EMMC-CSA

European Materials Modelling Council

Report

Sessions on

Industrial Integration and Economic Impact

within the

EMMC International Workshop 2019

FEB 25-27, 2019, Vienna Austria

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1. Executive summary

1.1 Description of the deliverable content and objectives

This report provides information on the sessions, organised by the EMMC Working Group '"Industrial Integration and Economic Impact" within the EMMC International Workshop 2019. A summary from the feedback received before the EMMC International Workshop 2019 on the discussion notes of the three sessions (Session 12, 15 and 18) and a summary of the discussions during these sessions are presented in this report.

1.2 Major outcome

Important topics related to the activities of the EMMC Working Group '"Industrial Integration and Economic Impact" were discussed and feedback obtained.
This outcome, together with the feedback from the rest of the sessions of the EMMC International Workshop 2019 will be used for preparing the EMMC RoadMap 2019.

2. Progress report (main activities)

In this chapter the main outcome of each EMMC Working Group '"Industrial Integration and Economic Impact" related session is given. The summaries provided are based on the impulse presentations, the discussions during the workshop and the input received via an online survey. The detailed input/minutes for each session are given in the Appendix.

2.1 Session 12: Raising the maturity level of materials modelling adoption in industry

Summary from the survey feedback received for Session 12:

- In economics, maturity modelling is part of the so-called Transition Science which describes certain Transition considering the technology, institutional, market and social domains.
- Decision making relies on the quantitative description of the transition including the technological, institutional, market and social domains. The danger with using traditional optimization modelling (as opposed to systems dynamics) is that it might lead to unintended consequences and inefficient or failed Transitions. Quantifying societal and environmental impacts of modelling as well as direct economic impacts is very important (for public and government support).
- To study Transitions quantitatively would require substantial data collection (e.g. of when companies in a sector have adopted materials modelling, how much they invested, for how long, and relate that to their outputs (e.g. patents/success/output of the related industry).
- For materials modelling to mature within a company it takes time and sustained investment, well planned growth and the right combination of staff, software and hardware resources.
- Considering the maturity model dimensions (People, Tools, Processes, Data), the following can be summarised:
- <u>People</u>: It is important to have a sustained growth to a group size that can get more broadly involved in materials modelling projects. Recruiting people with Translator skills (including the skill to talk to internal business stakeholders) and the ability to present and communicate well with the business is key. Collaboration with academic groups is important for underpinning science and for improving and influencing the direction of research. Research collaborations and projects can also help in the early stages to showcase the use of materials modelling and to increase the volume of modelling work. Collaboration of modellers within other internal groups is also key. For example, education of analytical

chemists using materials modelling tools can help establish the modelling in Analytical Science thus help bridging different disciplines.
Engineering knowledge relative to software capability can be a key barrier. Lack of knowledge is a major barrier to entry of using atomistic modelling in the engineering simulation field. Training can improve the understanding of physics-based problems (major issue).

- Tools: The maturity of tools enables solutions to more complex, realistic problems. Improving the (computing) infrastructure allows the experts to focus on science and materials modelling. Multiscale software could still be a challenge especially for multiscale processes. Marketplaces may help in the future to have a wider view on possible modelling tools for each specific case. Moving towards using cloud resources brings new legal and security challenges. Cloud security standards are continuously improving which can allow companies to build some activities on the cloud to deal with more complex workflows. License costs can still be an issue especially with the wide range of tools required. Open source software is generally regarded as too hard to use.
- Process: Maturity of modelling can grow by gradually branching into more areas: increasing visibility, becoming more useful, having greater accountability. With growth comes the opportunity to influence the direction of research (rather than being involved in hindsight). Project initiation forums inside the company can be set to avoid ‘nice to have’ projects and to focus on projects with impact. Investment in workflows for tool integration and data transfer between tools and processes is key. The need for new workflows can be quite frequent. For highly regulated industry, e.g. aerospace, modelling is often limited to non-regulated aspects and is often used for material/part optimization in advance for qualification. . Optimisation drives the use of materials modelling: “the more you optimise, the more you have to optimise”.
- Data: The maturity of data integration can be enhanced by company-wide digital transformation efforts, moving towards an integrated digital resource. Data science is a new and growing effort. Data transfer in complex simulation processes is key and interoperability is often poor. Reliability of material data (e.g. properties) which is often produced by academics may be an issue due to, for example, lack of accreditation/qualification of manufacturing processes, characterization methods and equipment. .

Summary:

- Maturity (and success) comes with time and steady investment. It takes time to build trust and expertise. Managing expectation is important.
- Important components for building maturity are: working closely with experimentalists, collaboration between chemists and engineers, being aware of what is happening more widely, working with external partners for expertise development, and having a strong infrastructure.
- Awareness of the modelers and their role can be increased via organization of national and international EMMC workshops, presentations of EMMC representatives at their organizations (companies, research institutes) and via spreading success stories using new media (EMMC YouTube channel etc.).
- Role of Translators in business: The senior company management needs Translators to communicate materials modeling results into value for the business.
- Modeling in education: More people have to actually do modelling themselves during their education, within their respective basic subjects.

- The roles/definitions of modelers: EMMC should define the subthemes that are out there in the business world and in the scientific challenges - name roles of people working within these sub-topics and link positions such as Translation. Distinguish data scientist from modeler.
- Sharing of software documentation: Many material modelling people consider their codes as their personal property. The benefit of sharing is not yet widespread. The contents that should be shared and documented should be the basic core of the code (physical model) and the modules that can routinely be used for pre and post processing - also for (slightly) different simulations. Adoption of a common format such as MODA or similar can help.
- Recommendations for the EMMC include: encourage open science, design and distribute modelling infrastructure (e.g. Translators, Market Places), to support quantitative economic models where there is often a lack of sufficient data with stakeholders' input to estimate the potential economic impacts of modelling and to support investment strategies and policy making

2.2 *Session 16: Business Decision Support Systems (BDSS): from concept to implementation*

The two H2020 project FORCE and COMPOSELECTOR presented their concepts and developments around the topic of BDSS.

