Collaborate for Faster Innovation with the 3DExperience Platform

Plenary Talk 6

Mike Haverty (Applied Materials, US)

Deploying Materials Modeling in Industry - Successes and Challenges

Session 1   MON, FEB 25, 2019   14:45-16:30   IMPERIAL BALL ROOM

Bridging physics-based and data-driven modelling

Chair
Kersti Hermansson (Uppsala University, SE)

Impulse 1
Bart Rijksen (Dow Benelux B.V., NL)
Pros and cons of physics-based and data-driven modelling in industry

Impulse 2
Signe Riemer-Sørensen (SINTEF Digital, NO)
Integration of machine learning (ML) and physics-based modelling

Introduction

Materials modelling within science and engineering traditionally use physics-based models, but currently there is much excitement about big data and machine learning in materials and molecular modelling, and about the opportunities that these approaches may bring. But are there also scientific shortcomings associated? Is this development in fact driving us towards "... numbers, not insights", i.e. away from the often quoted scientific wish for "... insights, not numbers"?! Can we come to an understanding in the community about how physics-based insight and data-driven analysis may complement each other?

Discussion points and questions
- What are the pros and cons of physics-based and data-driven modelling in industry?
- Which approaches are perceived as the most reliable and trustworthy - and why?
- Are there examples of successful integration of machine learning (ML) with physics-based modelling within different industrial sectors?
- Are there educational examples (successes or failures) of the use of machine learning (ML) within different industrial sectors?
- Will we be able to get deep scientific insights, or even physics theories, from ML?
- Where will we be 5 years from now? 10 years from now?

Session 2   MON, FEB 25, 2019   14:45-16:30   ROOM ÖSTERREICH

Digital Transformation of Materials R&D

Chair
Georg J, Schmitz (ACCESS, DE)

Impulse 1
Benedikt Ziebarth (Schott AG, DE)
Materials Informatics and Semantics for Glass Development

Impulse 2

Nadezhda N. Kiselyova (Russian Academy of Sciences, RU)

Machine Learning for Inorganic Compounds Design

Impulse 3

Egon Willighagen (Univ Maastricht, NL)

Nanomaterials ontologies: data integration and applications to risk assessment

Introduction

Investments in key enabling technologies projects have been creating a huge wealth of data and knowledge, which however remain largely within silos. Results not immediately exploited are typically lost to innovation. Even data deposited in openly accessible repositories remain largely out of view and are hard to re-use due to a lack of a common semantic basis. Impacting on innovation in materials, products and processes requires a strategic approach to digitalisation involving a wide range of stakeholders along value chains and deep knowledge in materials, processes and digital technologies.

Discussion points and questions

- How can we increase European manufacturing and process industry capacity to extract knowledge from data?
- How can we support leadership by digital transformation of data into knowledge?
- How can we achieve that manufacturing companies remain competitive (new products, high-added value) on the basis of knowledge extracted from wide-spanning data sets?
- How can we promote European benefits from data management, standardised documentation enabling interoperability and linking tools for enriching and enhancing the usability of data?
- What actions are proposed for a common semantic knowledge base in materials?
- What practical ways forward are there for industry to reap the benefits of digitalisation in materials?

Session 3	MON, FEB 25, 2019 14:45-16:30	ROOM UNGARN

Towards the Translator as a key professional

Chair

Denka Hristova-Bogaerds (DPI, NL)

Impulse 1

Ronan Le Goff (IPC, FR)

How to make an academic a professional translator?

Impulse 2

Yuri Kadin (SKF Research & Technology development, NL)

Modelling of surface defects in ceramics: translation of industrial challenge into modelling solution

Introduction

Within EMMC, translation is considered as the process of translating an industrial challenge/ problem into a solution with the help of modelling. The experts that are performing this process are called Translators. They provide a service for the companies and can be either academics, software owners/engineers, internal employees of the company or independent translators (not related to specific research/industrial institution). Translators are primary players at the interface between industrial end-users on the one hand and software owners and modellers on the other hand. Translators support the usage of materials modelling in industrial R&D to the same level as experiments are used today.