FORCE

- Making decisions is a process which starts with a "need" and includes analysis of the business situation, identification of possible options, and finally the selection and implementation of the best alternative. The need triggering the process is often related to a change of requirements from a customer, supply chain member, market, or government.
- The approach starts by searching available data and information (materials properties, economic data, etc.) to respond to the research or industrial question. Data may have been generated from previous simulations, experimental data, or other sources. In the absence of a solution, the data is then integrated with new materials modelling workflows to build the most relevant KPIs for the analysis of the business challenge. The complexity of the decision-making is handled by Multi Criteria Optimization (MCO) techniques.
- The BDSS architecture has been depicted as an open platform which connects several components, modelling tools, databases, user-friendly apps to easily explore results, data mining tools, MCO tools. The integration with databases allows access to reference data and to keep track of all activities performed for traceability and reproducibility.
- A demo was shown of how the BDSS resolves the use case using a native workflow manager, an intuitive app to visualize and filter the results of MCO, and how functionalities of the native BDSS tool can be enhanced by connecting commercial tools.

COMPOSELECTOR

- The BDSS architecture is conceptually divided in three layers, namely the business layer, the simulation layer, and the materials layer. Each layer identifies itself with specific end-user personas.
- The Business Layer is where the Business process is modelled. To this end the Business Process Model and Notation (BPMN) standard is used. Based on the business information, simple criteria (such as

simulation cost, expected accuracy, etc.) are used to select pre-designed simulation workflows stored in the materials information management system at the Materials layer.

- The selected simulation workflow is then executed by the Materials Layer. The Materials Layer stores use case information, all input/output of the simulations, physical test data for validation, and runs a workflow manager to send data and information to the Simulation Layer, and listens to receive the output.
- The Materials Layer workflow communicates with the open simulation platform (MuPIF) which is part of the Simulation Layer. MuPIF runs the simulation workflow which communicates with various remote, distributed simulation codes, and the results are automatically imported back in the database in a form that can be used for decision-making at either the Materials or Business layer depending the respective decision maker.
- A demo highlighting the main functionalities of the distributed BDSS system has been shown. The demonstration covered the full cycle from the definition of the business process to the section of the appropriate simulation workflow from the data management system, its execution on remote HPC resources, the automatized capture and storage of obtained data, the raw data elaboration in terms of KPIs and their presentation in a dashboard app.

Summary:

- Discussion about the economic data to be used in BDSS. Since a material design project can take several years to be completed, it is challenging to ensure that the economic information collected in the initial phases are still relevant at the end of the project. Because of this it seems that these types of BDSS are immediately applicable to shorter timeframe cases. The BDSS tools allowing long term predictions, for instance AI techniques, are still to be developed.
- A proposed alternative/complementary approach is to include information such as the price volatility of materials as a KPI since this is currently an influential criteria for materials and process selection. This could be interpreted as stability of the solution. The presenters have clarified that in principle everything can be included as a KPI once properly formulated.
- It was recognized that large software companies are taking similar approaches to decision support systems and simulation workflow selection.
- It has been suggested that to facilitate the adoption of these tools by industries it is important to keep the model of the business process at a sufficiently high level and to prove the advantages in using the tools before entering further discussion on the implementation details.

2.3 Session 18: Increasing the adoption of materials modelling with SMEs

- It is recognized that SMEs with a lot of expertise in materials modelling can act as translators to others; while SMEs that have no expertise in materials modelling are in need of translators to establish a modelling workflow for their challenges.
- Overall, it is argued that innovation is mainly driven by SMEs, an important element being augmented analytics where humans are playing central role in deciding how to apply analytics.
- It is acknowledged that data science and advanced analytics only brings value when used by domain experts – physicists, materials scientists, customer insights professionals. It is discussed that the future demands for very simple tools but with a lot of complexity behind for very simple use. Essential is the ability to simulate real-life situations.
- Among the factors that facilitate the use of modeling by SMEs are availability of subsidies for SMEs to hire translators for specific services and the software-as-a-service offerings on Market Places.

- Among the advantages of working with SMEs are more personal contact, easier to understand several aspects of the company, short response time, fast decision, log-term relation is easy to establish, their involvement and eagerness to find solution (e.g. the project to succeed), high intensity of communication and data sharing.
- The best approach is to start doing small projects with the SME, show a few achievements and step by step build larger projects and trustful relation.
- The SMEs are often eager to be involved in big funded projects (i.e. EU, national funding schemes) and a feedback on their participation decision is quickly given.
- The SMEs can be easily contacted via placing modelling success stories in industry-oriented magazines and participation in topic oriented fairs and conferences, e.g. coating shows.
- The narrow domain of SMEs is an opportunity to be complementary. Consider the option that higher software costs could be integrated in the modelling support that you can provide. Make use of Market Place solutions.
- Often there is increased interest for modelling from the SMEs after/during the modelling projects. Hiring of modelers of their own is not affordable for such small SMEs;
- The general barriers to adoption of materials modelling are discussed. Among these are:
  - Costs of hardware, software and training;
  - Higher risks related also to the fact that time-to-solution is not within their time-to-market.
  - Lack of internal expertise for translation of the modeling results into business value and integration of modelling inside the SME's workflows
  - The use of academic models which are less expensive but are also less well maintained/documented.
  - Difficulties to obtain experimental data for validation and specifically at the lower length scales;
  - The inconsistency of data formats in different tools
- Cloud computing can reduce the need for in-house capability investment. However, Big Data will need skilled people and data storage facilities.
- Among the frameworks requirements for the SMEs are open access Marketplaces and Test Beds for a shared infrastructure, validated characterization protocols, tools/hardware for HPC, simulation, visualization and data management, as well as scaled-down in-house tools/platforms to support digitalization and re-use of modelling outcomes for design decision-making.

Summary:

- There is a great potential for translation services offered on virtual marketplaces to SMEs that do not often use modeling.
- More flexible license options for commercial software should be made available to SME. If modelling has to be conducted in-house, it could be an option to discuss short-term or pay-per-simulation business models with software companies. Academic software is often way too complex to be understood easily by a person not familiar with it, making it usually more expensive on a full-cost view.
- Modelling in chemical engineering is much closer to product development and should be more useful to SMEs.
- For SMEs the external translators are more useful to present/demonstrate to them the benefits of material modelling and how to use it. Discussion whether it is possible/useful to have an internal translator at the SMEs who is experienced enough, without working full time in such a position.

- For SMEs it is crucial for the virtual marketplaces to attract communities of translators that are competent and ready to reach out to a substantial industrial user base.
- When SMEs have access to data that is available and if they are well assisted by translators, they can make intelligent choices regarding data access. It will help if there is integration of Databases into apps to guide SMEs in an automated way through the modelling and translation workflow decisions.
- Visibility of funding opportunities for materials modelling could be channeled through the marketplaces and communication means such as videos and podcasts.

3. Conclusions

Quantifying societal and environmental impacts of modelling as well as the direct economic impacts is very important. For this we need to encourage open science, the design and distribution of modelling infrastructure (e.g. Translators, Market Places) and to combine (quantitative) economic models with (qualitative) stakeholder input to determine impact and support decisions by companies and policy makers.

For modelling to mature within a company it takes time and sustained investment, well planned growth and the right combination of staff, software and hardware resources. It is important for companies to build expertise in Translation (business challenges into modeling workflows and the modeling results back to value for business) and hire people that are strong in communication between modelling and business. Academic collaborations and internal collaborations between modelers and experimentalist will contribute not only to the successful implementation of the modelling solutions but also to understanding the capabilities and the impact of modelling. EMMC should support learning and collaboration across disciplines.

For the modeling to mature it requires also development of the tools needed to implement and execute the modelling workflows, as well as workflows for tool integration and data transfer between tools. The increase of cloud security leads to performing wider activities on the cloud, especially useful for complex workflows. Data science is a new and growing effort. Data transfer in complex simulation processes is a key requirement for interoperability which is often underdeveloped. EMMC should support standardization of data documentation.

Further development of the BDSS tools is required to facilitate modeling informed decisions within the companies. Currently the BDSS tools under development are applicable to short-time scales and their further application to long-term business decisions is of importance.

The possibilities for SMEs to receive service from software and model developers applied for their specific cases, at favorable conditions will allow for wider adoption of modelling by the SMEs. The access of the SMEs to modelling and experimental/validation data is a way to stimulate and engage their interest in using modelling. The SMEs need to be stimulated to initiate modelling case studies and to be informed on possible tools for evaluating the benefits from modelling. Translation services offered on virtual Market Places are of crucial importance for SMEs that do not often use modeling and therefore require on-demand expertise.

The further establishment of the Market Places for material modelling will allow for accessing a network of experts and for making use of shared infrastructure, validated software and characterization protocols/tools and data.

4. Annex

4.1 Session 12 - 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

Rapporteur

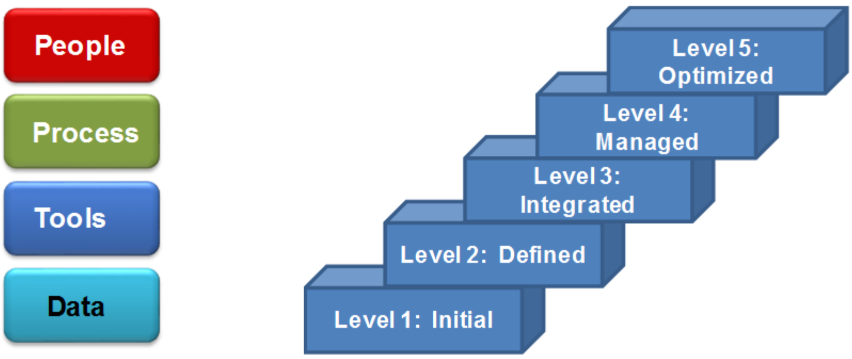
Denka Hristova-Bogaerds (DPI, NL)

Session presenter at Podium Discussion

Tom Verbrugge (DOW, NL)

4.1.1 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). It establishes a mapping of characteristics and behaviours in each of 4 key areas to a Maturity Level:



4.1.2 Objectives

Session 12 seeks to raise the maturity level of materials modelling adoption in industry by strengthening people, tool, process and data which can be seen as the four pillars of a successful deployment of materials modelling in the industrial community. The session aims to engage with leading modelling experts in industry in discussions to see how each of the pillars need to be strengthened in such a way to lead to a holistic solution for a deep and wide engagement of all involved stakeholders to make materials modelling a strong contender in their organisation. We are aiming to find suggestions that may lead to a stable/established deployment of modelling in Industry. Based on some examples for intermediate success our invited speakers had with materials modelling we will find first stepping stones to more impact in the long run. We are also looking forward to hear from opportunities and best practices our participants can share, but also some hurdles and barriers they encountered.

- Share what works very well and what barriers need to be overcome.
- Provide more insights and recommendations that will help to support future deployment of materials modelling in industry.

4.1.3 Background information and documents

Maturity level assessments are quite common in many fields, for example there is a useful one by PWC on Industry 4.0: https://i4-0-self-assessment.pwc.nl/i40/landing/ for a Digital Operations Self-Assessment. It helps to benchmark against others, set objectives and identify needs for action.
The actual questionnaire for the EMMC Materials Modelling Maturity Model can be found here https://ec.europa.eu/eusurvey/runner/MatModMatMod2018.