Discussion points and questions

- Translator role and modelling executor role: advantages and disadvantages. What would the client prefer?
- Internal and external translators: interactions, training, pros and cons?
- Business model for translators. Market Places and Open Translation Environment?
- Translation Cases: the benefits of having those and how to overcome the difficulties in preparing them?
- Translation Profile: How can Translators increase their visibility? How client can understand /estimate the level of the translation expertise?

Session 4　　MON, FEB 25, 2019　17:00-18:45　IMPERIAL BALL ROOM

Verification and validation as tools for promoting discrete models in industry

Chair
Roy Chantrell (UoY, UK)

Impulse 1
David Cebon (Granta, UK)
Uncertainty Quantification

Impulse 2
Jean-François Imbert (SIMconcept Consulting, FR)
Concepts of Verification and Validation

Introduction

In many industrial applications, materials modelling is not trusted as a predictive tool at small scale: Modelling is often seen just as a qualitative tool, useful for pre-screening. There are many reasons for this situation: besides the theoretical and computational limits of the existing models, industries suffer from a knowledge gap and a communication gap between experimentalists and modellers. In other to overcome these limits, we envision a more systematic verification and comparison with experiments (validation), e.g. by means of benchmarking and round-robin tests, blind tests and simulation challenges. This would lead to making available success stories and identifying dead ends.

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Discussion points and questions

- To what extent is a formal V&V process likely to enhance the uptake of materials models by European industry?
- How realistic is this in validating model performance in the case that initial and boundary conditions and input data are provided by the customer, and relate to a commercially sensitive application?
- To what extent is the V&V process limited by such incomplete feedback due to testing against proprietary information?
- This problem is often solved on a case-by-case basis, is it possible to formalize this process or at least define best practice?
- Comments please on the following roadmap
  - Initial V&V workflows validation & Verification
  - Towards ISO and formalized standards
  - CEN-Workshop on terminology…

Session 5 MON, FEB 25, 2019 17:00-18:45 ROOM ÖSTERREICH

Open Modelling Frameworks

Chair
Emanuele Ghedini (Università di Bologna, IT)

Impulse 1
B.P. Gautham (TCS Research, IN)

Standardization of representation of materials, manufacturing process and their simulation through metamodeling driven ontology

Impulse 2
Klaus Wolf (Fraunhofer SCAI, DE)

VMAP – A new and open Standard for virtual Manufacturing Workflows in 3D

Impulse 3
Adham Hashibon (Fraunhofer IWM, DE)

SimPhoNy: A framework integrating all types of models and computational representations.

Introduction

A large number of well-established integrated simulation environments exist, including commercial closed systems, commercials systems with APIs and open source environments. However, there is a lack of truly open modelling frameworks that enable end users to integrate any modelling, pre or post processing tools on a widely agreed, open standard footing for all types of models (electronic, atomistic, mesoscopic, continuum). At the very heart of an open modelling framework is the Open Simulation Platform (OSP) which is formulated as a set of common standards and related tools that form the basic environment on top of which compatible and compliant simulation workflows can be developed and run.

Discussion points and questions

- What modelling frameworks, open or otherwise are the most important ones to you and your community/organisation?
- What kind of standardisation is needed to use an OSP for interoperability?
- How would you want to use an OSP to fully automatize data transfer between models?
- Is full flexibility with tools that can link to it important to you?
- What would an OSP have to offer so that you would use it regularly?
- What would an OSP have to offer so that you would enable your software to link to it?