Impulse 1

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

4.1.4 Impulse 1 - Conclusion, Questions, Remarks

Christa Court provided an economist’s perspective on materials modelling as a field and on maturity modelling. In economics, maturity modelling is part of so-called Transition Science.
Modelling technology transitions (MTT) can be done at the micro-scale, i.e. for individual companies or macroscale, including how companies interact with the government or other institutions. Broad technology transitions (such as the wide-scale adoption of materials modelling) are affected by economic, social and political factors. Lessons learned from MTT in the US energy sector: Decision making relies on quantitative description of the transition including the technology, institutional, market and social domains. The danger with using traditional optimization modelling (as opposed to systems dynamics) is that it might lead to unintended consequences and inefficient or failed transitions. Quantifying societal and environmental impacts as well as direct economic impacts is very important (for public and government support).

To study Transitions quantitatively would require substantial data collection (e.g. of when companies in a sector have adopted materials modelling, how much they invested, for how long etc and relate that to their outputs (e.g. patents)/success/output of related industry).
However, there are important things that EMMC can do/is doing, see recommendations for EMMC (slide). In particular, a study similar to or building on that done by MGI (Plenary by Ben Anderson) would support the call for further public investment.

Recommendations for what EMMC can do include: encourage open science (see Workshop Session 5), design and distribute modelling infrastructure (e.g. Translators, Market Places), combine economic models with stakeholders input to estimate the potential economic impacts of modelling (plenary by Ben Anderson, RTI study for MGI)

Impulse 2

Glenn Jones (Johnson Matthey, UK)

Materials modelling in JM: a brief history and look to the future

4.1.5 Impulse 2 - Conclusion, Questions, Remarks

Glenn Jones provided an End User perspective on the adoption and maturity of materials modelling in industry. He reviewed how modelling has developed in the last 10 years and concluding that some maturity has been established, but that it takes time and sustained investment, well planned growth and the right combination of staff, software and hardware resources.

The hype around materials modelling in the 1990s was mentioned and its failure strongly related to the lack of capabilities (due to computing and algorithms) to treat realistic models. That situation has changed.

Modelling is used in different R&D segments, employing a range of models. Modelling is mature in (process) engineering outside of R&D. Fairly mature is the physics and chemistry-based materials modelling in R&D as well as engineering development. For further improvements e.g. in computational chemistry: important are enhancements of computing and predictive models. Relatively immature is the mathematical and statistical modelling, which is under development at JM.

Another key point regarding maturity development is that JM is engaged with materials modelling projects along the whole chain from academia to production. Academic interactions are important for underpinning science, new methods can be adapted to application. They improve and influences the direction of research, brings new talent and new ways to solve JM problems.

Research collaborations and projects also helped in the early stages to show case the use of materials modelling. Nowadays they are also important to increase the volume of work that can be done with JM involvement.

Likewise, it has been important to develop, gradually, an in-house capability. In the JM case, the opening of a modelling lab in South Africa with several staff was a key step forward, increasing the ability to take on a range of projects. Ensuring high impact project selection was and remains key.

Today, the group has expanded further and “moved out of ‘cottage industry’ to industrial materials science”. In addition, modelling has become established in Analytical Science as a consequence of education of analytical chemists using materials modelling tools (e.g. Solid-state NMR).

The success of materials modelling projects led to involvement in more mainstream projects. Also, modelling helps bridging different disciplines.

Considering the maturity model dimensions (People, Tools, Processes, Data), the following can be summarised:

People: Sustained growth to a group size that can get more broadly involved had been important. Collaboration is key, with academic groups and other groups internally. Also recruiting people with Translator skills (including talk to business internally) and the ability to present and communicate well with the business is important. People need to be able to sell the value and continually make the business case.

Tools: JM adopts state of the art tools. The maturity of tools has grown to a point that realistic problems can be tackled. Multiscale software and infrastructure is a challenge especially for multiscale processes (simulation and simulation time misalignment). More realistic is having ways to systematically averaging and do statistics, there are routine ways of doing that. A lot of software is there which needs to be glued together. Marketplaces may help in future.

Currently: not always go to multiscale, keep it simple. But in some case chemistry needs to propagate to engineering scales. Then for such case a show case is made to demonstrate its usefulness and need for investments. There is still a lot of learning to do.

License costs can still be an issue especially with the wide range of tools required. Improving (compute) infrastructure has also been key: scientists can nowadays focus on science and materials modelling rather than having to run compute infrastructure as well. Moving towards using cloud resources addressing new legal and security challenges. Cloud security standards have improved (are more standardised), cloud within the company is secure so it is already happening. Building some activities on the cloud to deal with continuous workflow.

Process: Maturity has grown by gradually branching into more areas: more visibility, more useful, greater accountability. With growth comes taking influence on direction of research (rather than being involved in hindsight). Also, JM now have project initiation forums as key part of their internal process: avoid just nice to have projects and focus on impact.

Investment in workflows is key: glue that binds different models/people/activities together. The need for new workflows is quite frequent. Fundamental problems pushed to business can be used to template such workflows (see also above).

Data: data integration is at relatively low maturity but this is likely to change as part of company-wide digital transformation efforts, moving towards an integrated digital resource. Data science is a new and growing effort, but still figuring out the best way forward.

Lesson learnt: maturity (and success) comes with time and steady investment. It takes time to build trust and expertise. Managing expectation is important.

Important are: working closely with experimentalists, collaboration between chemists and engineers, being aware of what is happening more widely, working with external partners for expertise development and having a strong infrastructure.