Session 6   MON, FEB 25, 2019   17:00-18:45   ROOM UNGARN

Translation for and by SMEs

Chair
Jesper Friis (SINTEF, NO)

Impulse 1
Amit Bhave (CMCL Innovations, UK)

Synthesis of desirable nanoparticles and reduction of unwanted nanoparticles: Translation process and learnings

Impulse 2
Nicola Gramegna (EnginSoft S.p.A., IT)

Material modelling in Design chain of lightweight components

Introduction

A wider use of material models will make European SMEs more competitive on the market. The potential of material modelling for shortening the product design phase and decreasing the production costs is recognized by the manufacturing industry across Europe, including SMEs (EMMC roadmap 2018). In this session we illustrate and discuss the importance of materials modelling for SMEs through successful examples.

Discussion points and questions

- How can we increase the *awareness* among SMEs of the benefits with materials modelling?
- How can we make translators, and thereby material modelling, *more accessible* to SMEs?
- What *additional challenges* does a translator face when performing translation for SMEs? Is there a need for training of translators tailored towards SMEs?
- How can materials modelling be made *more attractive* to SMEs, both in terms of making use of the results in daily operation and with respect to value creation.

Session 7   TUE, FEB 26, 2019   10:15-12:00   IMPERIAL BALL ROOM

Coupling & Linking of models towards industrial needs

Chair
Pietro Asinari (Politecnico di Torino, IT)

Impulse 1
Kwang-Ryeol Lee (KIST, KR)
The thematic platform as a multiscale simulation environment

Impulse 2
Ludovic Briquet (Johnson Matthey, UK)
The gaps and challenges in linking models: a perspective from catalysis

Introduction

Detailed modelling of physical phenomena inherently embeds dealing with different length and spatial scales, which in some cases become disparate. This multi-scale nature must be properly addressed for accurate modelling; however, accurate representation leads to stiff systems, causing a dramatic limiting factor for the numerical solution with standard methods (e.g. very small time-steps and/or very fine spatial discretization). This problem finally hinders modelling advancements for engineering and industrial applications; therefore, multi-scale methods able to address and overcome this limit are desirable. With this purpose, methods using Coupling & Linking (C&L) strategies have been - and are being - developed, together with and in parallel to model-reduction techniques (ROM, Reduced-Order Modelling). The aim of this session is to provide an overview of the currently available techniques for C&L and ROM, and their potential in industrial applications.

Discussion points and questions

- In your opinion, which are the most important current gaps to be filled with regards to C&L methods? Where to put more effort: discrete-discrete, discrete-continuum?
- About wide adoption of C&L methods in industry: which are the most relevant limiting factors? Lack of specific expertise in R&D departments? Lack of success stories about the benefits of adopting these techniques? Unawareness of their potentiality?
- In your opinion, which are the most relevant industrial sectors that may particularly benefit of C&L methods? Why? Which are the most relevant and urgent phenomena to tackle via C&L methods?
- About strengthening the collaboration and cooperation between the academic model developers and industrial researchers: how can synergy on C&L method development and application be promoted to achieve a win-to-win situation?
- Do you think that a more systematic V&V layout would boost industrial application of C&L methods? In your opinion, is V&V a critical issue for widespread use of C&L in industry?

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Session 8   TUE, FEB 26, 2019   10:15-12:00   ROOM ÖSTERREICH

International Materials Ontology

Chair
Gerhard Goldbeck (GCL, UK)

Impulse 1
Dimitris Kiritsis (EPFL-ICT, CH)

Industry Ontologies Foundry: foundations and industrial applications

Impulse 2
Toshihiro Ashino (TOYO Univ., Japan)

Materials Information Integration Based on Ontology

Impulse 3
Emanuele Ghedini (Università di Bologna, IT)

EMMO: an ontology for the physical sciences

Introduction

Interconnected, interoperable data and modelling resources are essential for advancing materials and manufacturing research, development, deployment and management.

The EMMC is seeking support of the entire materials community for the establishment of common standards underpinning not only materials modelling interoperability and but more widely integration of all types of materials as well as materials processing and manufacturing information. The aim is to facilitate FAIR access to materials resources including data concerning modelling workflows, materials properties and characterisation.

Achieving interoperability should be based on common ontologies. Ontologies also provide for concerted access to repositories of data and of services, and will also enhance interoperability between materials models and integration of services.

Discussion points and questions

- Are ontologies important to you?
- How can we get all relevant stakeholders on board?
- What is needed to keep the international materials ontology going (RDA, new projects/funding, forming a consortium,…)?
- Can we achieve "interoperability"? What does this mean to you?
- What sort of training/ dissemination/ would you like to see?

Session 9   TUE, FEB 26, 2019   10:15-12:00   ROOM UNGARN

Training for translators, with emphasis on economic concepts and skills

Chair
Natalia Konchakova (HZG, DE)

Impulse 1
Hein Koelman (DOW, NL)

What is expected from a Translator in a big company – examples and learnings

Impulse 2
Eliodoro Chiavazzo (POLITO, IT)

Artificial intelligence based tools to support translators in material modelling: The ongoing training test case at Politecnico di Torino and Politecnico di Milano

Introduction

Translators are professional profiles able to bridge industrial needs and state-of-the-art academic research to drive industrial innovation; thus, they present a multiplicity of skills spanning technical and economic knowledge, communication and soft skills. In this session, we provide an overview of the training scheme defined by the EMMC, with particular emphasis on the economic concepts and skills that Translators must have or acquire.

Discussion points and questions

- Do you think that the Translator profile identified by the EMMC is complete and meets exactly the expectations on their role in industry? If not, what can lead to a refinement of the role of these figures in industry?
- Do you think that the Training scheme for Translators identified by the EMMC is sufficiently complete or it can be improved by additional concepts? How?
- In your opinion, which are the most critical aspects in training of translators? Training should focus more on technical, economic aspects or both equally?
- Do you think Translators can have a central role in the digitalization of the European industry towards industry 4.0? If yes, how are they expected to contribute (e.g. main innovation areas and tools)?
- Which would be the additional training concepts that may be useful to provide to the Translators towards industry 4.0? Concepts about data-driven modelling? Concepts and tools for machine learning? Others?

Session 10   TUE, FEB 26, 2019   14:15-16:00   IMPERIAL BALL ROOM

Marketplaces: emerging business opportunities and impact on digital society

Chair
Donna Dykeman (Granta, UK)

Impulse 1
Takuya Kadohira (NIMS, JP)
Materials Integration

Impulse 2
Katri Valkokari (VTT TECHNICAL RESEARCH CENTRE OF FINLAND LTD, FI)
Novel business models for digital platforms

Impulse 3
Raimund Bröchler (INTRASOFT Intl., LU)
MARKET4.0 – A Multi-Sided Business Platform for Plug and Produce Industrial Product Service Systems - How do we build the manufacturing B2B marketplaces of the future

Introduction

Materials Modelling Marketplaces are emerging platforms that provide all stake holders-modellers, industry and translators - ample opportunities to interact, collaborate online and conduct transactions. Marketplaces host various services such as:

- Match making e.g., helping industry find and connect with modellers and experts (and vice versa),
- Modelling services e.g., as simulation tools as Software as a Service (SaaS) that enable industry to run and perform simulations online without the hassle of local installations or cutting thus licensing and maintenance costs,
- Development and use of customized simulation tools, workflows and Apps, e.g., enabling industry connecting to modellers to develop customized solutions for their workflows and providing this on the Marketplace platform or on premises behind a firewall,
- Training and education services,
- Data repositories and curation solutions,
- Collaboration services

Emerging Marketplaces should foster an ecosystem integrating all stakeholders and relevant or beneficial information in a sustainable and efficient manner. Marketplaces provide novel business opportunities for exploitation of modelling knowledge and related data.