Impulse 3

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

4.1.6 Impulse 3 - Conclusion, Questions, Remarks

The presentation provided and overview of the SimBest study of simulation current practice, best practice and barriers in seven different industry sectors, funded in UK, executed by NAFEMS. The findings are based on on-site interviews with simulation managers at 79 companies in the UK.

All seven sectors use modelling a lot and are relatively mature, in particular CAE is standard in automotive, aerospace and energy.

The objective was how to turn new users into experienced users and improve them.

Here we summarise some key results according to the Maturity Model dimensions.

People: Engineering knowledge relative to software capability was found to be a key barrier. Lack of knowledge will be a major barrier to entry of using atomistic modelling in the engineering simulation field. Lack of qualified engineering resource is also a barrier. Training can help: understanding the problem physics (major issue), correct modelling of the problem, understanding algorithms, advanced simulation technology.

Continuous learning and collaboration across disciplines are the key. Bringing people together with different expertise is exciting as many companies don't collaborate internally. Discussing a project can bring people together.

Tools: Software capability and price is also an important barrier in some field, though that was debated in the session (e.g. by auto industry representative) who claims that V&V/risk/uncertainty are more of an issue than cost/price. Open source is generally regarded as too risky to use.

Processes: Learning and collaboration across disciplines is essential to improve workflows.

Coupled and multi-physics: Barriers are tool integration and data transfer between tools and processes

Highly regulated industry can also be limitation, e.g. aerospace: modelling limited to non-regulated aspects, cannot be used for materials that is regulated e.g. in engine use.

Optimisation drives the use of materials modelling. "the more you optimise, the more you have to optimise". E.g. when a component is optimised, it will typically lead to the need to optimise the material in the component.

Data: Data transfer in complex simulation processes is key and interoperability is poor: data standards are part of the current VMAP project (see also Session 5).

Regarding material data (e.g. properties) companies takes data from academic and often they don't have much experience how reliable the data are. Some parts have statistically different properties than other if materials composition is different. This is complicated issues.

4.1.7 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?
  - A number of barriers and approaches to overcome them have been discussed in the session and are summarised above.
- How can we make a wider range of stake holders aware of the modellers and their role?

Survey respondents suggest:

  - national and international workshops
  - representatives (from EMMC) giving presentations within organisations (companies, research institutes)
  - spreading success stories via new media (EMMC YouTube channel) etc
- How can we promote the role of a translator?

The presentation by JM clearly demonstrated the role and value of translation within a company. Recruitment of staff with communication skills is key to promoting materials modelling inside the company and as such the role of Translator receives recognition.

- How can we promote the importance of early involvement between modellers and project teams?

The topic was discussed in the JM presentation. Survey respondents added:

  - By making sure the project team knows the potential of modelling. The need to see examples that are accessible to them of how modelling could help them. The benefit must be clear for both sides.
- As one needs longer term changes of mindsets, what should be on an "On-boarding package" for higher level management?
  It should include
  - Examples when complex and multiscale simulation model can give a benefit
  - Knowledge on how model developers have to be guides - and on translation procedures - the higher management need people that can transform the results into a value for business
- 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?

- More people have to actually do modelling themselves during their education - based on their respective basic subjects
- How can we enable the specialisation/differentiation on roles within modelling as “the modeller” is deemed too generic?
  - The term modeller is too generic and often confuses people. We should start by disciplining ourselves and use our specialization. Everyone is aware that there are many types of analytical chemist. There is no reason why they should not know there are many types of "modellers".
  - EMMC should define the subthemes that are out there in the business world and in the scientific challenges - name roles of people working within these sub-topics and in linking positions such as Translation.
- How can we support the fact that there is a difference between a data scientist and a modeller?
  - See above: clear role naming and description
  - via examples
- 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?
  - The topic was discussed in the presentations (see above).
  - Best practice means modelling being a part of the developing processes from the very beginning on - not seen as a "firebrigade" if everything else failed or as an add on that could do magic and explain ALL open questions
- 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?
  - Apply best practice experience from big software companies.
  - Many material modelling people considers their codes as their personal property. The benefit of sharing is not yet wide spread.
  - The contents that should be shared and documented should be the basic core of the code (physical model) and the modules that can routinely be used for pre and post processing - also for (slightly) different simulations.
  - Adopt a common format: MODA or similar.

4.2 Session 15 - *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.

Rapporteur

Davide Di Stefano (GRANTA, UK)

Session presenter at Podium Discussion

Glenn Jones (Johnson Matthey, UK)

4.2.1 Introduction

Sustaining and growing businesses requires 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.

4.2.2 Objectives

Session 15 will showcase the BDSS vision and developments from FORCE and COMPOSELECTOR projects which will demonstrate the combinations of open and commercial systems for integrating modelling decisions in new or existing business support systems, and a commercial system developed by Siemens. FORCE and COMPOSELECTOR provide materials modelling modules on all scales along with a suite of decision-making tools (optimization, cognitive computing, materials informatics) that can be used to build customised BDSS Apps or integrated into third party business decision tools. Siemens provides a mature/enterprise-level tool using mesoscale and continuum modelling accompanied by a suite of integrated tools for design and business decision-making.

The presentations will demonstrate:

- Reduction of company costs and increased performance and commercial impact based on effective materials models driven business decisions;
- Guidance to companies in developing their strategies with an effective, user friendly materials models driven business decision system;
- Increased industrial use of existing materials knowledge and effective materials models;
- Improved trust of industrial decision makers in materials modelling and their commercial advantage;
- Essential company savings in time and money, especially via the elimination of the need for (some) plant trials.