Discussion points and questions

- What are marketplace services that you would pay for?
  1. Fee for basic usage
  2. Online Consulting
  3. Match making: search for expertise

4. product search: search for available and suitable software products
5. Advertisements in general
6. Advertisements of products
7. Advertisement of your expertise
8. Data repository access
9. Software as a Service/ Hardware as a Service
10. Configuration and/or execution of simulations or simulation workflows
11. Other

- What license schemes for Apps and software services would you prefer?
- What would be the type of enterprise/institution profiting most from a Marketplace ?(e.g. academia, SME, industrial R&D labs, software vendors, academic software developers, others)
- How do you expect the marketplace to help do your job better?
- Can you imagine services/tools/expertise that you would like to exploit on such Marketplaces?
- Can you imagine services/tools/expertise that you would like to exploit on such Marketplaces?
- What requirements do you have for the marketplace regarding security / data privacy and confidentiality / performance / data storage?
- What must the marketplace absolutely offer for you to consider its use at all?
- Which functionality should a marketplace offer so that you would use it every day?

- If there would be more than one materials modelling marketplace – e.g. less comprehensive, but more focused ones - would this mean you are less inclined to use it? How would this impact the chances to use it?

Session 11	TUE, FEB 26, 2019 14:15-16:00	ROOM ÖSTERREICH

Progress in the Industrial Deployment of Materials Modelling Software

Chair
Erich Wimmer (MDS, FR)

Impulse 1
Anders Engström (Thermo-Calc, SE)
Progress in the industrial deployment of thermodynamic modelling software

Impulse 2
Brian Dron (MDS, DE)
Drivers for the industrial deployment of atomic-scale materials modelling software

Impulse 3
Stan van Gisbergen (SCM, NL)
Opportunities and challenges in the industrial usage of chemistry modelling software

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Introduction

This session will address the present status of industrial deployment of materials modelling software especially in Europe. Examples of both successful implementations of atomistic simulations in industrial contexts and the barriers to overcome will be discussed. We will also focus on measures to be taken by all stakeholders to promote the integration of materials modelling in industrial processes.

Discussion points and questions

- Deployment of materials modelling in different industrial sectors including automotive & aerospace, chemical & petrochemical, electronics, specialty materials, pharmaceutical
- What are the main drivers of industrial uptake of materials modelling?
- What type of software is being used and most effective?
- International comparison
- Software as a service
- Organizational aspects, e.g. central modelling groups, modelling embedded in business units, budget, staffing

Session 12 TUE, FEB 26, 2019 14:15-16:00 ROOM UNGARN

Raising the maturity level of materials modelling adoption in industry

Chair
Tom Verbrugge (DOW, NL)

Impulse 1
Christa Court (University of Florida, US)
Modelling technology transitions associated with materials modelling

Impulse 2
Glenn Jones (Johnson Matthey, UK)
Materials modelling in JM : a brief history and look to the future

Impulse 3
Gino Duffett (NAFEMS International, UK/DE)
Engineering modelling and simulation: best practice and state-of-the-art

Introduction

Maturity Modelling is a process improvement approach and benchmarking framework whose goal is to help organisations improve their performance. It serves as a reference system for objective mapping of "as is" and "to be" states for business activities and operations. The Materials Modelling Maturity Model used by the EMMC is based on a Maturity model developed by Accelrys (now Biovia).

Discussion points and questions

- Can we list barriers and suggestions to overcome these to enable businesses to transfer their modelling ecosystem to a higher level?
- How can we make a wider range of stake holders aware of the modellers and their role?
- How can we promote the role of a translator?
- How can we promote the importance of early involvement between modellers and project teams?
- As one needs longer term changes of mindsets, what should be on an "On-boarding package" for higher level management?
- Better education: How can we support the changes in the undergraduate education towards even more know-how towards modelling? How can we support the education of non-modellers via different channels?
- How can we enable the specialisation/differentiation on roles within modelling as "the modeller" is deemed too generic?
- How can we support the fact that there is a difference between a data scientist and a modeller?
- What could be the best practices how materials modelling shall feature in the process of a company? Can we suggest a metrics and KPIs for modelling?
- How can we encourage better documentation for tools via SWO channels or internal WIKI pages and who can we find out what should be in there?
- How can we promote the concept of Data Trusts?

Session 13   WED, FEB 27, 2019   10:15–12:00   IMPERIAL BALL ROOM

Innovation hubs: foundations of modelling services

Chair
Georg J Schmitz (ACCESS, DE)

Impulse 1
Leopold Talirz (EPFL, CH)

The AiiDA lab ecosystem for computational materials science

Impulse 2
Stephan Hojda (RWTH Aachen University, DE)

AixViPMaP® Realizing ICME in a user- and practice- oriented manner

Impulse 3
Esther Hurtós (EURECAT- FormPlanet Test Bed, ES)

Modelling in a materials characterisation Test Bed. FormPlanet case

Impulse 4
Borek Patzak (Czech Technical University in Prague, CZ)

MuPIF open simulation platform: architecture and applications

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Introduction

Digital Innovation Hubs (DIH) are eco systems that consist of small and large industries, start-ups, researchers, accelerators, and investors that aim to create the best conditions for long term business success for all involved stakeholders. DIH are focused on enabling and delivering digitalization and innovation capabilities to all by means of providing focused and customized central access to a multitude of relevant services providing a better framework for the digital industrial revolution.

Innovation Hubs are meant to be essentially one-stop-shops that enable all stakeholders including small and large industries, software owners, modellers etc., to access, obtain and deploy and implement modelling services more rapidly. The goal is that companies become more competitive in their business models, materials/products/production processes developments using online digital technologies.

Innovation hubs are based on state of the art cloud technologies (private and public) providing the infrastructure for online platforms, that are essentially like "virtual competence centres" or "virtual institutes" providing access to the latest knowledge, expertise and modelling advances across all domains. Such innovation hubs should also be connected to regional centres helping bringing and connecting all key players together to collate all expertise from all Europe into one vibrant hub.

Discussion points and questions

- How to stimulate the participation of modellers, software owners, and companies in using modelling services on innovation hubs?
- How to supporting Open translation environments and other hubs in addition to the marketplaces: what is needed?
- How to guarantee a long-term research investments in the development of advanced models and workflows for materials simulations, verification and validation?
- How can innovation hubs better support and boost the development of electronic, atomistic, mesoscopic, and continuum models towards more predictive modelling with new capabilities?
- Strategies to join up the methods and models to use data from different scales and different granularities, i.e. model interoperability, or Coupling & Linking?
- Is there a need to have one dedicated modelling innovation hub and how to connect it with other thematic hubs (like, innovation hubs for photonics, steels, light materials, etc…? How important are licensing scheme and access rights to software tools and services?
- What benefits would modellers/software owners/companies gain by sharing modelling workflows) and expertise? What are the conditions for sharing if at all?
- If you are a company, how would you utilise such innovation hubs (e.g., the marketplaces)?
- Advantages for software owners resulting from the innovation hubs?
- Importance of interoperability and EMMO for modelling services and digitalisation of workflows?

Session 14 WED, FEB 27, 2019 10:15-12:00 ROOM ÖSTERREICH

Business Models for Materials Modelling Software

Chair
Alexandra Simperler (GCL, UK)

Impulse 1
Hans Fraaije (Culgi, NL)
Software, Service, Data

Impulse 2
Thomas Schrefl (Danube University Krems, AT)
Magnetic materials modelling – Bridging the gap between academic software and industry needs

Impulse 3
Zlatan Stanojevic (Global TCAD Solutions GmbH, AT)
How to Fail Commercially in Materials Modeling

Introduction

Successful software for materials modelling has an expected lifetime of many decades. This long-term nature requires a sound legal and business foundation: the ownership of software must be clearly established and the license models need to be carefully thought through to ensure a sustainable development and maintenance of the software and impactful exploitation by both academic and industrial end-users. Different business models carefully need to be considered when developing a strategy for long term sustainability of software and sustainment of the operation.