4.2.3 Background information and documents

FORCE: Formulations and computational engineering (FORCE) is a new project, underway within the EU program Horizon 2020. The main goal of the consortium is to bring materials modelling to the heart of business decision making by integrating materials modelling into state-of-the-art business decision support systems (BDSS). The project will enable decision makers in industries to make more knowledgeable decisions based not only on existing legacy data, but also on new data generated by state of the art multiscale and multi-physics materials modelling. The main goals of the project are to: 1) Combine materials and business modelling to explore which technical solutions are economically viable; 2) Enable better utilisation of (the huge) dynamic data and information. https://www.the-force-project.eu/

COMPOSELECTOR: COMPOSELECTOR is an ambitious, innovative and timely project to develop, demonstrate and assess an integrated software platform based on a multi-disciplinary, multi-model and multi-field approach for decision-making in the selection, design and fabrication of micro-structured and macro-structured polymer-matrix composite materials. The project will enable greater strategic use and integration of materials and process modelling in business processes. The project combines technical and commercial expertise from academia, a Research and Technological Organisation (RTO) and industrial entities to support a new paradigm in micro-structured and macro-structured PMCs selection where it is crucial to identify concurrent material-selection factors within the value chain. The achievements of this project will improve material selection, design and process capabilities as it creates an accessible platform for the use of computational materials science and physics at the early stages of design. https://www.composelector.net/

Impulse 1

Adham Hashibon (Fraunhofer IWM, DE)

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

Adham Hashibon presented the concept, strategy and status of implementation of the Force BDSS system.

The main goal of the project is to support users in making decisions. The presenter explined that making decisions is a process which starts with a “need” and includes analyse the business situation, identify possible options, and finally choose and implement the best alternative. The need activating the process is often due to a related to change of requirements from customer, supply chain, market, or governments.

The main objective of the Force project is to enhance traditional BDSS systems with materials modelling to enlarge, possibly on the-fly, the knowledge base on which traditional systems relies.
In the project this will be demonstrated in three chemical formulation use cases:

- Personal cares
- Rigid PU foams
- Fast curing industrial inks

These use cases are talked from the point of view of the system. The aim of the consortium is not only to solve the use cases but is to solve them within the Force BDSS system.
The force approach starts looking at the available data (materials properties, economic data, etc.). The data are integrated with materials modelling data to build the most relevant KPIs for the analysed business challenge. The complexity of the data is handled by Multi Criteria Optimization (MCO) techniques. This approach allows to tackle concurrent and opposite requirements and produced a palette of “optimal compromises” (Pareto front), from which the decision maker can confidently select options.
The Force BDSS architecture has been depicted in the presentation as an open platform which connect several components, modelling tools, databases, user-friendly apps to easily explore results, data mining tools, MCO tools. The integration with databases allows access reference data and to keep track of all activities performed for traceability and reproducibility.

The status of the development has been showed in a demo based on an almost realistic chemical reactor process. The presented scenario included concurrent KPIs, such as maximize the purity of the product while minimizing the cost.
The presenter showed a demo of how the BDSS resolve the case using a native workflow manager, an intuitive app to visualize and filter the results of MCO, and how functionalities of the native BDSS tool can be enhanced by connecting commercial tools. In the demo this has been demonstrated by seamlessly storing the results of the MCO performed by the Force workflow manager into a commercial data management system.

Impulse 2

Salim Belouettar (LIST, LU)

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

Salim Belouettar presented the concepts, strategy and status of the implementation of the Composelector BDSS system.

The main idea at the base of the Composelector project is to use materials modelling to enable better business decisions. As in the Force project the starting point is the business need. Modelling activities are tailored and automatized to support the decision maker with relevant information on-demand.

The Composelector BDSS architecture is conceptually divided in three layers, namely the business layer, the simulation layer, and the materials layer.
The business layer is where the Business process is modelled. To this end the Business Process Model and Notation (BPMN) standard is used. The BPMN is a graphical representation for business processes. Based on the business information, simple criteria (such as simulation cost, expected accuracy, etc.) are used to select pre-designed simulation workflows stored in the materials information management system at the Materials layer. The selected simulation workflow is then executed from the Materials Layer which sends the request to the Simulation Layer represented by an open simulation platform (MuPIF) which communicates with a distributed eco-system of simulation software run on remote, distributed HPC resources. The results are automatically imported back in the database and used at the Materials and Business layers to support the decision maker. The data can be analysed by different tools including dashboards and multidisciplinary optimization tools.
A demo highlighting the main functionalities of the system has been shown. The demonstration covered the full cycle from the definition of the business process to the selection of the appropriate simulation workflows from the data management system, its execution on remote HPC resources, the automatized capture and storage of obtained data, the raw data elaboration in terms of KPIs and their presentation in a dashboard app.

4.2.4 Final remarks

Both presenters showed how, in the related projects, materials modelling can be integrated in Business Decision Support Systems. Even if the projects focus on different use cases and the implementations are independent, the main design principles are common and aligned to the EMMC directives.
Interesting points have been raised by the audience regarding the economic data to be used in BDSS. Since a material design project can take several years to be completed, it is challenging to ensure that the economic information collected in the initial phases are still relevant at the end of the project. Because of this it seems that these type of BDSS are immediately applicable to reformulation tasks, small variation of established product, which have much shorter timeframes. However, the experts in the audience do not exclude the possibility to develop tools allowing long term predictions using for instance AI techniques. A proposed

alternative/complementary approach is to include information such as the price volatility of materials as a KPI.

The presenters have clarified that in principle everything can be included as KPI once properly formulated.

The audience recognized that large software companies are taking similar approaches to decision support system and simulation workflow selection. However, it was also pointed out that challenges exist in trying to introduce new processes in companies where business processes are already well established. It has been suggested that to facilitate the adoption of these tools by industries is important to keep the model of the business process at a high level and to prove the advantages in using the tools before discussing the implementation details.

The need has been highlighted to connect to ERP systems. In both implementations, this can be done exploiting the functionalities of integrated commercial tools to connect to PLM systems which are usually already connected to ERP systems.