Discussion points and questions

- What do you consider the "perfect" ratio of services vs software sales?
- What can be done to use SaaS more as it regarded as a potentially way to attract customers who have not the means to get infrastructure and skilled staff in place?
- What attractive new ways are there to enable new materials modelling businesses?
- How is software sustainability best achieved?
- How can we enable a change in education and better recognition of the efforts involved in software sustainability?
- What role can Marketplaces play to facilitate a more dynamic materials modelling software ecosystem?
- How can Marketplaces be made sustainable, i.e. self-sustaining?
- What role could/should government support/EC play in sustaining marketplaces as a key facility for research and industry?

Session 15   WED, FEB 27, 2019   10:15-12:00   ROOM UNGARN

Business Decision Support Systems (BDSS): from concept to implementation

Chair
Glenn Jones (Johnson Matthey, UK)

Impulse 1
Adham Hashibon (Fraunhofer IWM, DE)

The FORCE: Integrating materials modelling in BDSS for applications in the field of chemical formulations

Impulse 2
Salim Belouettar (LIST, LU)

COMPOSELECTOR BDSS: An integrated business and material modelling framework for the selection and design of composites materials.

Introduction

Sustaining and growing businesses require continuous product innovation. Making meaningful business strategy decisions is an ever more challenging task in a global context. The combination of materials and business modelling to explore what technical solutions are economically viable is not yet exploited to the extent it could. The sheer volume of data and information combined with its dynamic nature demands an ever better understanding of possible options. There is a need for a Business Decision Support System (BDSS) that supports the selection of the optimal material and process, taking into account the implementation costs but also the associated risks, uncertainties and costs related to the modelling and simulation; a priority, especially for SMEs.

Discussion points and questions

- Tell us about your decision-making tool or methodology (BDSS) and how it integrates material model outcomes?
- What models are integrated in your BDSS: nature of the models – theory-driven (electronic, atomistic, mesoscopic, continuum) and/or data-driven.
- How does your solution integrate into existing BDSS?
- Who are the main actors using the BDSS, and what types of projects do they use it for?
- What are the main benefits, or key performance indicators, linked with integrating material model output with business decisions?
- Is your BDSS working successfully to include materials modelling outcomes? What is your vision of success?
- What are the business objectives/requirements in the product design process that your BDSS can support?
- What is the main value/business proposition for your BDSS?

Session 16   WED, FEB 27, 2019   13:00-14:45

Innovation hubs: next generation collaboration and services on marketplaces

Chair
Natalia Konchakova (HZG, DE)

Impulse 1
Marco Sebastiani (Roma Tre University, IT)
Open Innovation Environment in materials characterisation: the example from H2020 project OYSTER

Impulse 2
Alejandro Strachan (Purdue University, US)
Containerized scientific and engineering workflows in nanoHUB

Introduction

Innovation Hubs are meant to enable all stakeholders especially companies access to vast materials modelling related services including training, education, repositories of models and materials data, as well as collaboration and translator and translation platforms. The goal is that companies find information and connect to modellers (and vice versa) more efficiently and become more competitive in their materials/products/production processes developments using online digital technologies.

Innovation hubs are based on state of the art cloud technologies (private and public) providing the infrastructure for online platforms, that are essentially like "virtual competence centres" or "virtual institutes" providing access to the latest knowledge, expertise and modelling advances across all domains. Such innovation hubs should also be connected to regional centres helping bringing and connecting all key players together to collate all expertise from all Europe into one vibrant hub.

Examples of such hubs are the emerging Materials Modelling Marketplaces as envisioned by the EMMC. They provide foundations for collating all materials modelling expertise and assets, such as programs (commercial and open) on open and closed (behind firewall) online hubs.

Discussion points and questions

- How to stimulate the participation of modellers, software owners, and companies in using marketplace s and innovation hubs
- What kind of translation services and how to offer them on such hubs and market-places
- Can online translation work? And how?
- Match making: how to guarantee a level quality of services offered online?
- Privacy: as a user of an online hub or marketplace, what personal information would allow to be used for quality assurance purposes (name, expertise, past experience)?
- How important connections or integrations to services such as LinkedIn, research gate, google scholar, etc., would be to you?

- These hubs offer open discussion forum (like stack exchange, or see emmc.info/forums). In which scenarios would you use such forums actively?
- How would you envision education and translation services? How important and how to integrate with existing platforms (such as corsera)?
- Data sharing and exploitation? If you are a database owner what would convince you to link/host/share your database with or on such innovation hubs (and marketplaces)?
- As a modeller, what would convince you to upload your modelling workflows and data to such innovation hubs?
- Would you consider publishing data and preprints of your modelling on such innovation hubs?
- The EMMC created a MODA portal as a tool to document your simulation workflows, see http://emmc.info/moda. How would you envision a similar service to document your simulations and link your results to it? What improvements you would like to see in the moda or a similar tool?
- Would adding DOI and citation to MODA in addition to some peer review encourage you to use the online tool more?

Session 17　　WED, FEB 27, 2019　13:00-14:45　ROOM ÖSTERREICH

Open source and commercial software for Industrial Deployment of Materials Modelling Software

Chair
Kurt Stokbro (Synopsys, DK)

Impulse 1
Georg Kresse (University Vienna, AT)
The VASP Software GmbH: why did we go commercial

Impulse 2
Michael Haverty (Applied Materials, US)
Materials Integration: An All-Of-The-Above Approach

Impulse 3
Laurent Adam (e-Xstream engineering, BE)
Multi-scale continuum modeling with Digimat : 15 years journey from academia to industrial application

Introduction

This session will address the role of open source and commercially distributed software in the advancement of industrial usage of materials modelling software. The meeting is intended to be inspired by concise impulse talks addressing the following objectives, which are complemented by in-depth discussions on the points below.

Discussion points and questions

- How can open source software models be sustainable and benefit from industrial usage?
- Can the more immature fields of electronic and atomistic models learn from other fields (for instance continuum models) to progress industrial usage?
- Will we see new business models in the future, for instance cloud based?

Session 18　　　WED, FEB 27, 2019　13:00-14:45　　ROOM UNGARN

Increasing the adoption of materials modelling with SMEs

Chair
Amit Bhave (CMCL Innovations, UK)

Impulse 1
Katya Vladislavleva (Datastories, BE)
Materials modelling for, within and by SMEs

Impulse 2
Welchy Leite Cavalcanti (Fraunhofer IFAM, DE)
Working with SMEs: challenges and opportunities

Impulse 3
Donna Dykeman and Davide Di Stefano (GRANTA, UK)
Data availability and materials modelling market places for SMEs

Introduction

The wider and successful adoption of materials modelling by SMEs is currently rather limited. Among the hindering factors are the narrow domain of products/specialty of SMEs, their limited research budget, high software costs, lack of internal expertise (staff is limited), lack of data available for model validation and lack of robustness, accuracy and flexibility of the models. The confidence of the SMEs in the benefits of the modelling still needs to be gained. Therefore this session targets to discuss opportunities that can facilitate the implementation of modelling by the SMEs, such as material modelling market places, data availability and tools enabling evaluation of the benefits from modelling.

Discussion points and questions

- SMEs often lack sufficient internal expertise or experience to evaluate the modelling costs and to understand the possibilities of modelling. Therefore they may need help, for example from the translators, to identify the value of modelling for their business. However, this service may be too expensive and investing in internal experts to do this job (as additional expertise) could be a more valuable option. Discuss both possibilities and their advantages and drawbacks.
- For SMEs acquiring software license may be not be always good option because they often need it only for short period (project duration is short and the topics of the projects is often very different). How can they still make use of needed software at

favourable conditions? Is academic software an option or too specific/complex for most of the SMEs?

- How can the market places help SMEs to implement more extensively materials modelling?
- How to make SMEs aware of the possibilities to use already available data for their own challenges?
- For SMEs additional funding from various agencies is often desired. Are the SMEs sufficiently aware of different funding opportunities or they still need help for that and from whom?