4.3 Session 18 - *Increasing the adoption of materials modelling with SMEs*

Chair

Sandeep Namdeo (Airborne Oil&Gas, The Netherlands)

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

Rapporteur

Tom Verbrugge (DOW, NL)

Session presenter at Podium Discussion

Katya Vladislavleva (Datastories, BE)

4.3.1 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.

4.3.2 Objectives

- To discuss possibilities for SMEs to receive service from software and model developers applied for their specific cases, at favorable conditions.
- To discuss and identify opportunities for SMEs to have access to modelling and experimental/validation data, as a way to stimulate and engage their interest in using modelling.
- To stimulate SMEs in initiating modelling case studies and inform them on possible tools for evaluating the benefits from modelling.

4.3.3 Background information and documents

The short time frames and often the insufficient internal expertise on modelling inside the SMEs, for them it could be more interesting to engage in a **service**-type of activity rather than in research project, considering simple models that don't require experts and are not expensive. Such a service can be provided by the material modelling **market places** where the SMEs can navigate through the different modelling possibilities or to search for translators and software service providers for their specific case. Therefore it is of importance to create database of models, software and translators within the market places.
In order to assess the benefits of using materials modelling, the SMEs will need business cases including return on investment strategy for utilizing modelling data. Making **modelling and validation data accessible** to the SME prior a modelling project starts may convince them to further explore the benefits of modelling.
A set of **standard tools to assess the economic impact** of modelling, for example the financial impact with ROI, would be useful for SEMs to define their business cases. Tools such as spreadsheet, report/guide or video need to be made available for this purpose, as well as **case studies** from SMEs demonstrating the benefits of the modelling.

Impulse 1

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

4.3.4 Impulse 1 - Conclusion, Questions, Remarks

DataStories is an SME in the area of data science and data analytics. The presentation addresses 3 main topics: 1) possibilities for SMEs to receive service from software and model developers applied for their specific cases, at favourable conditions; 2) opportunities for SMEs to have access to modelling and experimental/validation data, as a way to stimulate and engage their interest in using modelling; and 3) stimulating SMEs in initiating modelling case studies and inform them on possible tools for evaluating the benefits from modelling.
In the experience of DataStories, they encountered 2 types of SMEs: 1) SMEs with a lot of expertise in materials modelling, that do not need their services, and can be translators to others; and 2) SMEs that have no expertise in materials modelling, where they can act as a translator. Overall, it is argued that innovation is mainly driven by SMEs. An important element in the offering of DataStories is what they call augmented analytics, i.e. placing the human element central to the analytics.

In their experience data science and advanced analytics only brings value when used by domain experts – physicists, materials scientists, customer insights professionals. This is also confirmed by attendees in the audience. Current offerings in this area are often either very simple tools for very simple users, or very complex tools for very advanced users, whereas the future demands for very simple tools but with a lot of complexity behind for very simple use. Essential is the ability to simulate real-life situations.
Incentives for SMEs to participate are discussed: 1) provide subsidy for SMEs to hire translators for specific services; 2) promote software-as-a-service offerings on market places (rigid software offers will disappear by themselves – the market will push them out) at favorable license fees; and 3) offer (and facilitate) trainings on specific applications of materials modelling in specific contexts (e.g. materials modelling for recycling cooling elements, applications of AI to speed up commercialization of new formulations in cosmetics, computational aspects of creating biodegradable inks for packaging industry, AI-driven material+ design).

Impulse 2

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

4.3.5 Impulse 2 - Conclusion, Questions, Remarks

IFAM is an institute that that provides research and development from the formulation of an adhesive to assembly and joining technologies. Two case studies are discussed. Positive aspects of SMEs that make attractive to work with them: 1) The visionary who created it, envisaged it, who is passionate, full of energy and enthusiasm, is more accessible; 2) Few employees, more contact, easier to understand several aspects of the company (from administration, management, research, products); 3) You can start doing small projects, few results, few achievements that can satisfy the client, and step by step getting bigger and building the relation; 4) In case of applying for big projects (i.e. EU, national funding schemes) when the opportunity comes you can easily know a feedback regarding participation without waiting too long; they can take decisions; 5) Short response time, fast decision; the interest is easily shown. You normally deal with the people who are taking the decisions; 6) You have a partner with whom you can work for a long time (years of relation), normally the person stays in the position, thus, new project still the same group working together; 7) They contribute to the success; and 8) You talk to the person who handles the application every day; 9) High intensity of communication, phone calls are seldom shorter than 30 minutes, i.e. a lot of information is given; and 10) They want you understand the challenge, they want to facilitate to find the solution.
How to engage with SMEs? Go to the target audience: inform about your success and tool capabilities in industry-oriented magazines; subscribe to receive Newsletters; participate in topic oriented fairs and conferences, e.g. coating shows; contact the customer to understand their needs; The narrow domain of an SMEs is an opportunity to be complementary; identify the list of requirements and topics for cooperation; identify small projects, funding opportunities to start with; identify the budget frame, time schedule for the solution and funding; higher software costs could be integrated in the modelling support that your provide; use marketplace solutions.
During the Q&A, there were further points provided: There is shared accountability when working with SMEs; It is all about people and thus communication; In general, there was increased interest for modelling from the SMEs following the projects; Hiring of modellers of their own is not affordable for such small SMEs; What is the

difference being a translator with large companies: also in that case we tend to be complementary to what they already have, but communication is very different, mostly it is much less compared to that with an SME.

Impulse 3

Donna Dykeman and Davide Di Stefano (GRANTA, UK)
Data availability and materials modelling Market Places for SMEs

4.3.6 Impulse 3 - Conclusion, Questions, Remarks

Granta Design, an ANSYS Subsidiary, is a leader in materials information technology — to advance materials engineering and education, and to enable better, greener, safer products. The presentation discusses 1) SME Market, including opportunities, barriers, and requirements to adopt materials modelling, 2) Strategies for SMEs to overcome barriers to adoption, including examples and future solutions.

General barriers to adoption of materials modelling are discussed: 1) Expertise (Translation): Individuals understanding models & connecting business value; Integration of modelling expertise inside design and engineering workflows; 2) Accessibility: Predominantly private solutions and data capture by large enterprises; Availability of data to reduce repetition, speed of discovery; 3) Code quality (Verification): Models predominantly developed by academia; Little software maintenance expertise applied to most models; 4) Validation: Difficult to test properties at the lower length scales; Relationship to high length scales often missing; and 5) Standards: Schema, data formats; Parameter definitions change depending on the length scale; Interoperability between corporate and research tools; Multiple open-source, disconnected tools.

Magnified barriers for SMEs are cost, expertise and risk: 1) Costs: Hardware: computing, storage; Software; Physical data; Training; 2) Expertise: External translators; Training; and 3) Risks: Return on Investment (ROI); Quality of results; Time-to-solution is not within their time-to-market.
SME digital readiness to adopt materials modelling: 1) E-commerce: Third party service, low barrier to entry; 2) Cloud Computing: Reduces the need for in-house capability investment; 3) ERP software: Needs software solutions and established business processes; and 4) Big Data: Needs skilled people, HPC and data storage.

It is argued that SMEs can adopt materials modelling when 1) models and simulations are at the most relevant length scale for their product or application, 2) models and modelling workflows are verified, validated (VV) in advance with appropriate uncertainty quantification (UQ), and 3) modelling outcomes (VVUQ'd virtual data) can be reused.

Frameworks requirements are discussed: 1) open access Market Places and Test Beds create a shared infrastructure (Reference data (virtual, physical) that is quality assured; Validated characterization protocols (virtual, physical); Model Software/code plugins; Tools/hardware for HPC, simulation, visualization and data management) and 2) scaled-down, in-house tools/platforms to support digitalization and re-use of modelling outcomes for design decision-making (SMEs can adopt models and simulations that represent the scale of their applications; SMEs can reuse data/knowledge within existing tools (designers, engineers, scientists)). At all times, quality of modelling outcomes needs to be clear, evidence-based.

4.3.7 Discussion points and questions

The following questions summarize the issues for this session.

- 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.
    - The services of translators are likely less expensive than hiring a person whenever, on average over time, much less than one full person is needed. This will usually be the case for small enterprises that do not focus on materials modelling right away; for medium-scale enterprises, it may often be the case. There is a great potential for translation services offered to such clients on virtual marketplaces.
    - Some types of modelling (such as atomistic) are linked to very fundamental questions and it may not be in the SME's interest to engage in that as their R&D time frame is too short. Modelling in chemical engineering is much closer to the product development and should be more useful to SMEs.
    - Internal Translator: High cost, long training, skilled personnel. In an SME the person will not have a full time translator role, so the training might be for a part time role of the person only. Extern Translator: If the benefit of material modelling is visible to the SME this presents the on-demand version for the SME to use materials modelling.
    - The key question is: is it possible to have an internal expert for this specific question who is experienced enough to still have a good overview, without working full time in such a position.
    - Internal translation might be short-sighted and then is not a valuable solution. Training of SMEs towards materials modelling basics and advantages should absolutely be free and open"

- For SMEs acquiring software license may not be always the good option because they often need it only for short periods of time (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 license conditions? Is academic software an option or too specific/complex for most of the SMEs?
    - “Too complex" does not exist if you have good advice. Hire academic or independent translators to advise you and to develop workflows tailored to specific economic and materials-related boundary conditions.
    - If they have internal experts, using open source academic versions should not be insurmountable. But more flexible license options for commercial software should be made available to SME.
    - Academic versions will most likely be too undocumented for novice use and/or at SME. Licencing concepts together with computational power on-demand and as-needed (much like CPU24 for example).
    - A good translator should aim at specifically designed solutions for SMEs, with short contracts and software licensing included. If modelling has to be conducted in-house, it could be an option to discuss short-term or pay-per-simulation business models with

software companies. Academic software is often way too complex to be understood easily by a person not familiar with it, making it usually more expensive on a full-cost view.
- The solution is to put the software (and needed database) access on a market place with case by case use and payment.

- How can the market places help SMEs to implement more extensively materials modelling?
  - The marketplace can help to connect the SMEs with the SMEs with the help of translators, but it will depend on the visibility of the marketplace and relevant use cases.
  - What will be the added value of the marketplace? Today you can already find a lot via the web. The value of the market place is likely a collection of experts.
  - By reaching out to the SMEs, and this cannot be the activity of the virtual marketplace itself, it needs to be mainly conducted by the translators that operate on the virtual marketplace. For this reason, it will be crucial for the virtual marketplaces to attract communities of translators that are competent and ready to reach out to a substantial industrial user base, and this is how the virtual marketplaces eventually help the SMEs best.

- How to make SMEs aware of the possibilities to use already available data for their own challenges?
  - Portioned small-scale data access should be one of the tradeable objects available at the virtual marketplaces. These need to be appropriately screened and indexed, where presumably some assistance from the data providers will be required. When SMEs can "see" what data are available, and at what cost, and if they are well assisted by translators, they can make intelligent choices regarding data access
  - Integration of Databases (free and pay) into apps to guide SMEs automated trough the modelling and translation workflows

- 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?
  - Difference between marketplace and digital marketing. Visibility of funding opportunities (both European and regional) for materials modelling could be channeled through the marketplace to make the market place more visible.
  - How the communication is done is key (videos and podcasts).

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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	SINTEF AS	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
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